INTEGRATING DECISION SUPPORT AND DATA MINING FOR RISK EVALUATION AND MANAGEMENT: A METHODOLOGICAL FRAMEWORK AND A CASE STUDY IN AGRICULTURE

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Doctoral Dissertation
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Doctoral Dissertation

INTEGRACIJA PODPORE PRI ODLOČANJU IN PODATKOVNEGA RUDARJENJA ZA VREDNOTENJE IN UPRAVLJANJE TVEGANJA: METODOLOŠKI OKVIR IN ŠTUDIJ PRIMERA IZ AGRONOMIJE

Doktorska disertacija

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Abstract

The thesis addresses a challenge in decision analysis that deals with risk and uncertainty as well as automation of decision support in this context.

The problem is motivated by complex decision making problems that encounter risk and uncertainty, requiring risk analysis during the decision making process. The starting point is risk analysis and common risk analysis approaches, i.e., ex-ante and ex-post approaches, which have been identified with certain limitations and potential for improvement in the context of automating decision support. On the one hand, ex-ante is a prospective approach that evaluates the potential risk at the beginning of the period in question and tries to describe the state of the world at the end of that period by using projection, simulation or foresight approaches. It is heavily based on information about the state of the world that is clearly known but incomplete and, on a basic level, does not consider the level of certainty of that information. On the other hand, ex-post is a retrospective approach that evaluates risk at the end of the period in question, by considering the real (observed) state of the world. Therefore, the former approach relies on incomplete or imperfect information, whereas the latter has at its disposal complete pieces of information. In a real-world problem, making a decision at the beginning of the period of interest is of higher priority and in some cases is the only solution, so the ex-post approach is not suitable. To improve the ex-ante approach by considering additional ('what is certainly known') information with quantified low uncertainty, we propose an integration of predictive and diagnostic models that introduce a predictive and a diagnostic layer in the scope of the ex-ante approach, respectively.

The second point of motivation is the evaluation of alternatives in accordance with a state of the world that would take place when a corresponding alternative is realized. Traditional methodologies for decision modeling do not explicitly offer the possibility to consider the state of the world in the evaluation of alternatives. The work presented in the thesis allows individuals to express preferences over an outcome of an alternative and a state of the world upon application of an alternative.

Furthermore, existing approaches to decision analysis require many steps to be executed and a wide range of tools to be used for each of them. However, having a decision support tool or a system that can handle most of these simultaneously is highly desirable. Therefore, we propose a methodological framework for decision analysis that connects all required steps and delivers the desired support. The proposed methodological framework deals with decision making under risk and uncertainty and consists of two modules: risk assessment and risk management. The risk assessment module implements the proposed extended ex-ante approach to risk evaluation. The risk management module uses a set of predefined functions to produce the desired support.

The proposed methodological framework is applied in a case-study scenario from the domain of surface and ground water protection from phytochemicals used in agriculture. The outcome of the case-study is a decision support system with a web-based interface. Extensive performance evaluation of both modules of the methodological framework's im-

plementation is performed using data collected on agricultural fields that are part of an experimental site located in Western France. The resulting decision support system considers a description of a particular application of pesticides on a field as input, and proposes a set of agricultural practices to be performed on the field, in order to avoid surface and ground water pollution with phytochemicals.

Povzetek

Doktorska naloga obravnava izzive s področja analize in avtomatizacije odločanja, pri katerem se soočamo s tveganjem in negotovostjo.

Naloga se osredotoča na kompleksne probleme odločanja, katerih sestavni del sta tveganje ter negotovost, ki ju je potrebno analizirati in obvladati že med odločitvenim procesom. Tovrstni pristop najprej upošteva analizo tveganja z uporabo standardnih metod ex-ante in ex-post. Pri dosedanji uporabi omenjenih metod za podporo odločanju se je pokazalo, da sta podvrženi nekaterim omejitvam in ju je zato mogoče nadgraditi. Ex-ante je metoda, kjer ocenimo odločitveno tveganje na začetku obravnavanega obdobja in poskusimo opisati stanje na koncu tega obdobja. Končno stanje ocenimo bodisi s projekcijo, simulacijo ali s strokovnimi napovedmi. Nasprotno je ex-post retrospektivna metoda, kjer ocenimo odločitveno tveganje na koncu obravnavanega obdobja, pri čemer upoštevamo začetno (opaženo) stanje. Ex-ante se torej zanaša na nepopolne informacije o prihodnosti, medtem ko ex-post uporablja popolnoma znane informacije o minulem obravnavanem obdobju. V primerih, kjer je potrebno odločitev sprejeti na začetku obravnavanega obdobja, kar je včasih tudi edini možni pristop, je uporaba ex-post metode za obvladovanje odločitvenega tveganja neprimerna. Za takšne primere nam preostane samo pristop ex-ante, ki ga pa v našem primeru izboljšamo z vključitvijo dodatnih zanesljivih informacij, ki jih pridobimo s pomočjo napovednih in diagnostičnih modelov. Na ta način v ex-ante metodo obvladovanja odločitvenega tveganja vpeljemo napovedni in diagnostični metodološki nivo.

Dodatno obvladovanje odločitvenega tveganja izboljšamo z ocenjevanjem možnih alternativ glede na stanje, do katerega bi prišlo, če bi dano odločitev realizirali. Pri ocenjevanju alternativ s trenutno uveljavljenimi metodami odločitvenega modeliranja tega stanja ne moremo neposredno upoštevati. V nalogi pokažemo, kako lahko odločevalec izbere, katerim alternativam daje prednost glede na izid in stanje, do katerih pripeljejo.

Uveljavljene metode za analizo odločanja so tudi sestavljene iz mnogih korakov, za njihovo izvedbo pa potrebujemo številna orodja. Da bi ta proces poenostavili, smo razvili metodološki okvir za odločitveno analizo, ki za zagotavljanje podpore pri odločanju združi vse potrebne korake in omogoči, da odločanje upošteva tudi tveganje in negotovost. Okvir sestavljata sklopa za ocenjevanje in upravljanje tveganja.

Za ocenjevanje tveganja uporabljamo predlagano razširitev pristopa ex-ante, za upravljanje s tveganjem pa izkoristimo množico vnaprej definiranih funkcij, ki omogočajo želeno podporo pri odločanju.

Predlagani metodološki okvir je preizkušen v raziskavi o zaščiti površinskih vod in podtalnice pred onesnaženjem s fitofarmacevtskimi sredstvi, ki se uporabljajo v kmetijstvu. Končni rezultat raziskave je sistem za podporo pri odločanju, ki je uporabnikom dostopen preko spletnega vmesnika. Obširen preizkus predlaganega metodološkega okvira za obvladovanje odločitvenega tveganja smo izvedli na podatkih, pridobljenih na eksperimentalnih kmetijskih pridelovalnih površinah zahodne Francije. Vhodni podatki v sistem za podporo odločanju so opisi načrtovane uporabe fitofarmacevtskih sredstev. Sistem oceni stopnjo tveganja za onesnažene vode in v primeru tveganja predlaga nabor zaščitnih ukrepov.

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Abbreviations

ACC	...	Accuracy
AS	...	Active Substance
BMT	...	Bagging of Model Trees
BRT	...	Bagging of Regression Trees
CIPER	...	Constrained Induction of Polynomial Equations for Regression
DP/MIM	...	Dual-Permeability/Mobile-Immobile
DRSA	...	Dominance-based Rough Set Approach
DSS	...	Decision Support System
ER	...	Error Rate
FPR	...	False-Positive Rate
GIS	...	Geographical Information System
GUI	...	Graphical User Interface
KOC	...	Soil Adsorption Coefficient
KW	...	Kinematic Wave
LR	...	Linear Regression
MACBETH	...	Measuring Attractiveness By a Categorical Based Evaluation
MCDA	...	Multi-Criteria Decision Analysis
MCDM	...	Multi-Criteria Decision Making
MDL	...	Minimal Description Length
MT	...	Model Tree
PCQE	...	Pratiques Culturaleset Qualité des Eaux
PDA	...	Preference Disaggregation Principal
PNEC	...	Predicted Non-Effect Concentration
PPDB	...	Pesticide Properties Database
PR	...	Polynomial Regression
PRC	...	Precision-Recall Curve
PREC	...	Precision
RMSE	...	Root Mean Squared Error
ROC	...	Receiver Operating Curve
RRSE	...	Root Relative Squared Error
RT	...	Regression Tree
RZWQM	...	Root Zone Water Quality Model
SDP	...	Spring Drainage Period
SWHC	...	Soil Water Holding Capacity
T/V	...	Test/Validation
TPR	...	True-Positive Rate
UTA	...	UTilité Additive
WDP	...	Winter Drainage Period
WHO	...	World Health Organization
ZAPROS	...	Closed Procedures near Reference Situations

Chapter 1

Introduction and Background

In everyday life we repeatedly face situations that require us to select a belief or action among several alternative possibilities. These situations present us with decision problems. The act of selecting an alternative among the given possibilities and the cognitive process underlying it are both referred to as decision making. Each decision problem is characterized with an objective, according to which alternatives are evaluated. This can be a simple objective that is expressed with a single criterion or a complex objective that utilizes multiple criteria. Both simple and complex objectives are the subject of the study of decision analysis, a field of operations research that investigates the possibilities of structuring and solving decision problems. Multi-criteria decision analysis (MCDA) is a sub-field of operations research, concerned with structuring and solving decision problems that involve multiple criteria (Zopounidis & Pardalos, 2012).

In general, one of the main challenges in decision analysis is dealing with potential risk and uncertainty, which can derive from different sources within the scope of decision problems (Chateauneuf, Cohen, & Tallon, 2010). The scope of a decision problem (application area) is defined as a domain that describes a current or expected state of nature (further referred to as *world*), on which a decision should be made. It is described with a set of rules and situations (further referred to as *state of the world*) that can be well or partially known, i.e. accompanied with perfect or imperfect information, respectively. Imperfect information about the state of the world is one potential source of uncertainty within a decision making process.

The objective of decision making is to choose the best alternative (also referred to as option or action in the literature) among many alternatives, considering multiple, possibly conflicting criteria. The term *best* in the definition emphasizes the subjective nature of the problem, but formally, it is defined as an alternative that satisfies a certain set of criteria of the decision maker (further referred to as *individual*). The defined set of criteria maximizes what the individual expects to gain from the state that the world evolves to, when the decision is made (Roeser, Hillerbrand, Sandin, & Peterson, 2012). The property of an alternative to satisfy such criteria is said to be the rationality of the alternative, philosophically referring to so called instrumental rationality (Peterson, 2009).

In order to check the rationality of an alternative, it is required to be evaluated over a given state of the world. Evaluation of all defined alternatives results in a *set of outcomes*. The set of outcomes is another possible source of uncertainty, due to consequences unknown in advance.

In the thesis, uncertainties due to lack of information about the state of the world and unknown consequences constitute the main subject of the study and are further referred to as *uncertainty*. There exist other potential sources of uncertainty, described in Section 2.2, but they are excluded from detailed research in the thesis.

As previously stated, the uncertainty appears due to lack of information about state or consequences. Such lack of information is formulated as imperfect knowledge that influences the whole decision making process. The imperfect knowledge involved causes risk of unknown behavior of the world under different outcomes (Roeser et al., 2012; Aliev & Huseynov, 2014). In decision theory, the individual's degree of control over risks is often problematic and difficult to model. Thus, risk analysis is required.

The incorporation of risk analysis into decision theory has been reviewed by Kaplan and Garrick (1981). They defined risk in its various formats with corresponding decision-theoretic counterparts. Apostolakis (2004) defines the term *risk-informed decision making* as decision making informed by risk analysis. This notion is adopted throughout the thesis and further referred to as decision making.

Risk analysis consists of two main parts: risk assessment and risk management. The former tries to uncover hidden assumptions of what level of evidence we need to act as if the uncertainty is minimal. In other words, risk assessment attempts to assess uncertainties and prioritize and quantify them as level of impact of estimated uncertainty on the decision making process. Risk management assumes that risk is quantified correctly, and tries to mitigate such risk to tolerable or acceptable level, by implementation of different techniques (Haimes, 2015).

A literature survey exposes two approaches for risk assessment in revealing potential risk and uncertainty evaluation: ex-ante (before the fact) and ex-post (after the fact) (Keeney & Winkler, 1985b; Kolstad, Ulen, & Johnson, 1990; Kamin & Rachlinski, 1995; Neely, 2003; Todd & Wolpin, 2008). Ex-ante is a prospective approach that evaluates potential risk at the beginning of the period in question and tries to describe the state of the world at the end of that period, by using projection, simulation or foresight approaches. On the other hand, ex-post is a retrospective approach that evaluates the potential risk at the end of a period, considering the real (observed) state of the world. Therefore, the former uses incomplete or imperfect information, unlike the latter, which uses complete information (Fleurbaey, 2010; Fleurbaey & Peragine, 2013).

The ex-ante approach focuses on an individual's expected utilities or preferences over beliefs and actions, due to the lack of information or imperfect information. The ex-post approach, on the other hand, computes the expected value of actions and the focus is shifted to preferences over outcomes (Roeser et al., 2012). From the decision making point of view, the ex-ante approach has limited resources for good estimation of the rationality of alternatives, whereas the ex-post approach deals with known states of the world. Another limitation of the ex-ante approach is the fact that an individual's true preferences under incomplete or imperfect information about the state of the world can differ significantly from the individual's preferences given perfect information. This limitation affects the rationality of decisions driven by preferences, by a combination of the individual's interests and correct information about alternatives (Weirich, 2004).

From the above, it would appear that the ex-post is preferable to the ex-ante approach. However, in real-world problems, making a decision at the beginning of a period of interest is of higher priority, and in some cases is the only option. For example, for the problem of whether we should take an umbrella or not when going out, knowing that it will rain half an hour after leaving home is of higher priority when we are still at home (at the beginning of the period when we will be out) than later, when we will be already out.

In addition, some real-world decision problems do not only require evaluation of an alternative as is (at time point t), but also evaluation of the state in which the world will be, after application or implementation of an alternative (action) - time point $t+1$. In such a case, the ex-ante approach is severely limited with the resources available and only the ex-post approach can be used.

Most real-world decision problems have a complex nature that requires incorporation of different sources of information, projections and simulations in order to accomplish the goal of a decision making process that deals with uncertainty. Such decision problems are hard to solve by hand and mostly require support throughout the decision process. Such support can be given in different forms: structuring problems into smaller sub-problems that are easy to be solved, building a model to be used each time an evaluation of alternatives is required, performing algorithmic risk analysis, etc. A system built to support a decision making process is called a decision support system (Keen, 1980; Bohanec, 2001). Traditional decision support systems (further referred to as *DSS*) consist of three parts: knowledge base, decision or utility model and user interface (D. J. Power, 2008; D. Power, Sharda, & Burstein, 2015). However, in the case of decision making processes that require risk analysis, traditional approaches to building DSS do not offer appropriate integration and must be customized with an appropriate knowledge base or decision model.

The goal of this thesis is to study and develop a new methodological framework in the domain of decision analysis and decision support that will narrow down the limitations of ex-ante risk assessment in the process of decision making by introducing a predictive level that will integrate both decision support and data mining methodology in order to improve the estimate of the state of the world. As such, the methodology covers the uncertainty due lack of information about the state of the world, and will allow the ex-post approach to be applied over the predicted state of the world (so called *quasi ex-post risk analysis*). Thus, the problem of ex-ante risk assessment is transformed to a problem of quasi ex-post risk analysis. For example, using the same decision problem, whether to take an umbrella or not if we consider weather forecast before leaving home, we will act as if we traveled into the future and hypothetically know that it is raining at the time we are out. Therefore, we will take an umbrella. This brings more accurate information about the state of the world into the process of decision making, where certainty will be quantified with the accuracy of models used at the predictive level.

In risk analysis, risk management is a stage that tries to mitigate the assessed risk. On the other hand, when wrapped within a decision making process, risk management delivers support to the individual in order to make a decision. Therefore, it should be structured in a form that will be understandable to the individual. *A second goal of the thesis is to make the proposed methodological framework applicable to decision problems that require building decision support systems, which will be able to consider all the decision making tasks stated by Roy (2005): choosing, sorting and ranking tasks.* The choice task is to select one "good" alternative or a small set of "good" alternatives from the set of all alternatives. The sorting task is to assign each alternative from the set of alternatives to a category of a predefined set of categories. Ranking task aims at defining a complete or partial order on a given set of alternatives.

The aforementioned defines the methodological scope of the study and the thesis. In addition, the study requires a use-case (case-study) where the developed methodological framework will be implemented and discussed. Thus, the thesis encompasses a case-study development and results that define the practical scope of the thesis.

The methodological framework is applied in a case-study scenario from the domain of surface and ground water protection from phytochemicals (referred to as pesticides) used in agriculture. In 2000, the EU Water Framework Directive (European Parliament & Council, 2000) introduced an innovative, integrated and holistic approach in the form of a policy, with the ultimate goal to improve the quality of surface and ground water bodies. This policy triggered a re-organization of water management on a high (conceptual) level among all EU members. It is thus characterized by a high level of complexity, requiring involvement of numerous decision makers operating at different levels, and a large number of

stakeholders with different preferences and judgments (Lahdelma, Salminen, & Hokkanen, 2000).

Room for improvement regarding methodologies and tools therefore exists, in order to support the Directive as closely as possible, on different levels or sectors (such as environment, energy, industry, agriculture, and tourism) involved in the challenge of meeting the Directive's obligations and implementation requirements. Due to the fact that about 70% of the world's fresh water is consumed by agriculture (Clothier, Green, & Deurer, 2008), supporting the Directive in agriculture, given a pre-defined budget of investment acceptable for farmers, turns out to be a great challenge. Since agriculture is a major contributor to water pollution, the use of pesticides has to be implemented in accordance with safe and environmentally sound agricultural crop management. Their use must be consistent with the Directive on the sustainable use of plant protection products (European Parliament & Council, 2009a) in order to provide the most effective protection of surface and ground waters through the implementation of best crop management practices.

Although crop management uses active substances previously approved for commercial use, i.e. respecting EU regulations (European Parliament & Council, 2009b) and permitted according to the Commission Implementing Regulation (European Parliament & Council, 2011), they can still be found in surface and ground water in concentrations above the threshold allowed for drinking and technically safe water. While each approved and permitted active substance has passed very rigorous ecological risk evaluation during its registration process (the procedure for preregistration risk evaluation is described in detail by authorities such as the European Food Safety Authority) (European Parliament & Council, 2009c), the post-market risk evaluation of pesticides used in agriculture is not regulated at the same level. To make progress on this issue, the European Commission (through the environmental program LIFE ("LIFE programme," 2014)) and the "European plant protection industry association" (2016) (ECPA) launched the project TOPPS (Train the Operators to Promote best management Practices and Sustainability) (Roettele, 2008), which aims to reduce water pollution due to improper use of pesticides. The TOPPS project addresses point-source and diffuse-source water pollution by pesticides and tries both to diagnose the level of pollution risk and provide instructions for mitigation measures that would reduce and prevent the pollution of water with pesticides. Even though decision makers (agricultural advisers and farmers) benefit from the TOPPS project, its first results are very difficult to use at the field level and decision makers are not given much flexibility in terms of selecting a set of proposed mitigation measures.

Thus, the underlying concepts of the above mentioned Directives and Regulations and, in particular, the way it has been implemented in practice, have received major criticism from politicians, water managers and scientists (Moss, 2007, 2008; Dufour & Piégay, 2009; Josefsson & Baaner, 2011), with the development of locally-adapted evaluation and management methods was emphasized as the weakest point.

To overcome the problem of water pollution with pesticides at the field level, we apply the proposed methodological framework deriving to a web-based decision support system comprised of risk assessment and risk management modules for pesticides approved for use in agriculture.

It is assumed that farmers and farmer advisers evaluate the risk of pesticide transfer from the agricultural field to surface and ground water bodies in their planning period, when detailed crop and protection practices should be defined. In fact, they should perform ex-ante risk assessment, since the state in the field is only known at the time of planning (beginning of period under consideration). This can be improved by transforming the analysis from ex-ante to quasi ex-post risk analysis, as this thesis suggests.

The risk management module consists of a finite space of possible mitigation mea-

sures formalized as alternatives, defining the scope of agricultural practices (e.g. crop management, soil cultivation, time and dose of pesticide application, etc.) that should be considered in order to reduce the assessed ecological risk of pesticide transfer into water bodies.

The implementation of DSS is usable at the field level and allows individuals (e.g., farm advisers) better flexibility regarding the choice of mitigation measures from the proposed ordered set. Finally, partial tasks from the DSS, developed in this thesis (in particular from risk assessment) are compared with state-of-the-art models or systems.

1.1 Aims and Hypotheses

The aim of the thesis is threefold. First, to *develop a methodological framework for decision making under risk and uncertainty that will reduce the limitations of ex-ante risk assessment by introducing a predictive or diagnostic layer.* The predictive (diagnostic) layer would add more accurate information about the state of the world at the end of period of interest, which will allow ex-post risk analysis over predicted states of the world (quasi ex-post risk analysis) to be applied.

Second, to *upgrade the methodological framework towards a platform for building decision support systems, which will allow assessed risk to be managed, including output that will satisfy criteria for ranking or sorting a defined or chosen sub-set of alternatives.*

Finally, to *implement and evaluate the developed methodological framework on a specific decision problem.* The evaluation is done with a case-study implementation in the domain of post-market risk assessment and management of pesticides used in agriculture.

The overall aim is addressed through the following main objectives:

Objective 1
Develop a methodological framework for decision making under risk and uncertainty that will be suitable for solving decision problems in which a potential state of the world (at the end of a period in question) should be considered in alternatives' evaluation.

Objective 2
Define a quasi ex-post risk analysis that will be integrated in the decision analysis and will improve efficiency and rationality in a process of decision making under risk and uncertainty. This relies on predictive or descriptive models, out of which additional information can be extracted for the purpose of ex-post assessment of a potential risk and uncertain states.

Objective 3
Evaluate the developed methodological framework for decision making under risk and uncertainty.

The last objective (Objective 3) is further subdivided into objectives strongly related to the scope of the case-study:

Objective 3.1
Definition of the problem of pesticides transfer in surface and ground water to be managed in accordance with the EU Water Framework Directive (European Parliament & Council, 2000) and regulations (European Parliament & Council, 2009b, 2011) about pesticides used in agriculture.

Objective 3.2
Representation of mitigation measures in the form of complex alternatives.

Objective 3.3
Development and validation of the proposed DSS including quasi ex-post risk analysis (risk assessment and risk management modules).

Objective 3.4
Evaluation of the built DSS's performance and comparison with state-of-the-art models and expert systems.

The aforementioned objectives are supported with three hypothesis. A confirmation of the hypothesis accomplishes the given objectives. They are addressed in the thesis as follows:

Hypothesis 1
Introducing quasi ex-post risk analysis provides additional information with quantified degree of certainty that fills the gap of imperfect knowledge, which better describes the state of the world, at the beginning of a period under consideration (time of decision making).

Hypothesis 2
Introduction of a risk management module improves the evaluation of alternatives in accordance with the estimated state of the world that will potentially take place if the evaluated alternative is applied (state of the world at time point $t+1$). Furthermore, with a predefined set of criteria of how the output (support) should be designed, the risk management module is able to deliver desirable support in decision analysis.

Hypothesis 3
The developed methodological framework can solve decision problems characterized by the presence of risk and uncertainty about the state of the world after an alternative is applied, and in terms of alternatives' consequences (outcomes).

1.2 Contributions to Science

The development and implementation of the methodological framework for decision making leads to four scientific contributions:

Contribution 1
Introduction of quasi ex-post risk analysis that enriches the process of decision analysis with additional information with quantified degree of certainty, which fills the gap of imperfect knowledge in a decision problem.

Contribution 2
Introduction of a risk management module with conditional output that delivers output (support) along with the decision maker's expectations and the possibility to evaluate alternatives over the state of the world that would take place upon implementation of the corresponding alternative (in time $t+1$).

Contribution 3
Formalization and development of a novel methodological framework for decision making under risk and uncertainty composed of quasi ex-post risk analysis (including both risk assessment and risk management modules), which allows subsequent implementation and embedding within a decision support system.

Contribution 4

Development of a decision support system as a case-study in the domain of agriculture and environmental protection for the problem of surface and ground water pollution with pesticide used in agriculture. The results of this implementation contribute in the development of the domain of the case-study.

The first contribution includes investigation of different approaches to handling uncertain, imperfect or incomplete knowledge that introduces risk in the decision making process. Such imperfect knowledge arises the need to consider risk analysis in order to find out 'what is unknown' and how it influences the decision making process. Furthermore, risk analysis requires extensive research of the state of the world and uses simulation or projection to estimate the influence of risk on the final decision, represented as ex-ante risk assessment. Unlike ex-ante, ex-post risk assessment provides assessment at the end of period under consideration, which is hardly suitable in most real-world decision problems, where assessment and reaction are required at the beginning. Introducing quasi ex-post risk analysis effectively preserves the use of ex-ante risk assessment. It improves knowledge by introducing a predictive (diagnostic) layer that contains predictive (diagnostic) models built from data (expert knowledge).

The second contribution introduces a management module that autonomously tries to solve the problem of assessing risk by extensive search through the alternative set. The risk management module evaluates all possible alternatives that result in a set of outcomes and a set of possible states of the world that can take a place upon implementation of a particular alternative, over which the decision maker's preference relation can then be expressed. Furthermore, the management module can take other steps that additionally support the decision making process, if it is provided with proper models. These steps include sorting (categorizing alternatives within a predefined set of categories), choosing (selecting a sub-set of alternatives that satisfy given conditions) and ranking (creating a complete or partially ordered set of alternatives). These steps can also be combined in order to provide maximum support with the decision making process. The models that need to be provided for each step are not constrained by type or dependent variables, so the management module can depend on the state of the world, alternative or outcome parameters, or their combination. The risk management module delivers outcome (support) in a format appropriate to the decision maker's policies or expectations.

The third contribution formalizes quasi ex-post risk analysis (including both risk assessment and risk management modules) into a methodological framework that allows further development and implementation in a wide variety of decision problems in different domains. The methodological framework for decision making under risk and uncertainty can be delivered as the core of a DSS that can be filled with required models and ready to be covered with a graphical user interface for wider usage. The framework can also be integrated or embedded into existing decision support systems as a completely autonomous part.

Finally, the forth contribution is a multidisciplinary contribution over the domains of decision making (decision support), environmental science, ecology and agriculture. From the perspective of decision making and decision support, the developed decision support system provides an opportunity to completely evaluate the proposed methodological framework for decision making under risk and uncertainty. Furthermore, it validates the ability of the methodological framework to solve complex decision problems of an autonomous or semi-autonomous nature. On the practical side, from the environmental, ecological and agricultural point of view, the implementation of the methodological framework over the decision problem in the domain of water protection from pesticides, contributes to filling the gap between EU Directives and Regulations (European Parliament & Council, 2009a,

2000) for water protection, which are characterized as very general but still complex and restrictive. In addition, the farmers suffer collateral damage from implementation of these regulations. Namely, the active substances previously approved for commercial use, i.e. respecting EU regulations (European Parliament & Council, 2009b) and permitted according to the Commission Implementing Regulation (European Parliament & Council, 2011), appear to be among the most important pollutants of water bodies in the environment. Thus, the developed decision support system covers the post-market risk evaluation of pesticides used in agriculture. Such a system allows farmers to immediately evaluate risk when planning plant protection and obtain suggestions of mitigation measures to consider in case the plan is assessed to be risky.

1.3 Organization of the Thesis

The thesis is divided into two parts. The first part is dedicated to reviewing the theory of decision making and risk analysis, and the methodology used in developing the methodological framework, as well as the framework itself and its formalization. The second part elaborates the case-study implementation of the methodological framework.

The complete organization of the thesis is shown in Figure 1.1. The core of the thesis is the development of the methodological framework for decision making under risk and uncertainty. Branches of the central node (*methodological framework*) indicate the main parts of the thesis, with corresponding chapters, arranged clockwise. Each chapter starts with a sibling bounded with a black circle that describes the subject of the chapter.

The thesis starts with the *methodology* part consisting of four chapters (*Chapter 2* to *Chapter 5*) that provide an overview of *decision analysis*, *risk analysis*, *decision modeling* and *machine learning and data mining*. This part concludes with *Chapter 6* that has an important role in the thesis and formalizes the *methodological framework* and its modules, used in the next part (*case-study*). *Chapter 7* introduces and formulates the decision problem under consideration. The implementation of the methodological framework for this decision problem is then described in *Chapter 8*, where each module is described and defined. The chapter finishes with a technical description of the graphical user interface of the decision support system built over the implementation of the methodological framework. The case-study part concludes with *Chapter 9*, which evaluates and validates modules from the implementation of the methodological framework. A comparison between the models built within the framework's modules and state-of-the-art models is also provided. The thesis concludes with Chapter 10, where conclusions, remarks and suggestions for further work are given.

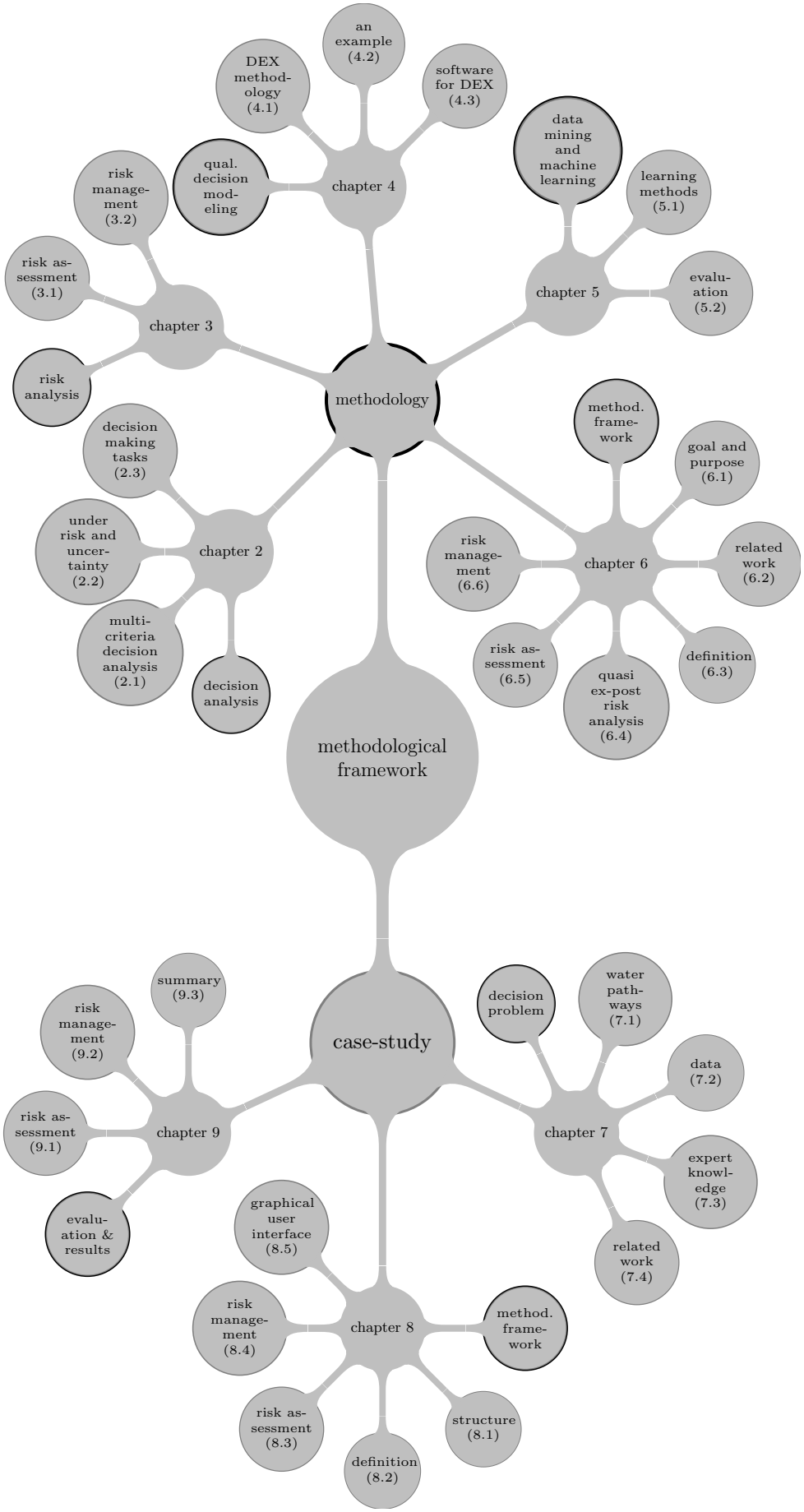


Figure 1.1: Organization of the thesis.

Part I

Methodology

Chapter 2

Decision Analysis

Decision problems can be simple or complex, depending on the circumstances under which a decision needs to be made. To make decisions, simple or complex processes may be required, which may be intuitively or formally described as part of the decision analysis. Decision analysis is a discipline that deals with structuring decision problems and decision making processes, based on decision theory. Decision analysis is also known as "applied decision theory". Decision theory aims to describe the human cognitive functions involved in rational (optimal) decision making, and to establish a general framework that guides the decision analysis and the process of decision making.

Decision making is the process of selecting preferred alternative(s) by the decision maker. In recent decades, as technology advances and intelligent machines appear, the human being is not the only decision maker. In other words, the invention of smart agents opens the issue of replicating the human brain functions that will allow machines to make decisions as humans do, in an autonomous and automatic manner. Decision making by human beings is studied by the discipline called *Decision science*, while decision making by machines is covered by *Decision systems*. The former is further divided into normative decision sciences (Decision theory, Utility theory, Game theory, theory of Choice, etc), descriptive decision sciences (Cognitive Psychology, Social and Behavioral Sciences, etc.) and decision support in building frameworks and tools to support humans in the decision making process (Bohanec, 2001). In the remainder of the thesis, human decision making is simply refereed to as decision making.

Terry (1971) defines the process of decision making as "a process of selection, based on some criteria from two or more possible alternatives" and introduces an alternative space to summarize the task. Massie (1958), further introduces the desired result as the purpose of the activity, defining the decision making process as "a course of alternative consciously chosen from available alternatives for the purpose of the desired result". In addition, McFarland (1970) tries to include the circumstances into the definition and defines it as "an act of choice, wherein an executive forms a conclusion about what must be done in a given situation. A decision represents a course of behavior chosen from a number of possible alternatives".

The definitions above introduce the shape of the problem in decision making. A decision making process is constrained by its alternative space, purpose of the activity, and circumstances under which a decision is made. A decision is an act of selection of an alternative that will satisfy the desired objective of the decision problem, under given circumstances.

The alternative space is a set of alternatives designed to address the objective(s) of the decision problem. Alternatives should reflect substantially different approaches to the problem or different priorities across objectives, and should inform decision makers with real options and choices. Good solutions are not possible without good alternatives.

Usually, what decision makers need is good information about a small, carefully chosen set of alternatives – their consequences, key differences (trade-offs) in their consequences, and the response of key agents with respect to these trade-offs. Generating good alternatives is a source of important insights both from a technical perspective and a values perspective.

When dealing with more than one objective, the decision problem is defined as multi-objective or multi-criteria decision problem. Multi-criteria decision problems are the subject of study in Multi-Criteria Decision Making (MCDM) or Multi-Criteria Decision Analysis (MCDA) disciplines of operations research (Figueira, Greco, & Ehrgott, 2005).

2.1 Multi-Criteria Decision Analysis

The main objective of MCDA is to provide decision makers with a tool for multi-criteria decision problem solving, where several conflicting criteria are taken into account. In each application area (world) described with a set of rules and situations (further referred to as "state of the world"), the objective of decision making is to choose the best alternative among many alternatives, considering multiple possibly conflicting criteria or attributes.

Roy (1996) defines a multi-criteria decision problem as a situation in which, having defined a set A of alternatives and a family F of criteria, the decision maker wishes: to determine a subset of alternatives considered to be the best with respect to F (choice problem); to divide A into subsets according to some norms (sorting problem); to rank the actions of A from best to worst (ranking problem); to describe actions and their consequences in a formalized and systematic manner, so that individuals can evaluate those actions (description of issue).

For simplicity, all kinds of decision making problems have a common stem which is represented and mathematically formalized by the main elements of any decision making problem. The first element is a set A of alternatives, formalized as

$$A = \{a_1, ..., a_n\}; n \geq 2 \tag{2.1}$$

where $n \geq 2$ demands that at least two alternatives should be placed in the set, in order that a problem is considered a decision problem.

The next element is the objective condition, previously defined as the state of the world. Namely, a set of states of world S defines the world itself: $S = \{s_1, ...s_m\}$, where $s_j, j = 1, ..., m$, is a possible objective condition or state of the world. Savage (1972) considered the world as a space of mutually exclusive and exhaustive states, stating that all possible states of the world (possible conditions in the future) are known and only one of them $s_j, j = 1, ..., m$, will take a place.

In multi-criteria decision analysis, alternatives and states of the world have a complex nature and consist of sets of attributes or criteria. An attribute is an atomic element that is used to define an alternative or a state of the world. Throughout the literature, an attribute or criteria can be seen as a single perspective or a point of view on a given decision problem. The set of attributes of an alternative and a state of the world is called *definition* of an alternative and state of the world, respectively.

Throughout the course of the thesis, an attribute of an alternative will be denoted as g_a, and the set of attributes as G_a, while an attribute of a state of the world will be denoted as g_s and the set of attributes as G_s. Thus, the complex nature of an alternative $a \in A$ and a state of the world $s \in S$ is written as:

$$G_a = \{g_{a1}, g_{a2}, ..., g_{ak}\}, \tag{2.2}$$

$$G_s = \{g_{s1}, g_{s2}, ..., g_{sl}\}. \tag{2.3}$$

A set of values that an attribute takes a value from is called the *domain* or *value scale* of an attribute. A function that assigns a value from the set of values to a particular attribute is denoted as D. Thus, a value assigned to an attribute g_{ai} of an alternative $a \in A$ is $a_i = D(g_{ai})$. Similarly, a value assigned to an attribute g_{sj} of a state of the world $s \in S$ is $s_j = D(g_{sj})$.

A set of values assigned to each attribute of an alternative a_i or state of the world s_j is said to be a *description* of the alternative a_i or the state of the world s_j, respectively:

$$a_i = \{a_{i1}, a_{i2}, ..., a_{ik}\}; a_i \in A. \tag{2.4}$$

$$s_j = \{s_{j1}, s_{j2}, ..., s_{jl}\}; s_j \in S. \tag{2.5}$$

If attributes are considered as random variables, in probability theory, the description of alternatives and states of the world is called *realization*, and the assigned values *observations*.

The third element is the outcome of an alternative in various states of the world. Outcomes are also referred to as consequences. Any application of an alternative results in an outcome (leads to some consequence) in any state of the world. A set of outcomes is commonly denoted as χ. If the outcome $x_i \in \chi$ is a result of alternative a_i taken over a particular state of the world s_j, it is formalized as

$$x_i = f(a_i, s_j); a_i \in A; s_j \in S; i = 1, ..., n; j = 1, ..., m \tag{2.6}$$

where f is a function whose domain is the set of alternatives A and the world S, and the range is the set of outcomes χ:

$$f : (A, S) \to \chi. \tag{2.7}$$

In order to evaluate or assess an alternative $a \in A$, it is necessary to formally measure all its possible outcomes $x \in \chi$. For this purpose, a function u:

$$u : \chi \to \mathbb{R}, \tag{2.8}$$

is used to express the utility that an individual gains from a particular outcome. This function is called the *utility function* and its input is the outcome of an evaluated alternative. Depending on the decision problem, the range of a utility function may not be the set of real numbers $\mathbb{R}$, but a finite set of nominal values (e.g., $\{good, useful, desirable\}$) that expresses preferential values of an individual. In multi-criteria decision analysis, the utility function includes an aggregation function across alternatives' attributes, which can be of different types, e.g., additive, multiplicative, linear value function, etc (French, 1988).

The final element of decision making are preferences of an individual. Preferences describe an individual's subjective likeliness (attitude) over the set of alternatives. Given alternatives $a_1, a_2 \in A$, an individual regards as more preferable alternative a_1, in comparison to a_2 written as $a_1 \succ a_2$. Indifference between them is written as $a_1 \sim a_2$. In case a_1 is as good as a_2, this is written as $a_1 \succeq a_2$. Mathematically, preferences are described as a binary relation (Definition 2.1):

$$\succeq \in A \times A. \tag{2.9}$$

Definition 2.1 (Binary relation). Let A be a finite set of elements (a_1,a_2,a_3,...,a_n). A binary relation R on the set A is a subset of the cartesian product $A \times A$, that is, a set of ordered pairs (a_i,a_k) such that a_i and a_k are in $A : R \subseteq A \times A$.

The preference relation is then defined as in Definition 2.2.

Definition 2.2 (Preference relation). Let A be a finite set of alternatives $A = \{a_1, a_2, a_3, ..., a_n\}$ with a corresponding set of outcomes $\chi = \{x_1, x_2, x_3, ..., x_n\}$ over a given state of the world, and u a defined utility function. A binary relation $\succeq$ between two alternatives is a preference relation if and only if:

$$\forall (a_i, a_j) \in A \times A : u(x_i) \geq u(x_j) \Leftrightarrow a_i \succeq a_j. \tag{2.10}$$

Based on preference relations, an individual is able to make a choice and decide what alternative best suits his or her requirements. However, the result of decision analysis is not always one single alternative that appears to be the best, but can be a set of different alternatives as well. An overview of possible outputs from decision analysis is given in Section 2.3.

Most decision problems can be represented with a so-called decision table that encompasses the above elements of the decision making process (Table 2.1) (French, 1988).

	s_1	s_2	...	s_m
a_1	$u(f(a_1, s_1))$	$u(f(a_1, s_2))$	...	$u(f(a_1, s_m))$
a_2	$u(f(a_2, s_1))$	$u(f(a_2, s_2))$	...	$u(f(a_2, s_m))$
.	.	.	...	.
.	.	.	...	.
.	.	.	...	.
a_n	$u(f(a_n, s_1))$	$u(f(a_n, s_2))$	...	$u(f(a_n, s_m))$

Table 2.1: General form of a decision table.

The general form of a decision table expresses the use of utility function u over each combination of alternative $a_i \in A$ and state of the world $s_i \in S$. However, this representation does not include information on what state could possibly take place. Accordingly, there are three different cases: we know what state will take place (*true state*), we know what chance of occurring does each state of the world have, or we don't know anything about the chances of occurring for each state of the world.

Savage (1972) summarized the world S as a space of mutually exclusive and exhaustive states, where the future is known and only one state will occur. This is not always true in the case of decision making at the beginning of a period under consideration. In some real-world problems the future is incompletely known. Such an environment of imperfect information about the future of S affects the decision of choosing the most preferred alternative. Namely, under imperfect information about the future of S, the true interest of the individual lies in what his preferences would command under perfect information and not under the available information.

The main issue here is to impose some reasonable assumptions on properties of the individual's preferences. The properties critically depend on the type, amount and correctness of information about S, where several typical cases arise (Aliev & Huseynov, 2014):

Decision making under uncertainty or complete ignorance

The case when no information on probabilities of states of S are available (Table 2.1)

Decision making under risk

The case when the objective probability of occurrence of each state of S is known (Table 2.2)

Decision making under ambiguity or ignorance

Case when difficulties in assessing precise probabilities of states of S are present (e.g.

when a state of the world has an attribute that represents an event that is hard to observe or estimate)

Decision making under certainty
The idealized case, when it is known which state of S will occur, known as the *true state* (Table 2.3)

	s_1	s_2	...	s_m
a_1	$u(f(a_1, s_1))$	$u(f(a_1, s_2))$	...	$u(f(a_1, s_m))$
a_2	$u(f(a_2, s_1))$	$u(f(a_2, s_2))$	...	$u(f(a_2, s_m))$
.	.	.	...	.
.	.	.	...	.
.	.	.	...	.
a_n	$u(f(a_n, s_1))$	$u(f(a_n, s_2))$	...	$u(f(a_n, s_m))$
	$p(s_1)$	$p(s_2)$	...	$p(s_m)$

Table 2.2: Decision table for decision making under risk.

	s
a_1	$u(f(a_1, s))$
a_2	$u(f(a_2, s))$
.	.
.	.
.	.
a_n	$u(f(a_n, s))$

Table 2.3: Decision table for decision making under certainty.

Imperfect information is defined as information which is imprecise, uncertain, incomplete, unreliable, vague or partially true in one or more respects (Zadeh, 2001). In addition, Aliev and Huseynov (2014) clarify that imprecision and uncertainty are the most critical concepts of imperfect information, and that decision making under risk and uncertainty are related cases that can be differentiated only by the amount of available information. This leads to merging both circumstances into one and considering it as decision making under uncertainty. The latter implies motivation to study closely decision making under uncertainty.

2.2 Decision Making Under Risk and Uncertainty

Uncertain information is defined as information without complete certainty that results from lack of information about S for deciding whether a statement is true or false (Smets, 1997). Furthermore, uncertainty can be classified as objective or subjective, depending on the source of information, whether coming from evidence or an individual's opinion on the likelihood of states of S. Objective uncertainty may be probabilistic or non-probabilistic, where probabilistic uncertainty is related to randomness, i.e. probability of an event related to its tendency to occur. Subjective uncertainty is an individual's belief on the likelihood of the occurrence of an event.

In the scientific field of risk analysis, risk is defined as a measure of the probability and consequence of uncertain future events that have a chance of an undesirable outcome. The

outcome can appear in the form of hazard or opportunity. Given both of them, risk consists of two components: chance or probability of a state of S to take place, and an undesirable outcome or consequence. Furthermore, Yoe (2011) stated that uncertainty gives rise to risk, so the essential purpose of risk analysis is to help in making better decisions under conditions of uncertainty.

For simplicity, risk can be defined as the product of the probability of a state to take place and it's consequence (Yoe, 2011). Therefore, if a state of S of any consequence has no probability of occurrence, there is no risk. Likewise, if there is no consequence or undesirable outcome, then there is no risk.

The definition given tries to distinguish the probability of a state of S from the probability and type of an outcome. Accordingly, two cases of uncertainty in the decision making process can be identified:

- Uncertainty due to lack of information about the probability of occurrence of a state
- Uncertainty due to lack of information about possible outcomes or consequences

In both cases uncertainty can critically affect the process of making decisions and it is highly recommended to consider both of them and analyze, in-depth, the source and level of uncertainty.

In decision making theory it is important to separate 'what is known' from 'what is unknown' and try to minimize the latter. However, this is not always possible. The first and most important distinction to make in 'what is unknown' is that between natural variability and knowledge uncertainty (National Research Council, 2009). The former is uncertainty that deals with the inherent variability in the physical world. Variability is often attributed to a random process that produces natural variability of a quantity over time and space or among members of a population. It can arise because of natural, unpredictable variation in the performance of S. It is, in principle, irreducible. However, characterizing such variability might introduce additional knowledge, by using descriptive statistics over evidence of particular natural processes (Bonta & Cleland, 2003), extracting a context and guidance for further management of particular problems (Landres, Morgan, & Swanson, 1999) or various techniques for their representation and quantification (Reagan et al., 2004; le Maître, Knio, Najm, & Ghanem, 2001).

Knowledge uncertainty is the uncertainty attributed to a lack of knowledge about the states of S and their outcomes. It is reducible in principle, although it may be difficult or expensive to do so. Furthermore, knowledge uncertainty is divided into three main "piles" (World Health Organization, 2006):

Scenario uncertainty
: Uncertainty in specifying the risk scenario that is consistent with the scope and purpose of the assessment.

Model uncertainty
: Uncertainty due to gaps in scientific knowledge that hamper an adequate capture of the correct causal relations between risk factors.

Parameter or input uncertainty
: Uncertainty involved in the specification of numerical values (be it point values or distributions of values) for the factors that determine the risk.

The most commonly encountered uncertainty is parameter (input) uncertainty (Yoe, 2011). Thus, some quantities have a true or factual value, while others do not. Instead of a true value, they have a best or most appropriate value that reflects some subjective judgment.

The search for a true value is an objective one, while the search for a best value is subjective. In such a case, the source of uncertainty could be again knowledge uncertainty or natural variability, where reduction of the latter appears to be a complex task.

Because uncertainty gives rise to risk, the essential purpose of risk analysis is to help an individual to make better decisions under conditions of uncertainty. This is done by separating what we know about a decision problem from what we do not know about it. We use what we know and intentionally address those things we do not know in a systematic and transparent decision-making process that includes effective assessment and management of risks.

2.3 Decision Making Tasks

The term problematic (literal translation of the French "problematiqué") is used in decision theory to describe what type of problem a decision analysis can solve. We will use the term "decision making task" instead. In general, decision analysis is described as a field that deals with solving problems of choice. However, this statement is only partly true, since decision analysis can also be exploited by elaborating an appropriate set of alternatives or potential actions A. In other words, the outcome of a decision analysis is not strictly defined as a choice (Roy, 2005).

Consequently, Roy (2005) thoroughly studied this space of possible types of outcomes and proposed four different decision making tasks that describe all possible types of outcomes of decision analysis: description, choice, sorting and ranking.

The description task of decision making aims to build a suitable family of criteria that can be used in determining an alternative's performance. Such performance can be later completed by additional information like discrimination thresholds, aspiration or rejection levels, or weights. The outcome of decision analysis as conceiving descriptive tasks and not prescription or recommendation is said to be the description task.

The choice task of decision making is oriented towards selecting one "good" action or a small set of "good" actions or alternatives from A. The selection is not necessarily oriented towards the determination of one or all the alternatives of A, which can be regarded as optimum, but can also perform pair-wise comparison among all alternatives from A in order to justify elimination of a large number of them. Selected alternatives are the most satisfying and remain non-comparable to each other.

The sorting task of decision making aids with the assignment of each alternative from A to a category that belongs to a predefined set of categories. Assignment is done via judgment and various criteria (sometimes conflicting) that guarantee that all alternatives assigned to a particular category are "nearest" by their appropriateness. The outcome can have the form of an ordered list of categories with sorted alternatives from A. In a sense, this task conflicts with the classification task. However, Kadziński, Greco, and Słowiński (2014) argued that classes (categories) in a classification task are obtained throughout the analysis, parallel to the nominal classification problem, unlike the sorting task where classes (categories) are defined before the assignment procedure is run.

The ranking task of decision making is oriented towards imposing a complete or partial order on A, which can be regarded as an appropriate instrument for comparing alternatives. Comparison can be done based on predefined preferences or can be induced by a model that depend either on preferences or input in the decision making process.

However, there has been criticism of the aforementioned scheme of decision making tasks, to the effect that they are interconnected. Krantz, Suppes, and Luce (2006) stated that if an individual is able to select the best alternative a_i for any set of alternatives, then there exists a rank order of all alternatives in A. Figueira et al. (2005) noted the reverse

statement: "Ordering relations is the natural basis for solving ranking or choice problems". Therefore, for completing the task of choosing the best alternative a_i among all given in A, it is necessary to constitute an order of the set A by evaluating all possible alternatives.

An ordering relation is a set relation that for a given set A establishes how each alternative $a_i \in A$ compares to each other alternative $a_j \in A$ from a preference perspective, which leads to obtaining an order that can be used to make either a choice of an alternative from A (to identify the best alternative) or to rank the set A. In general, an ordering relation is defined as a preference structure (Figueira et al., 2005):

Definition 2.3 (Preference structure). A *preference structure* is a collection of binary relations defined on the set A such that:

- for each pair $(a_i,a_j) \in A \times A$; $i, j = 1, ..., n$; at least one preference relation is satisfied
- for each pair $(a_i,a_j) \in A \times A$; $i, j = 1, ..., n$; if one preference relation is satisfied, another one cannot be satisfied.

The total order structure consists of an arrangement of objects from the best one to the worst. Furthermore, a preference structure can be associated with partial, weak, semi- or interval order (Figueira et al., 2005).

Chapter 3

Risk Analysis

Risk analysis is a systematic process that deals with uncertainties to formulate alternatives and assess their various distributional impact. It is usually performed in three steps or tasks: risk assessment, risk communication and risk management, where risk assessment and management are obligatory (Haimes, 2015).

Risk analysis influences an individual's thinking by making it more analytical. This simultaneously limits the "damage" that human reasoning can inadvertently do when making decisions. Risk analysis is a useful and evolving way to think about and solve risky and uncertain problems. It separates 'what is known' from 'what is unknown' (the uncertainty), and it focuses appropriate attention on the latter and how that might affect decision outcomes, and therefore, the decision itself. Thus, risk analysis should be an integral part of the decision making process, rather than an add-on technical analysis (Haimes, 2015).

The process of risk analysis is iterative and schematically organized as in Figure 3.1. Risk assessment is a systematic process for describing the nature, likelihood, and magnitude of risk associated with some substance, situation, action, or event that includes consideration of relevant uncertainties. It tries to answer the following questions: "What can go wrong?", "What is the likelihood that it could go wrong?", "What are the consequences?", "What is the time domain?" (Haimes, 2015). Risk assessment can be qualitative, quantitative, or semi-quantitative (a mixture of both).

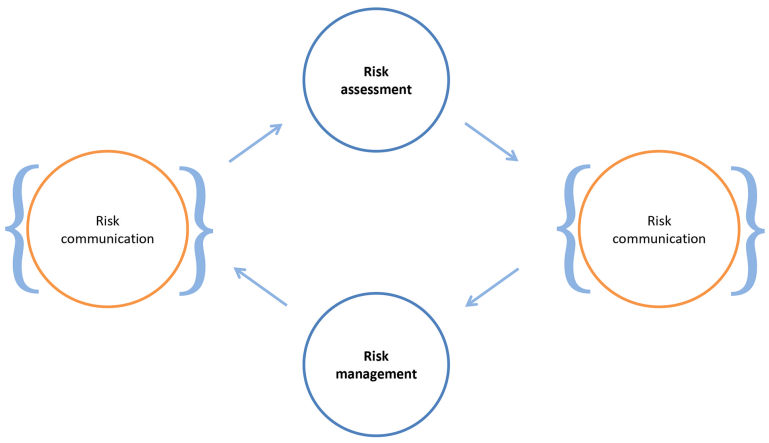


Figure 3.1: Risk analysis. Schematic organization of the process.

Risk management is a process of evaluating risks and initiating action to identify, eval-

uate, select, implement, monitor, and modify actions taken to alter levels of unacceptable risk to acceptable or tolerable levels (Lund, Solhaug, & Stølen, 2010). In terms of questions, it tries to find answers for: "What can be done and what options are available?", "What are the associated trade-offs in terms of all costs, benefits, and risks?" and "What are the impacts of current management decisions on future options?" (Haimes, 2015). The goals of risk management are often said to include scientifically sound, cost-effective, integrated actions that reduce risks while taking into account economic, environmental, social, cultural, ethical, political, and legal considerations (Yoe, 2011).

Risk communication is more of an organizational step in performing the analysis than part of the analysis itself. This step or task is not considered for further review here.

3.1 Risk Assessment

Risk assessment is a component of risk analysis that answers the individual's questions about the risks. It provides the objective information needed for decision making, including a characterization of the relevant uncertainty that could influence the decision. An assessment is done to get an understanding of potential risk and to measure and describe it as much as possible. It provides an objective, unbiased treatment of the available evidence in well-organized and easy to understand documentation that clearly links the evidence to its conclusions. It also describes and addresses uncertainty in intentional ways.

Risk assessment is based on ordinary reasoning. It is a set of logical, systematic, evidence-based analytical activities designed to provide individuals with the best possible identification and characterization of the risk associated with the decision problem. Evidence can be considered to encompass all available data regarding the decision problem under consideration. It is a methodical process with specific steps that provide for a thorough and consistent approach to the assessment of risks. It also provides a reduction of the uncertainties that attend those risk. Because it includes the best available scientific knowledge, it is science based (Yoe, 2011).

At its simplest, risk assessment estimates the risks associated with different hazards, opportunities for gain, or alternatives. The most robust and detailed definition is given by Health (1983), stating that risk assessment can be divided into four major tasks: hazard identification, dose-response assessment, exposure assessment and risk characterization. In a similar way, the World Health Organization (2006) define risk assessment as "a scientifically based process consisting of four steps: hazard identification, hazard characterization, exposure assessment and risk characterization".

In the context of food-safety regulations, hazard identification is identification of biological, chemical and physical agents capable of causing adverse health effects that may be present in a particular food or group of foods. Its characterization includes qualitative or quantitative evaluation of the nature of adverse health effects. Dose-response is determination of the relationship between the magnitude of exposure to a chemical, biological or physical agent, which represent the dose, and the severity of associated adverse health effects that cover the response. Exposure assessment includes qualitative or quantitative evaluation of likely intake of biological, chemical and physical agents via food. The final step is defined as estimation of the probability of occurrence and severity of potential adverse health effects in a given population.

In addition, Yoe (2011) came out with a reduced list of steps in risk assessment on a general level, where four general steps in the assessment of a potential risk are: hazard or opportunity identification, consequence assessment, likelihood assessment and risk characterization. Hazard or opportunity identification is a framework for identifying the hazards that can cause harm or the opportunities for gain. Next, consequence assess-

ment identifies who or what may be harmed or benefited, as well as in what ways it can be done. Likelihood assessment includes assessment of the likelihood of various adverse and beneficial consequences with qualitative or quantitative characterization. Finally, risk characterization preforms estimation of the probability of occurrence, the severity of adverse consequences and the magnitude of potential gains. As before, characterization can be done qualitatively or quantitatively.

While hazard or opportunity identification can be done manually by the individual, consequence and likelihood assessment require gathering and analyzing relevant data that can be done in a computational environment, the outcome of which will feed the step where risk is characterized. Risk characterization, by itself, can be done by a predefined guide or instruction built in accordance with domain policies.

Consequence and likelihood assessment characterize the nature and likelihood of the harm or gain caused by a hazard, and the gain possibility. Both are highly linked to the presence of uncertainty. Lack of domain knowledge in the former may lead to an incomplete list of possible consequences. The latter analyzes the manner in which undesirable consequences of hazards or desirable consequences of opportunities occur, so they can characterize the likelihood of the sequence of events that produce these outcomes. Therefore, the lack of observability or measurability of the outcome introduces another level of uncertainty at this stage.

In practice, consequence assessment is done by carefully identifying the consequences and linking them to the hazards and opportunities by application of various conceptual iterative models. In such an iterative process, some aspects become better understood, while uncertainty is reduced. On the other hand, assessing the likelihoods of the consequences associated with identified risks can often be aided by developing a risk hypothesis, which is a model or scenario that explains in detail how the source of risk can lead to the consequences of concern. Alternatively, it estimates the probability that an alternative does yield a favorable outcome.

Both consequence and likelihood assessment can be done in qualitative or quantitative manner. On the conceptual level, a survey of the literature exposes two approaches to consequence and likelihood assessment: ex-ante (before the fact) and ex-post (after the fact) (Keeney & Winkler, 1985a; Kolstad et al., 1990; Kamin & Rachlinski, 1995; Neely, 2003; Todd & Wolpin, 2008). Ex-ante is a prospective approach that evaluates the potential risk at the beginning of a period in question and tries to describe the state of the world by using projection, simulation or foresight approaches. On the other hand, ex-post is a retrospective approach that evaluates the potential risk at the end of the period in question, considering the real (observed) state of the world. Therefore, the former uses incomplete or imperfect information, unlike the latter, which has at its disposal complete pieces of information (Fleurbaey, 2010; Fleurbaey & Peragine, 2013).

From the decision making point of view, the ex-ante approach focuses on an individual's expected utilities or preferences over beliefs, hazards and opportunities, due to lack of information or imperfect information. The ex-post approach, on the other hand, computes the expected value of the hazard and opportunities and the focus is shifted to preferences about the outcome (Roeser, 2012). An important limitation of the ex-ante approach is the fact that the individual's true preferences under incomplete or imperfect information can significantly differ from the individual's preferences given perfect information. Such a limitation has an effect on the rationality of decisions driven by preferences. This results from the combination of the individual's interests and correct information about possible alternatives (Weirich, 2004). Both approaches can be applied in decision problems with presence of both sources of uncertainty, about the state of the world S and about decision consequences or outcomes.

Representing both approaches on a timeline (Figure 3.2) shows that ex-ante is performed at the beginning of the period of interest (denoted by a point in time, t), while the ex-post approach is performed at the end of the period under consideration (at time $t+1$).

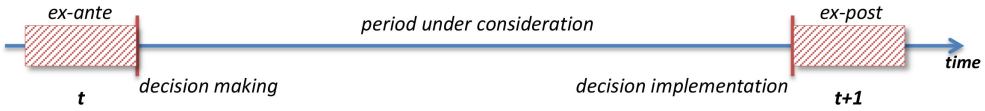


Figure 3.2: Ex-ante and ex-post on a time line.

When considering the timeline (Figure 3.2), the time point t is also considered as the point at which a decision is made, while the time point $t+1$ is considered as the time point at which the decision is implemented. The period bounded by the time points t and $t+1$ is defined as the period of interest or the period under consideration.

For example, let $s_t \in S$ be a state of the world at time t (beginning of the period under consideration) and $a_t \in A$ an alternative that needs to be chosen. At time t, the individual doesnt́ know what the consequence will be of choosing a_t and what state $s_{t+1} \in S$ will take a place (end of period under consideration). If ex-post risk assessment is made, then the individual performs assessment and analysis at time of s_{t+1}, and his or her preferences are based on the outcome derived from the chosen alternative a_t (implemented decision) and known state of the world s_{t+1} at time $t+1$: $u(f(a_t), s_{t+1})$. Unlike ex-post, ex-ante is performed at time point t and faces uncertainty over s_{t+1}. The utility function u should take such circumstances into account and perform evaluation based on the alternative a_t and the state of the world s_t: $u(f(s_t, a_t))$. However, the ex-ante approach can take into account some projection method in order to obtain insight into the probability of a state of the world taking place.

On the implementation level, ex-ante is mostly applied with probability elicitation, Monte Carlo analysis and Probabilistic Scenario analysis (Yoe, 2011), while ex-post is performed by Error Propagation equations (Mandel, 2012), Scenario analysis (van der Heijden, 2005) and Sensitivity analysis (Saltelli et al., 2008).

3.2 Risk Management

Once the risk has been profiled, evaluated and the decision context understood, the process continues with management of evaluated risk. Risk management is required if the risk has been evaluated to be non-acceptable. An acceptable risk is a risk whose probability of occurrence is so small, or whose consequences are so slight, or whose benefits (perceived or real) are so great that individuals or groups in society are willing to take or be subjected to the risk that the event might occur. Acceptable risk requires no risk management; it is, by definition, acceptable. Risk that is not acceptable is therefore unacceptable, and by definition must be managed or reduced to the level of acceptable or tolerable risk. A tolerable risk is a non-negligible risk that has not yet been reduced to an acceptable level. The risk is tolerated for one of three reasons: inability to reduce the risk further; the costs of doing so are considered excessive; or the magnitude of the benefits associated with the risky activity are too great to reduce it further. Overall, the reduction of the assessed risk to an acceptable or tolerable level is the main objective of risk management (Chavas, 2004; Haimes, 2015).

In order to achieve the risk management objective, an individual should consider strategies that describe specific ways of achieving it (Yoe, 2011). A strategy in decision making is an alternative a, and a set of strategies is the set of alternatives A, introduced earlier. Risk management consists of formulating a set of alternatives A and choosing an alternative that will satisfy the risk management objective.

Formulating a set of alternatives is a comprehensive task that should be constrained within the domain of the decision problem. Yoe (2011) states the key point that nobody can be sure to have the best alternative, unless many of them are not considered. Therefore, at this point, a set of proposed alternatives is necessary. More importantly, the alternatives have to be evaluated. A lot of research in the domain of decision analysis is concerned with methods to aid the evaluation of A and choosing right alternative $a \in A$. The methodology developed for this task in the context of MCDA is called preference modeling (Figueira et al., 2005).

Chapter 4

Decision Modeling

Decision analysis (Nagel, 1993; Skinner, 2009) is a discipline that proposes a framework for analyzing decision making problems. In order to analyze and provide aid or support to individuals in their search for satisfactory solutions to the multi-criteria decision problem, it becomes necessary to construct some type of model to represent individual preferences and value judgments. Such models (further referred to as decision models) can be distinguished mainly by the number of attributes or criteria that they can consider, and the type of the input/output space, whether quantitative or qualitative. Therefore we differentiate single-attribute vs. multi-attribute (criteria) decision models that are based on qualitative or quantitative input/output space.

Multi-criteria decision (MCDA) models seek to take explicit account of multiple, conflicting criteria and help to structure the decision problem with complex alternatives (Belton & Stewart, 2002). Typically, alternatives perform well with some criterion or subset of criteria and perform poorly with others, so unique solution (single attribute that perform best) can rarely be proposed. Finding a trade-off among many well performing alternatives is the purpose of MCDA. Furthermore, MCDA models provide a process that leads to rational, justifiable, and explainable decisions.

Belton and Stewart (2002) classify MCDA models into three broad categories: *Value measurement models*, *Reference level models* and *Outranking models*. Value measurement models construct a utility value (nominal or numeric) in order to represent the degree to which one alternative may be preferred to another. This category includes the following most popular methods: Kepner-Tregoe (Kepner & Tregoe, 1981), UTA (UTilitiés Additives) (Jacquet-Lagreze & Siskos, 1982), MACBETH (Bana e Costa & Vansnick, 1999) and DEX (Bohanec & Rajkovič, 1990).

Reference level models assign desirable or satisfactory levels of achievement to each criterion. The analysis then tries to discover alternatives that are closest to achieving these desirable goals. The most used method is Goal Programming (Charnes & Cooper, 1957) and its variants like Interactive Sequential Goal Programming (Hwang, Paidy, Masud, & Yoon, 1979), Linear Goal Programming and General Goal Programming (Belton & Stewart, 2002).

Outranking models compare alternatives in a pairwise fashion, initially in terms of each criterion in order to identify the extent to which preference for a particular alternative can be asserted over another alternative. There are variations that perform the pairwise comparison of alternatives over aggregated relevant criteria. Typical methods within this category are AHP (Analytic Hierarchy Process) (Saaty, 2005; Saaty & Vargas, 2014), ZAPROS (Larichev & Moshkovich, 1995; Larichev, 2001), DRSA (Dominance-based Rough Set Approach) (Greco, Matarazzo, & Slowinski, 2001, 2002) and methods that belong to the ELECTRE and PROMETHEE families. A complete overview of these families can be

found in Greco, Ehrgott, and Figueira (2016).

Figueira et al. (2005) extend the above classification with: the *Dissagregation-aggregation approach* and the *Rule preference approach*; while others are renamed as: *Value system approach*, *Multiobjective optimization approach* and *Outranking approach*, respectively.

In the thesis, qualitative MCDA models are considered. Since the thesis comprises a case-study in the domain of environmental modeling, related studies and decision problems are reviewed. There are many aspects of decision making with environmental modeling that cannot be described adequately, or predicted deterministically, such as: future states and conditions of natural systems, risk, and human subjectivity in judgments (dÁngelo, Eskandari, & Szidarovszky, 1998; A. Kangas & Kangas, 2004). All these factors contribute to uncertainty in decision-making, often not considered because of data unavailability and costs (Malczewski, 1999). Data unavailability is a common problem in this domain, due to the cost of data collection if each criterion needs to be provided with data. In such situations qualitative estimations and expert judgments can be considered for better informed decision analysis.

Qualitative MCDA models are characterized by using qualitative attributes, whose value scales contain a finite predefined set of qualitative (or nominal) values, unlike quantitative models that use numeric value scales for attributes and preferences. There are two groups of qualitative MCDA models which differ in the way knowledge is acquired from an individual when the decision model is built (Boose, Bradshaw, Koszarek, & Shema, 1993; Bohanec, Aprile, Costante, Foti, & Trdin, 2013): methods based on interactive questioning for obtaining the individual's preferences, and methods that acquire the individual's preferences directly. Representative methods for the former are MACBETH and ZAPROS, and DRSA and DEX for the latter.

In this work, the DEX method for building qualitative decision models is considered. The following section describes DEX in more detail.

4.1 DEX Methodology

The DEX (Decision EXpert) method (Bohanec & Rajkovič, 1990; Bohanec & Rajkovic, 1999; Bohanec et al., 2008, 2014; Trdin & Bohanec, 2015) is a qualitative multi-criteria decision modeling method that enables an individual to structure the decision problem into smaller measurable concepts (attributes). DEX models consists of attributes, *scales of attributes*, *hierarchy of attributes* and *utility functions*.

Attributes are variables that represent basic features and assessed values of decision alternatives. They use qualitative scales, which consist of a finite set of nominal values, such as "bad", "good" and "great". Attributes in DEX comprise a *hierarchical structure* that represents a decomposition of the decision problem into less complex sub-problems, with the assumption that they will be easier to solve. The hierarchical structure is represented as a tree of attributes or directed acyclic graph with one or more *root* attribute(s) and a set of *input* attributes.

Basically, there are two types of attributes in DEX: input and aggregated attributes (including root attribute(s)). The former are used for describing alternatives and do not have any child attributes. The latter are obtained by aggregating input and/or other aggregated attributes and represent solutions or evaluations of a particular sub-problem and its alternatives. Aggregated attributes that do not have any parent attributes are called root attributes.

The hierarchical structure assumes that each attribute within the structure is indirectly connected to the root of the tree by only one traversal path. In addition, top-down traversal assures that such a path defines the hierarchical dependencies of particular attributes at

each level in the hierarchy. Namely, at each level of the hierarchy there is an attribute, which depends on its immediate descendants in the structure. Aggregation that defines the dependency is represented with a *utility (aggregation) function.*

The utility function is defined by a *decision table*, which consists of *decision rules.* It needs to specify an output value for every combination of descendants' values. Typically, such functions are prepared by the decision maker in accordance with his or her preferences.

Formally, a DEX model M is composed from a set of attributes $V = \{v_1, v_2, ..., v_n\}$, where n is number of attributes. They are structured hierarchically: each attribute $v \in V$ may have descendants (children) and predecessors (parents) in the model. The relationship is represented by utility functions I and O referring to the input and output of attribute v, respectively. The former is parametrized with a set of attributes that is used in the construction of a particular attribute v, while the latter results in a set of attributes in the aggregation of which that particular attribute v is included.

Each attribute $v \in V$ is accompanied with a value scale $sv \in Sv$, where sv is a set of qualitative values, from which attribute v takes a value, and Sv is the set of all value scales applicable for the given model M. Assigning a value from sv to attribute v is formally described as a function D that maps the attribute v to the corresponding value scale sv:

$$D : V \mapsto Sv. \tag{4.1}$$

With respect to an individual's preferences, scales can be either ordered (increasing or decreasing) or unordered. An ordered scale is a set of values that are preferentially ordered according to their contribution to the quality of alternatives, and the difference among values corresponds to meaningful distance represented in the appropriate space. An unordered scale by contrast, is a set of values without any meaningful relation, or the relation is unknown (undefined). The ordering of scales is important for constructing utility functions, and simplifies the definition of decision rules (Bohanec, 2013).

The aggregation of an attribute $v \in V$ with value scale $sv \in Sv$ and input attribute set $\{v_{j1}, v_{j2}, ..., v_{jk}\}$ $k < n$, is a relation I defined as:

$$I : sv_{j1} \times sv_{j2} \times ... \times sv_{jk} \mapsto sv, \text{ where } sv_{jt} = D(v_{jt}), t \in [1, k]. \tag{4.2}$$

An alternative $a \in A$, described with a set of input attributes, is evaluated by performing bottom-up aggregation of model inputs toward model outputs in accordance with the model's hierarchical structure and corresponding aggregation (utility) functions. The output of alternative's evaluation is a value from the root attribute's scale. Such a value expresses an individual's preference for the evaluated alternative and can be further used in the comparison and ranking of alternatives.

4.2 An Example

The following example illustrates every part of a DEX decision model described above. It addresses the decision problem of choosing an active substance to be applied in a field that will not pollute the environmental waters and be affordable for the budget that an individual has.

The model has one root attribute, *active substance* that expresses the preferences of an individual (farmer) for a particular active substance (Figure 4.1). In order to assess the "*goodness*" of a given active substance, the model decomposes the problem of selecting appropriate active substance into two sub-problems, represented as intermediate attributes: *cost* and *pollution.* Cost is assessed using *price* and *efficiency* of the active substance, while pollution considers the *required dose* and *DT50* - the property of an active substance that expresses the time to reduce to half its initial dose.

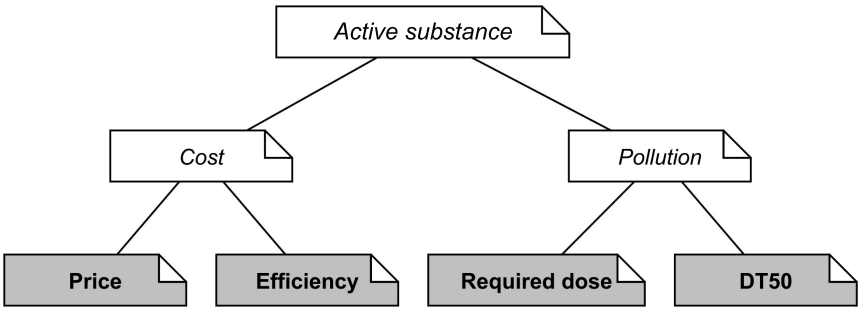


Figure 4.1: Hierarchical structure of the DEX model for evaluating active substances.

Attribute	Scale
Active substance	**bad**; accept; good; ***excel***
Cost	**high**; medium; ***low***
Price	**high**; medium; ***low***
Efficiency	**low**; medium; ***high***
Pollution	***low***; accept; medium; **high**
Required dose	***low***; medium; **high**
DT50	***low***; medium; **high**

Figure 4.2: Attribute value scales of the DEX model for evaluating active substances.

The root attribute is active substance with four possible values: *bad*, *accept*, *good* and *excel*. *Bad* active substance refers to substance with high cost and most likely to pollute surrounding watersheds, while *excel* refers to excellent/safety and low-cost active substance. The value scale is thus ordered from "bad" to "good" outcomes (increasing order). Figure 4.2 gives ordered scales for all attributes. Values given in red are considered not satisfactory outcomes/values, in contrast with satisfactory outcomes/values given in green. If the order were from "good" to "bad", it would be said to have decreasing order.

Table 4.1: Pollution aggregation.

Required dose	DT50	Pollution
low	low	low
low	medium	low
low	high	accept
medium	low	low
medium	medium	accept
medium	high	medium
high	low	accept
high	medium	medium
high	high	high

The aggregation of qualitative attributes in the hierarchical structure of the model is given in Tables 4.1, 4.2 and 4.3. The last table represents the utility function for the root attribute and shows that in some cases some of the alternatives can have the same evaluation, although they have different input values. This represents a trade-off in decision

making.

Table 4.2: Costs aggregation.

Price	Efficiency	Costs
high	low	high
high	medium	high
high	high	medium
medium	low	medium
medium	medium	medium
medium	high	low
low	low	medium
low	medium	low
low	high	low

Table 4.3: Active substance aggregation.

Costs	Pollution	Active substance
high	low	accept
high	accept	accept
high	medium	bad
high	high	bad
medium	low	good
medium	accept	accept
medium	medium	bad
medium	high	bad
low	low	excel
low	accept	good
low	medium	bad
low	high	bad

The DEX model is now defined and can be used to evaluate active substances. Table 4.4 gives the evaluation of four different active substance, named: *AS1*, *AS2*, *AS3* and *AS4*. For the sake of clarity the selection of active substances is done with the assumption that they are applicable to the same type of crop, and that they complement each other.

Table 4.4: Evaluation of four alternatives.

Active substance	Price	Efficiency	Required dose	DT50	
AS1	high	high	high	low	**accept**
AS2	medium	low	low	low	**good**
AS3	low	medium	high	medium	**bad**
AS4	low	high	medium	low	**excel**

Considering the evaluation of alternatives (Table 4.4), no active substances receive the same value. Since the scale of the root attribute *active substance* is preferentially ordered, the most and least preferred active substance can be read out. An individual would most likely prefer active substance *AS4*, since it is evaluated as excellent; the least preferred is *AS3*. The alternatives would be ordered by the individual's preference as follows:

$$AS4 \succeq AS2 \succeq AS1 \succeq AS3, \tag{4.3}$$

The above example is built using the DEXi software that is described in the following section.

4.3 Software for DEX

The DEX method has three different implementations. The first is DEXi (Bohanec, 2013; Bohanec et al., 2014) and is the one that is mostly used for modeling with DEX. The second is proDEX (Žnidaršič, Bohanec, & Zupan, 2006) that extends DEX with probabilities during evaluation. The third is DEXx, an implementation developed by Trdin and Bohanec (2015), which includes a variety of extensions of the traditional DEX method. DEXi and DEXx are the implementations that this work is based on.

The DEXi implementation is an interactive computer program for multi-attribute decision making. It supports two basic tasks: the development of qualitative decision models and their application. The graphical interface allows defining attributes, scales, tree structures and utility functions as part of the development task.

The application of developed decision models includes evaluation and analysis stages, both supported in the DEXi implementation. It supports defining the values of input attributes that define an alternative, and the evaluation of such alternatives from the bottom to the top (root) attribute. Furthermore, DEXi allows analysis of alternatives using "what-if", "plus-minus-1" analysis and selective explanation:

What-if
: Comparison of alternatives triggered by changes of input attribute values.

Plus-minus-1
: Checking to which extents alternatives are affected by small changes to input attribute values.

Selective explanation
: Emphasizes the strong and weak attributes of each alternative - the sub-trees where all attributes have the best (or worst) possible values.

The DEXx implementation is a library that provides a better and more powerful core structure for decision making with DEX. It is a new implementation of the DEX method, supporting four extensions: full hierarchies, numeric attributes and general aggregation functions, probabilistic and fuzzy distributions and relational models (Trdin & Bohanec, 2015).

Full hierarchies
: Support of full hierarchies, i.e. directed acyclic graphs. DEXi only supports them indirectly, using the concept of "chaining" or "linking" nodes.

Numeric attributes and general aggregation functions
: The DEX methodology supports only qualitative input attributes. This extension allows development of decision models that can consider both quantitative and qualitative attributes.

Probabilistic and fuzzy distributions
: Simple qualitative and quantitative input attributes are extended to include complex data, such as sets and intervals of values, fuzzy sets and distributions.

Relational models
: Support for relational aggregation of alternatives, for decision problems dealing with alternatives composed of several sub-components.

The DEX method and its extensions are integrated into a unified method, called DEXx. The library implementation additionally supports several utilities for individuals, for further presentation and analysis of the developed models and identified alternatives - outside the scope of the DEXx unified method. It is worth mentioning that the DEXx library does not include a graphical user interface and as such can be easily integrated in development custom decision support systems.

Chapter 5

Machine Learning and Data Mining

Machine learning is one of the most active research areas in the field of artificial intelligence. It studies computer programs that automatically improve with experience (Mitchell, 1997). It also has numerous applications in the field of environmental and agricultural sciences (Debeljak & Džeroski, 2011).

In general, machine learning tasks can be classified into three groups: supervised, unsupervised and semi-supervised learning. Supervised machine learning tries to find a rule that maps the input, represented with examples to the output desired label or class of examples. Unsupervised machine learning works over unlabeled examples that appear as input and tries to find a structure or hidden patterns among them.

The input data are usually given as a set of examples (instances). An example represents one observation, object or measurement. Each example is described with a set of values of attributes. The attributes can be continuous or discrete if they have numeric or nominal values, respectively. Input to machine learning algorithms is commonly given in the form of a single flat table (such as a spreadsheet table) using a number of variables or features (columns) and instances or examples (rows). Less commonly, the input is given in the form of data streams or relational tables.

Supervised machine learning methods construct a function that maps each instance (a vector of input variables) from the input space to an output (target) value (Figure 5.1). The construction of the function that maps the input values to output values takes as input example pairs of input/output values. In other words, the goal in supervised learning is to construct a model that is able to predict the value of a variable that is of special interest (called dependent or target variable). The main assumption is that the future can be predicted if only the past or history is considered. The history is described with examples or instances. Depending on the type of the target variable, we can distinguish between two major supervised learning tasks: regression and classification. If the values of the target variables are from a continuous scale, then the task at hand is regression. On the other hand, if we have nominal values, belonging to a finite set of values, then the task at hand is classification.

The function can have different forms, e.g. decision trees, rules, equations, or probabilistic graphical models. Such models are meant to complement or even replace the knowledge-driven models that describe the physical behavior of the observed process.

Unsupervised learning aims to find hidden knowledge among data and examples, such as clusters, independently from a target attribute.

Validation of models built using supervised learning is performed by comparing the predicted values for the target variable against its real observations. The objective way of comparing them is over a set of examples that were not included in the learning phase, i.e. unseen examples. However, it is also useful to compare the predictions over already seen

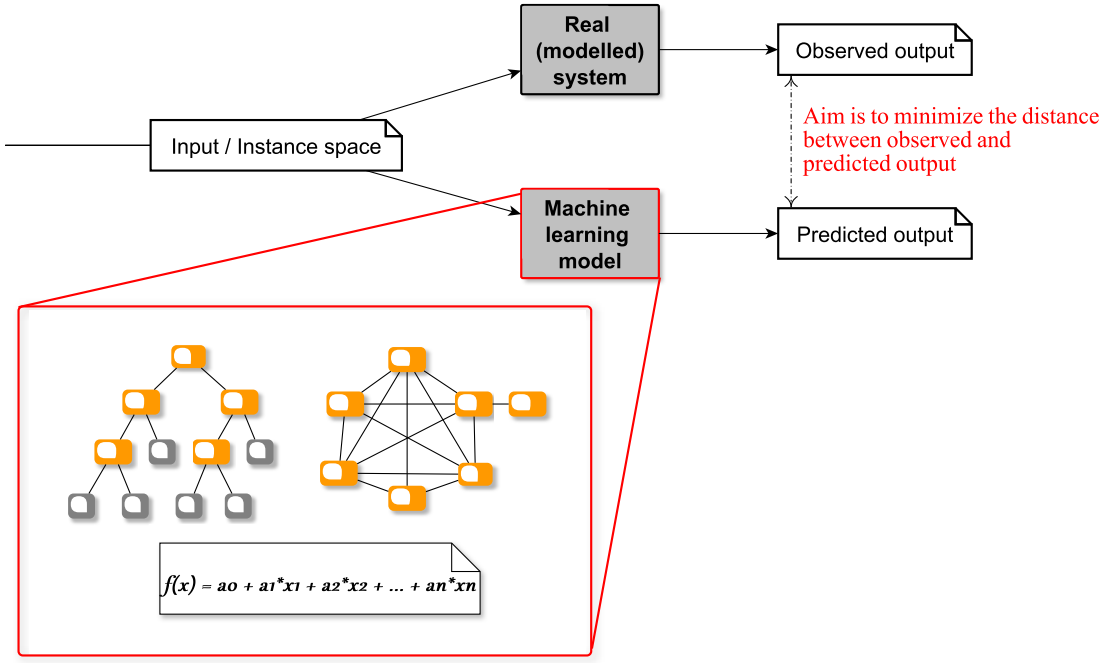


Figure 5.1: Scheme of the modeling approach using machine learning methodology.

data, as well. Validation over seen data or data included in the learning phase refers to the performance of a model over a training data set, while validation over unseen data refers to the performance of a model over a test data set. In between, there can also appear a validation set, which helps in unbiased representation of a model's performance. These data sets can be extracted from the complete data set in a different way, as reviewed later in this chapter.

How well a learned model predicts a target variable is expressed with a set of performance metrics. In the reminder of the chapter, performance metrics used in this study are presented.

An important issue that needs to be taken into account when learning models is so-called bias-variance tradeoff on model performance. It represents a tradeoff between learning a too general or a too specific model. The former is represented by the appearance of underfitting, while the latter is related to overfitting the model to the data used for learning. Overfitting means that the model performs very well on the training data set, while giving poor predictions on instances in the test data set (i.e., very low testing performance). If the model shows weak performance on both training and testing data set, then it is said that the model underfits the data. Thus, we need to select a model that generalizes well on both the training and the testing data, i.e. a model that has a high predictive performance on both data sets. To achieve this, various learning constraints need to be applied in the model construction phase. These learning constraints are different for different learning algorithms. In the following section (Section 5.1) each method used throughout the course of the thesis is described.

5.1 Learning Methods

Supervised machine learning comprises a variety of regression and classification approaches or methods, such as linear regression (Draper & Smith, 1981), regression and model trees

(Quinlan, 1992), classification trees (Breiman, Friedman, Stone, & Olshen, 1984; Quinlan, 1986), support vector machines (Cortes & Vapnik, 1995) and ensembles of different regression and classification models as base models (Breiman, 1996). In accordance with the goals of the thesis, both regression and classification methods are considered. We consider linear regression, classification trees, regression trees, model trees, and ensembles of classification, regression and model trees as the most suitable learning methods in accordance with their interpretability and effectiveness. All the methods applied in the study are implemented in the WEKA data mining suite (I. H. Witten & Frank, 2005) and CLUS software package (Blockeel & Struyf, 2003; Struyf & Džeroski, 2005), except polynomial regression, which is implemented within the CIPER tool (Džeroski, Todorovski, & Ljubič, 2003; Todorovski, Ljubič, & Džeroski, 2004; Pečkov, Todorovski, & Džeroski, 2006). A brief description of these methods is given below.

5.1.1 Linear regression

Linear regression is a model of the form of (5.1), which expresses the target variable as a weighted linear combination of input (independent) variables. The model is represented as a linear combination of terms. A term consists of an input variable and a weight (in the form of a real number) that gives a specific importance to the corresponding variable. The weights (referred to as parameters) are calculated from the training set in the process of learning the model. A comprehensive study of this method has been provided by Lawson and Hanson (1995).

$$\boldsymbol{f(x_1, x_2, x_3, ..., x_n)} = a_0 + a_1 \cdot x_1 + a_2 \cdot x_2 + a_3 \cdot x_3 + ... + a_n \cdot x_n, \tag{5.1}$$

The parameters are calculated using various optimization approaches for parameter fitting. Typically, the least squares method is used.

A major drawback of this model is its assumption of linearity, since most of the modeled systems in the real world are complex non-linear processes. This drawback results in learning linear models with poor generalization abilities (low variance and high bias). On the other hand, overfitting is a potential issue for linear regression if the observed system is a simple linear process and can be controlled by using a parameter that penalizes the higher values of the weights (Ridge parameter).

However, accordingly to the so-called Occam's razor principle (Anderson, Michalski, Carbonell, & Mitchell, 1986) (as simple as possible, but no simpler), linear regression models are used as baseline models for making comparisons with other regression methods.

5.1.2 Polynomial regression

Polynomial regression models are represented by polynomial equations. These are simple models and yet can be highly accurate on standard regression tasks. The method used for inducing a polynomial model is called CIPER — Constrained Induction of Polynomial Equations for Regression (Džeroski et al., 2003; Todorovski et al., 2004; Pečkov et al., 2006). It searches heuristically through the space of possible equations for solutions that satisfy the initially given constraints. The output of CIPER consists of a polynomial equation that satisfies the complexity constraints and best fits the data.

In the space of polynomial equations of arbitrary degree, an equation with small error on the training data can always be found. However, such an equation will be very complex and strongly overfitted (high variance and low bias) on the training data (and will consequently have low generalization power). To find an optimal trade-off between complexity of the model and well fitting the data, CIPER uses the Minimal Description Length (MDL) principle as a search heuristic (Pečkov et al., 2006). Furthermore, CIPER allows control

of the complexity of models by constraining the right hand side of an equation by limiting the maximum depth of a single term and the maximum number of terms. In the thesis, the learning process is constrained by controlling the maximum depth of a single term, and the value that maximizes the performance of the learned model is selected.

5.1.3 Decision trees

A decision tree is a classifier expressed as a recursive partition of the instance space. The decision tree consists of nodes and leaves. The top-most node is the root node. A node that has a child node is referred to as an internal or test node. All other nodes are called leaves (also known as terminal or decision nodes). A node is labeled with an input variable name and an arc with a valid value of the input variable associated with the node from which the arc originates. Each leaf is labeled with a class (prediction for the target variable) or assigned a real value. In a decision tree, each node splits the instance space into two or more sub-spaces according to a certain discrete function of the input variable values. In the simplest and most frequent case, each test considers a single variable, so that the instance space is partitioned according to the variable's value. In the case of numeric variables, the condition refers to a range.

Given a new instance, for which the value of the target variable should be predicted, the tree is interpreted from the root. In each inner node, the prescribed test is performed, and according to the result, the corresponding subtree is selected. When the selected node is a leaf, the value of the target variable for the new instance is predicted according to the model in this leaf. Terminal nodes (leaves) of a tree contain models defining the values of the target variable for all instances falling in a corresponding leaf. Models can have different forms for different learning tasks.

Decision trees can be easily overfitted to the training data. This can be resolved by a technique called pruning, which constrains the growth of the tree structure. There are pre-pruning and post-pruning techniques. The former constrains growth during the learning phase, typically by using the "minimal number of instances in a leaf" parameter of the algorithm implementation. This parameter requires tuning since very low values may introduce overfitting, while high values can generate very simple decision trees that introduce high bias in the modeled system. Post-pruning allows the tree to grow as much as possible and then applies pruning by removing sections of the tree that provide little power to classify or predict instances.

Depending on the learning task, a decision tree can be a regression or classification tree. The former, based on the model applied in the terminal nodes, can be differentiated as a regression or model tree, while the latter uses a simple majority model.

A regression tree is a decision tree that contains a simple model in the leaves (constant real value), most often an average value of the target variable for the instances that reach that particular leaf. Model trees are decision trees, whose leaves contain a linear regression model. A classification tree is a type of decision tree that contains a simple model in the leaves. Such a model assigns a nominal label to the instances that is found to be the majority in particular leaf during the learning process.

Due to the structure of the model tree and linear regression models in its leaves, the complexity of their structure is one of their disadvantages and a reason to consider regression trees in some circumstances instead of model trees. However, model trees have an advantage over regression trees in terms of predictive performance. Finally, model trees are able to make predictions outside the range of the target variable encountered in the training instances, which is not the case with regression trees.

In the thesis, the implementations M5 (Quinlan, 1992) and M5P (Wang & Witten, 1997) for regression (regression and model tree, respectively) and the J48 (I. H. Witten &

Frank, 2005) implementation of C4.5 (Quinlan, 1993) for classification are used.

5.1.4 Ensemble methods

Ensemble methods are machine learning methods that construct a set of predictive models (e.g., regression trees or models trees) and combine their outputs into a single prediction. In the literature, ensembles are also referred to as multiple classifier systems, committees of classifiers, classifier fusion, combination or aggregation (Schapire & Freund, 2012; Wolpert, 1992; Breiman, 1996; Džeroski, Panov, & Ženko, 2009). The main idea is to follow the behavior of wise people when making critical decisions. They usually take into account the opinions of several experts rather than relying on their own judgment or that of a single trusted adviser. The same principle is followed by ensemble methods: learning an entire set of models and then combining their predictions. This approach is computationally more expensive than learning just one simple model, but predictions are usually more accurate.

By building an ensemble that takes into account several diverse models and aggregates their predictions, the prediction of a dependent variable can be improved (Džeroski & Ženko, 2004). Overfitting can, in theory be an issue, but in practice, for some techniques overfitting or underfitting is not often an issue (Mitchell, 1997).

The learning of ensembles consists of two steps. In the first step, we learn the base models that make up the ensemble. In the second step, the base models (or their predictions) are combined into a single prediction. The base models need to be diverse, i.e. make different errors on the same learning instances. Combining identical or very similar models clearly will not improve the predictive accuracy of the base models. Moreover, it increases the computational cost. Learning diverse models and combining their predictions can result in more accurate predictions as compared with the predictions of a single model.

The most commonly used technique for combining predictions for classification models is voting, which combines predictions according to a static voting scheme that does not depend on the training data or the base models. In the case of regression, we take the average or a linear combination of the models' outputs.

The most prominent ensemble learning approaches are bagging (Breiman, 1996), boosting (Freund & Schapire, 1996), and random forest (Breiman, 2001). In the thesis, the bagging approach and random forest are used.

In bagging, averaging over the base predictive model outputs is used. The multiple base predictive models are learned on different bootstrap replicates. If the training set causes significant changes in the models learned, then bagging can improve the predictive performance of the base predictive models. Similarly, the random forest learns models using different instance subsets. Unlike the bagging method, the random forest considers subsets of the feature space as well. Therefore, sampling is done randomly over both dimensions instance and feature space.

5.1.5 Cost-sensitive learning

In general, the classification task aims to maximize the accuracy or to minimize the error. This is valid for misclassifications that have equal cost, which is not the case in most real-world problems, where the costs of a misclassification are often unequal.

Cost-sensitive learning (Ling & Sheng, 2010) is a type of learning that takes misclassification costs into consideration. The goal is to minimize the total cost, while treating different misclassifications differently.

The most prominent and popular method of cost-sensitive learning is Rescaling or Rebalance (Elkan, 2001). The method tries to rebalance the classes, such that the influences

of different classes are in accordance with their cost. Rescaling can be realized by re-sampling, where lower-cost class examples can be under-sampled so that the number of examples of lower-cost and higher cost classes are in proportion to their misclassification costs, respectively. Other forms of implementation include re-weighting training examples so that examples from the minority class will dominate by their weights.

In all case, cost-sensitive learning relies on a so-called cost matrix, where re-sampling weights for examples are specified in accordance with misclassification cost. Examples that are considered misclassified can be either false positives or false negatives. The former case refers to negative examples that were classified as positive, while the latter refers to positive examples classified as negative. Therefore, the costs specified in the cost matrix are considered penalties for the false positives and false negatives. The cost matrix for the binary classification problem has dimension 2×2, while in general it has dimension $n \times n$, where n is the number of class labels.

In the thesis, we consider only the binary classification task and use the implementation of cost-sensitive learning available as part of the WEKA suite (I. H. Witten & Frank, 2005). The cost-sensitive matrix is arbitrarily tuned starting with default values: cost equal to 1 for false positives and false negatives, and cost equal to 0 for true positive and true negative examples.

5.1.6 k-Nearest neighbor

k-Nearest neighbor (k-NN) is a type of instance-based learning, or lazy learning, where the function is only approximated locally and all computation is deferred until classification. The k-NN algorithm is among the simplest of all machine learning algorithms (Fix & Hodges, 1951; Cover & Hart, 1967; Tang & He, 2015).

The k-NN learning assumes that data which are close togethe, based upon some metric such as Euclidean distance, are more likely to belong to the same category. This type of learning is considered non-parametric method, because it requires only the value of k (the number of examples to be specified as a neighborhood) to be specified in advance. There are also extensions of the initial method that try to estimate the initial value of k (Tang & He, 2015).

Throughout the study performed in the thesis, we consider the regression task using the k-NN method. Its simplest form is aggregation of the neighborhood's target variable values, for an example to be predicted. The aggregation we used is an average of the values found in the target variables of the neighborhood.

5.2 Evaluation

Given a set of data, part of it is typically used to perform an evaluation of the learned model. This part is referred to as the testing set. The remaining part is reserved for learning the model and is called the training set. The testing set is used to estimate the performance of the model on unseen data. In some scenarios, it is possible to introduce a validation set, to be used for an unbiased selection of the model with highest performance. This means that if a best performing model is selected using a validation set, it is recommended that additional comparison is made with other models over new examples (not seen in the training phase, or the phase where the best performing model was selected). Splitting approaches that divide a complete dataset into a training, testing, and optionally a validation set are described in the following subsections.

One of the most important properties when designing a training and a testing set is that their intersection should be the empty set. This means that both data sets should

not have any overlap in the instance space.

A model's performance is expressed with performance metrics that represent quantification of *erroneous* or *accuracy* of the corresponding model. The set of performance metrics that we use throughout the course of the thesis is described below.

5.2.1 Evaluation approaches

Evaluation approaches define training and testing datasets (Japkowicz & Shah, 2014). Selecting an evaluation approach typically depends on the amount of data available for a given task or problem. If the problem deals with a vast supply of data, using a simple random sampling without replicates can be considered. Otherwise, if the problem deals with a limited dataset with respect to the number of instances or examples, another evaluation approach could be more appropriate.

A simple random sampling without replication guarantees that the sampled datasets will be mutually exclusive, with no examples found in their intersection. Typically, the instance space is divided into two datasets, one for learning a model and another one for evaluation of its performance. Another possibility is to introduce a validation set that will be used in finding the best parameters of a learning method (I. H. Witten & Frank, 2005). In such a context, the testing dataset is used for comparison of the model learned with the best parameters of the learning method, against other models.

In the case of a limited dataset with regards to size, cross-validation is typically considered for designing training and testing datasets. Cross-validation includes a process that repeatedly performs random sampling without replication and constructs a training and a testing dataset (Japkowicz & Shah, 2014). In the basic approach, called n-fold cross-validation, the training set is split into n smaller sets (folds). The following procedure is followed for each of the n folds: A model is trained using $n - 1$ of the folds as training data and the resulting model is validated on the remaining part of the data (i.e., used as a test set to compute a performance measure). At the end, the performances are aggregated in some way, e.g., by averaging across all learned models. This approach can be computationally expensive, but does not waste too much data (as the case when fixing an arbitrary test set), which is a major advantage in problems where the number of examples is very small.

Since cross-validation includes random sampling of examples, it is always better to set a greater value of n. Most frequently, 10-fold cross-validation is used, or 3-fold cross-validation for datasets that rely on a well estimated distribution of values that defines how much they are representative of a given population (I. H. Witten & Frank, 2005).

Another variation of cross-validation is leave-one-out cross-validation that considers a fold to be a single example from the complete dataset. Another approach that can be used is bootstrapping (I. H. Witten & Frank, 2005), based on a statistical procedure of random sampling with replacement.

5.2.2 Performance measures

A performance measure is a quantifiable indicator used to assess how well a learned model is achieving its desired objectives. In general, performance measures are grouped into measures for classification tasks and measures for regression tasks. The following is a description of measures used throughout the study. First, performance measures for classification are given, then measures for regression.

5.2.3 Classification task

There are different kinds of performance measures, primarily categorized by the type of information they consider or the format of the input (Figure 5.2). Performance measures can be based on a confusion matrix, classifier uncertainty, cost-ratio or skewness of the class distribution, and alternate information such as: interestingness or comprehensibility (Japkowicz & Shah, 2014).

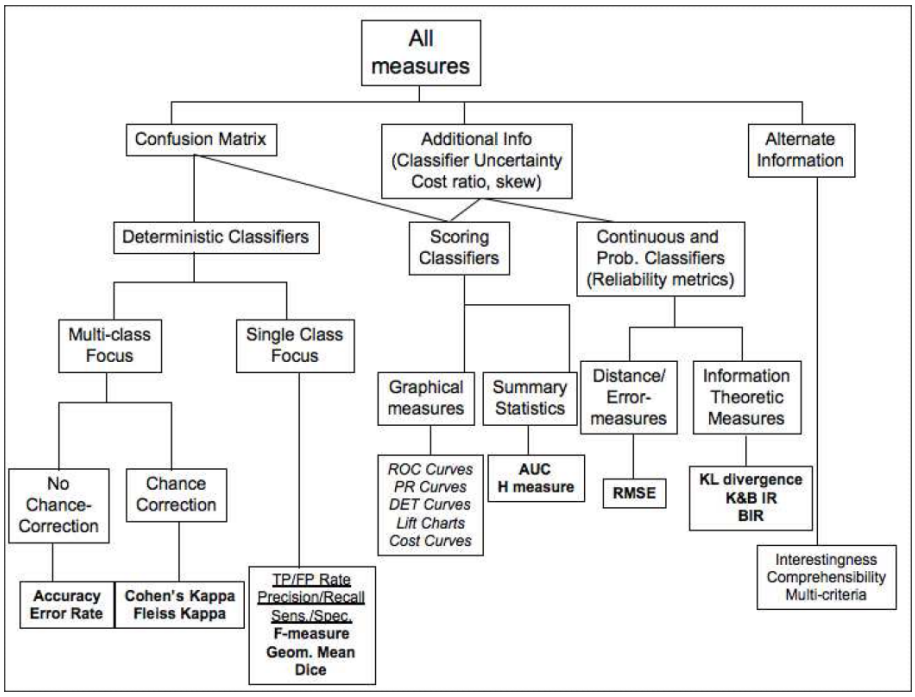


Figure 5.2: Overview of Performance Measures (Japkowicz & Shah, 2014).

A confusion matrix is also known as a contingency table, and consists of columns that represent instances in a predicted class, and rows that represent the instances in an actual class. Most of the popular performance measures are based on a confusion matrix, and further categorized by the type of classifiers used, and the focus of a particular measure. The type of a classifier can be deterministic or scoring, and the focus of a measure can be set to a single class or a multi-class. Multi-class focused performance measures include *Accuracy* (*acc*) and *Error Rate* (*er*), while single-class focused measures are: *True Positive* (*tpr*) and *False Positive* (*fpr*) rates, *Precision*, *Recall*, etc.

From a confusion matrix, simple metrics can be derived, which explore the number of instances that were classified correctly and those that were not. They are given in Table 5.1, where *TP - True Positives*, *FP - False Positives*, *TN - True Negatives*, *FN - False Negatives*, *P - Total Positives* and *N - Total Negatives*. Since we use only binary classification, the given confusion matrix is valid for a binary classification problem, with only a positive and a negative class.

The following performance measures can then be defined:

$$accuracy = \frac{TP + TN}{P + N}, \tag{5.2}$$

$$error\ rate = 1 - accuracy = \frac{FP + FN}{P + N}, \tag{5.3}$$

Table 5.1: A confusion matrix for binary classification task.

	Actual positive	**Actual negative**
Predicted positive	TP	FP
Predicted negative	FN	TN
	P=TP+FN	F=FP+TN

$$\textit{true positive rate} = \frac{TP}{P}, \tag{5.4}$$

$$\textit{false positive rate} = \frac{FP}{N}, \tag{5.5}$$

$$\textit{precision} = \frac{TP}{TP + FP}, \tag{5.6}$$

$$\textit{recall} = TPR = \frac{TP}{P}. \tag{5.7}$$

Scoring classifiers are suitable in evaluation using visual analysis and summary statistics. The former encompass *ROC Curve* (Receiver Operating Curve), *PR Curve* (Precision-Recall), *Lift Curve* and *Cost Curve*, while the latter covers *Area Under ROC Curve* (*AUC*) and *Area Under PR Curve* (*AUPRC*).

Curve analysis moves the score threshold between 1 and 0. It plots the value of the *tpr* against that of the *fpr*, and *recall* against that of the *prec*, for *ROC Curve* and *PR Curve*, respectively. Integration of such curves results in summary statistics measures such as *AUC* and *AURPC*.

5.2.4 Regression task

Performance measures for regression tasks are used with continuous and probabilistic classifiers, which rely on distance or error metrics. Throughout the course of the thesis the following are used: *Root Mean Squared Error* (*RMSE*), *Root Relative Squared Error* (*RRSE*) and *Pearson correlation* (r).

The *RMSE* is a measure that captures the squared residuals (differences between predicted and measured values) over the total number of instances:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(p_i - a_i)^2}{n}}, \tag{5.8}$$

where n is the number of instances (examples), p_i is the predicted value for the i-th instance and a_i is the actual (measured) value of the i-th instance.

The *RRSE* measure considers the squared residuals relative to residuals of the simple average model, and is defined as:

$$RRSE = \sqrt{\frac{\sum_{i=1}^{n}(p_i - a_i)^2}{\sum_{i=1}^{n}(a_i - \bar{a})^2}}, \tag{5.9}$$

where n is the number of instances (examples), p_i is the predicted value for the i-th instance, a_i is the actual (measured) value of the i-th instance and $\bar{a}$ is the average of the values in the target variable of the training data sets.

The Pearson correlation coefficient (r) captures the correlation between observed and predicted values of the target variable:

$$r = \frac{S_{predicted/observed}}{\sqrt{S_{predicted} \cdot S_{observed}}}, \tag{5.10}$$

where

$$S_{predicted/observed} = \frac{\sum_{i=1}^{n}(p_i - \bar{p})(a_i - \bar{a})}{n-1}, \tag{5.11}$$

$$S_{predicted} = \frac{\sum_{i=1}^{n}(p_i - \bar{p})^2}{n-1}, \tag{5.12}$$

$$S_{observed} = \frac{\sum_{i=1}^{n}(a_i - \bar{a})^2}{n-1}, \tag{5.13}$$

n is the number of instances (examples), p_i is the predicted value for the i-th instance, a_i is the actual (measured) value of the i-th instance, $\bar{p}$ is the average of the predicted values and $\bar{a}$ is the average of the values of the target variable of the data sets used for the test.

Chapter 6

Methodological Framework

Over the course of the present thesis, we formalized a methodological framework for multi-criteria decision making (MCDA) under uncertainty and risk. The formalization provides a better core structure for building decision support systems based on the DEX methodology, with integrated risk analysis and predictive models.

This chapter introduces the formalization of the methodological framework, implemented on a case-study in the domain of ecological and environmental modeling. First, the goals and purpose of the formalization are given, then the definition for each component or element of the framework; finally, the modules of the methodological framework are described.

6.1 Goal and Purpose

The main purpose of developing a methodological framework for MCDA integration with risk analysis is to facilitate and simplify the building of decision support systems for decision problems under uncertainty and risk, which were previously hard to address in a single system. The methodological framework is able to cope with different types of models for the purpose of risk analysis or decision analysis. Its implementation can be adjusted to deliver outputs according to expectations of the individuals that will use the decision support system.

The main questions we try to answer, throughout the course of the study, are:

- How to deal with decision making in a world that is characterized by changes that appear too fast?
- How to consider such changes as part of the decision analysis and include them in the evaluation of alternatives?
- How to evaluate alternatives in accordance with the state of the world that will take place upon implementation of the corresponding decision, and not only in accordance with their outcome?

The first two questions are related to decision problems that deal with a fast-changing world. Such decision problems should be analyzed so that the actual state of the world, at the time of decision making, is differentiated from the state of the world that takes a place when the corresponding decision is implemented or applied.

The third question is related to decision problems that require consideration of the state of the world that will take a place upon implementation of the corresponding decision. This is the case when the preferences of an individual correlate with both the outcomes

of alternatives and with the state of the world that takes a place upon application of the decision.

Therefore, in this study, we differentiate three significant points in time: t, t' and $t+1$ (Figure 6.1). The first refers to the time of decision making, the second refers to the time of the application of a decision, and the third refers to a time after the application of a decision, when outcomes or consequences of the applied decision can be quantified.

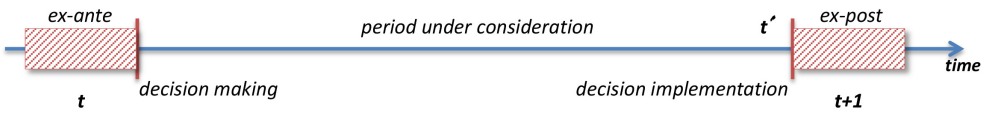


Figure 6.1: Time points t, t' and $t+1$ on a time line.

Consequently, the goal of the methodological framework is to provide capabilities to integrate risk analysis and MCDA into a system, which utilizes additional information provided by predefined predictive and diagnostic models. Thus, the methodological framework allows preferences (at time point t) to be evaluated with regard to the outcome (consequence) of an applied alternative or state of the world that takes place at the time of application of a decision (at time t') or upon the application of a decision (in time $t+1$).

6.2 Related Work

Facilitating decisions under conditions of uncertainty and risk requires choice about how this uncertainty is to be modeled. This involves choosing an uncertainty format (a way of representing the likelihood of possible consequences) and a related choice of a decision model in which preferences will be represented. Different formats exist for representing uncertainty, and for each of these formats many possible decision models have been developed.

The general form of a decision table (Table 2.2) can be viewed as the starting point for these considerations, as classical decision theory has pointed out (A. Kangas & Kangas, 2004). Namely, different individuals can take different attitudes towards risk and uncertainty, which may lead to different priority ordering of alternatives. A common strategy in the case of risky choices is *maximization of expected utility* (von Winterfeldt & Edwards, 1986). Similarly, the well-known von Neumann-Morgestern utility function (von Neumann & Morgenstern, 2007) considers risk attitudes implicitly in describing an individual's attitude toward risk. However, this requires to estimate the probabilities associated with consequences of choice alternatives or probabilities associated with appearances of states of the world. Both methods consider risk assessment implicitly.

Another group of methods considers risk assessment explicitly by introducing a risk model. A literature overview (A. Kangas & Kangas, 2004; Aven & Kørte, 2003; Yousefpour, Jacobsen, Thorsen, & Hanewinkel, 2012; Mendoza & Martins, 2006; Durbach & Stewart, 2012; Broekhuizen, van Til, Hummel, & IJzerman, 2015) finds wide usage of two theories that explicitly handle risk in a way suitable for inclusion in MCDA: *Bayesian decision theory* and *Fuzzy set theory*.

6.2.1 Bayesian decision theory

The Bayesian approach treats all attributes of alternatives and states of the world as random variables, where the randomness of the attribute describes its uncertainty (Carroll,

Ruppert, & Stefanski, 1995). The randomness of the attributes does not necessarily mean that the attributes' values vary randomly, but rather that the values of the attributes are not known. This allows making probability statements about the values of attributes based on the data at hand and prior beliefs of the individual (Carlin & Louis, 2010).

In Bayesian theory, models have two stages. The first is prior information concerning uncertain attributes θ of a state of the world $s \in S$ that can be described with a prior distribution $\pi(\theta)$. The second is the likelihood function of observed values y, given attributes θ: $likelihood(y|\theta)$. Then, the posterior distribution of attributes, given their observed values, is:

$$p(\theta|y) = \frac{likelihood(y|\theta)\pi(\theta)}{\int likelihood(y|\theta)\pi(\theta)d\theta}. \tag{6.1}$$

The tuple (a_i, s_j) is associated with a loss function $L(a_i, s_j)$. The decision that minimizes the expected loss (posterior risk) is given in the form:

$$L(a_i) = \sum_j p(s_j|a_i)L(a_i, s_j). \tag{6.2}$$

Another option is to consider a utility function $u(a_i, s_j)$ instead of the loss function. Then, the decision is required to maximize the utility (posterior gain).

Bayesian decision theory has advantages in pair-wise comparison of alternatives and estimation of their consequences across all possible states of the world. Additionally, it allows integration with classical decision modeling methods, e.g., AHP and MAUT (Mendoza & Martins, 2006).

Bayesian decision theory can also be used as an approach to ex-ante and ex-post risk analysis, depending on what probability distribution will be chosen for the analysis. If only a priori probabilities are considered, then the approach is based purely on degrees of belief concerning the values of attributes θ; this is the ex-ante approach. If empirical observations are not available, a priori probabilities describe only the individual's subjective beliefs about the appearances of states of the world (Carlin & Louis, 2010). If a posteriori probability distribution is considered, then Bayesian decision theory for risk assessment behaves as the ex-post approach (A. Kangas & Kangas, 2004).

6.2.2 Fuzzy set theory

Fuzzy set theory has been developed by Zadeh (1965), with uncertainty that has more to do with vague definitions of attributes than randomness. The basis of the theory is a membership function μ that describes the degree to which a certain statement is true (Zimmermann, 1991).

In the context of decision analysis, the uncertainty of an attribute can be described with fuzzy numbers which indicate that an attribute's value is approximately some given value (Ells, Bulte, & van Kooten, 1997). These fuzzy numbers are typically described with a triangular function (Cox, 1994).

Decision making in a fuzzy environment is a process where attributes can be represented with fuzzy sets. A membership function μ describes the degree of performance of the alternatives with respect to states of the world with uncertain attributes, and is based on fuzzy evaluations (Goumas & Lygerou, 2000).

Fuzzy set theory has an advantage in qualitative pair-wise comparisons of alternatives and integration with classic decision modeling methods, like AHP (Durbach & Stewart, 2012). However, due to the fuzzy nature of alternative evaluations, their ranking is often non-trivial and requires an additional step where the ranking procedure is considered

(Chen & Hwang, 1992). Fuzzy set theory is applicable in decision analysis as ex-ante risk assessment approach.

6.2.3 MCDA frameworks

Durbach and Stewart (2012) divide risk models or formats into five groups based on how risk is further incorporated into a decision model:

Probabilities
A multivariate probability distribution can lead the joint evaluation of all alternatives and states across all attributes.

Decision weights
Weighting the importance of uncertain consequences by factors (decision weights) which are typically not linearly related to associated probabilities. This is often described as an extension of the probability approach.

Explicit risk measure
Captures the impact of uncertainty on preferences by means of one or at most a small number of summary measures. In effect, this group of methods/frameworks tries to decompose overall preferences into 'value' and 'risk' components, both described with a particular model or measure.

Fuzzy numbers
Modeling imprecision or uncertainty by using fuzzy set theory and expressing imprecision with fuzzy numbers.

Scenarios
Incomplete descriptions of how the future might unfold. Based on causal reasoning that allows an individual to gain understanding of the problem at hand and generate insights into possible courses of actions.

Probabilities and decision weights are often used together, in a decision model that can handle such factors. Almost certainly the most widely-known model for decision making under uncertainty and risk is *expected utility theory* (von Neumann & Morgenstern, 2007), or *MAUT* (multi-attribute utility theory) (Keeney & Raiffa, 1993) in MCDA context. The aim of MAUT is to produce a function such that an alternative is preferred to another if and only if its expected utility is greater. Multivariate probability distributions are used for expressing expectations. This requires (a) construction of a marginal utility function u_j for each attribute c_j from an alternative that will satisfy the von Neumann-Morgenstern axioms, and (b) aggregation of the marginal utility functions into a global utility function U, such that the expected utility hypothesis is still satisfied (Durbach & Stewart, 2012). Typically, additive aggregation $U(a) = \sum_j w_j u_j(a)$ is employed, requiring preferences over particular attributes to be dependent only on marginal distributions and not on any interactions between attributes. More complex aggregation forms are also applicable, but they are rarely employed in practice (Keeney & Raiffa, 1993).

Another method from the group of methods using probabilities or decision weights is the so-called *stochastic outranking method* or *dominance-based method* that utilizes a stochastic dominance relation - pairwise comparison of the probability distributions (Zaras, 2004; Martel, d'Avignon, & Couillard, 1986; Azondékon & Martel, 1999; Dendrou, Dendrou, & Houstis, 1980; Fan, Liu, & Feng, 2010; Liu, Fan, & Zhang, 2011).

Acquiring a probability distribution is usually based on belief functions (subjective probability distribution), Bayesian decision theory or simulation using the Monte Carlo

approach (Spetzler & von Holstein, 1975; von Winterfeldt & Edwards, 1986; Belton & Stewart, 2002; A. Kangas & Kangas, 2004).

A representative way of combining methods that use fuzzy set theory is AHP with fuzzy numbers. Its suitability comes from the fact that AHP uses a qualitative pairwise comparison of alternatives (Durbach & Stewart, 2012). The original approach (Ubando et al., 2016) used the principal eigenvalue of the matrix of assessed memberships, whereas later estimation methods use a least squares (Jensen, 1984) or logarithmic least squares optimization (Kwiesielewicz, 1996). All three estimation approaches are modified to make use of fuzzy input data (Triantaphyllou & Lin, 1996; Wang & Chin, 2006; Wang, Elhag, & Hua, 2006). Typically fizzy geometric means are used for marginal evaluation across all available attributes (Buckley, 1985), but there are other options as well, as shown in Deng (1999), Mikhailov (2000), Mikhailov and Tsvetinov (2004), Leung and Cao (2000).

The group of methods or frameworks that use an explicit risk measure or model in order to express the level of risk can use a combination of different types of risk models and decision models. There is no general pattern of how these methods are built (Durbach & Stewart, 2012). The following is a description of a framework from this category.

Khadam and Kaluarachchi (2003) propose a methodology that integrates probabilistic risk assessment and MCDA into a comprehensive framework for water contamination management. The information needed for risk assessment are collected from a hydro-geologic model of water flow and transport incorporating spatial variability and a population model that allows variability of population characteristics. The information derived from the probabilistic risk assessment is then incorporated into the MCDA model. Each remedial alternative is tested against the decision criteria, and then the alternatives are ranked to determine the best alternative.

Probabilistic risk assessment (using a risk model as described in Bogen and Spear (1987)) incorporates the variability and uncertainty of risk attributes in the risk estimate. Input attributes are described through probability distributions, and the solution provides the statistical distribution of the risk estimate. The risk due to joint uncertainty and variability of input attributes are computed using the modified two-stage Monte Carlo simulation (Cohen, Lampson, & Bowers, 1996). The decision analysis is done in two parts: explicit and implicit decision analysis. The former consists of a filtering and ranking stage using a measure of efficiency for alternatives. The latter utilizes an importance order of criteria (IOC) (Clemen, 1996), or fuzzy dominance and resemblance (FDR) (Wenger & Rong, 1987; Kaufmann, 1975).

The methodology proposed by Khadam and Kaluarachchi (2003) is not obviously applicable to quantitative MCDA. Additionally, the two-stage simulation using Monte-Carlo is computationally demanding.

The overview of related methodologies and frameworks given above, shows that preference modeling largely prevails over consequence modeling. The methodological framework proposed here introduces the possibility to evaluate alternatives over consequences and states of the world, namely at time points t, t' and $t+1$. The related work considers only the state of the world given at time point t (at the time of decision making).

The motivation for our approach comes from the context of reinforcement learning (Sutton & Barto, 1998) and Markov decision processes (Bellman, 1957; Feinberg & Shwartz, 2012). When we have sequential points in which a decision should be made, we should always consider the state (at time point $t+1$) that will arise as a result of performing the set of actions (in MCDA defined as alternative) chosen at the previous time point t. In reinforcement learning, the consequence consists of a reward r_t estimated using a reward function r over the state s_t and the chosen set of actions a_t: $r_t = r(s_t, a_t)$. It is supposed that the performed set of actions results in state s_{t+1}: $s_{t+1} = f(s_t, a_t)$, whereas in decision

modeling the performed alternative emphasizes the utility that the individual will gain.

The aforementioned applies in the context of sequential actions that should be performed, i.e. sequential decisions made. This is usually not required in decision modeling, so we do not focus on sequences of decisions. We do, however, take into account the fact that decisions are made in time, so that action at time t has an effect on the state of the world at time $t+1$, which can influence preferences or gained utility.

Another issue to consider is decision making over a fast-changing world. Similarly, for decision making where a decision should be made long before it is actually applied. In these contexts, the individual faces the problem of the uncertain state of the world $s_{t'}$ at the time of application (t') of the alternative a_t chosen at time t.

In the reminder of this chapter, the complete formalization of the methodological framework is given. First, all relevant components are defined. Then, the methodological framework is formalized. Finally, the modules of the methodological framework are presented.

6.3 Definitions

The following defines the components that a decision analysis consists of, with extensions for the purpose of building an improved methodological framework.

6.3.1 State of world

As stated in Section 2.1, a state of the world in MCDA is complex and consists of a set of attributes or criteria G_s. An *attribute* $g_s \in G_s$ of a state of the world $s \in S$ is the most basic element that defines the domain or scope of S. In other words, an attribute defines the state at a most basic or atomic level. Accordingly, it is formalized as follows:

$$G_s = \{g_{s1}, g_{s2}, ..., g_{sl}\}. \tag{6.3}$$

A description of a state of the world $s \in S$ (a state of the world s) is said to be the assignment of a value to each attribute $g_{sj} \in G_s$:

$$s_j = D(g_{sj}), g_{sj} \in G_s. \tag{6.4}$$

Thus, a state of the world s is formalized as:

$$s = \{s_1, s_2, ..., s_l\}; s \in S. \tag{6.5}$$

In accordance with the available information, a state $s \in S$ can be described at any point of time. Recall that the decision making problem is oriented toward future events, so a state is defined in the future, as well. Consequently, it evolves into a state $s \in S$ defined with uncertainty:

Definition 6.1 (Uncertain state of the world). $s \in S$ is uncertain if at least one of its attributes is uncertain, or if its true value is unknown:

$$\exists g_{sj} \in G_s : s_j = \nabla\nu, \tag{6.6}$$

where $\nabla\nu$ is an unknown or estimated value.

Let ∇G_s be the set of all uncertain attributes for state s. If a description of s includes an estimated value for uncertain attribute $g_{sj} \in \nabla G_s$ with accuracy of estimation $\langle s_j \rangle$, then s is said to have an overall accuracy defined as:

$$\langle s \rangle = \frac{\sum_{g_{sj} \in \nabla G_s} \langle s_j \rangle}{|\nabla G_s|}, \tag{6.7}$$

where $|\nabla G_s|$ is the number of uncertain attributes in s. The estimation accuracy of a state of the world subtracted from 1 $(1 - \langle s \rangle)$ is the quantification of its uncertainty.

For example, let state $s \in S$ represent a state of a particular agricultural field. Furthermore, let s be defined with three attributes: $g_{s\_tillage}$ - is tillage performed; g_{s_crop} - what type of crop is present in the field; and g_{s_water} - how much water is flowing through a drainage network per day. The attribute g_{s_water} is unknown, since its depends on potential rainfall, while the others are described with certain values (e.g., $s_{tillage} = yes$ and $s_{crop} = wheat$). Therefore, the set of uncertain attributes is $\nabla G_s = \{g_{s\_water}\}$. Assume that the amount of water that will flow through a drainage network tomorrow (time point t' - the day when a decision should be applied) is estimated (using a particular estimator) to be *1.5 mm* with accuracy $\langle s_{water} \rangle = 0.9$. Then, the overall accuracy of the state s is $\langle s \rangle = 0.9$. Accordingly, the quantification of uncertainty of s is $1 - \langle s \rangle = 1 - 0.9 = 0.1$. Finally, we can say that the state s, defined with $G_s = \{g_{s\_tillage}, g_{s\_crop}, g_{s\_water}\}$ at the time of decision (t) will be described with the following vector of values $\{yes, wheat, 1.5\ mm\}$ with quantified uncertainty of 0.1.

6.3.2 Alternative

An alternative is an action or set of actions that can be performed over a state of the world. Like states of the world, in MCDA, alternatives are composed of a set of attributes or criteria G_a. An *attribute* (criteria) g_a is a specific point of view according to which an alternative is evaluated (Figueira et al., 2005). Accordingly, an attribute $g_a \in G_a$ is formalized as:

$$G_a = \{g_{a1}, g_{a2}, ..., g_{ak}\}. \tag{6.8}$$

A description of an alternative $a \in A$ is said to be the assignment of a value to each attribute $g_{ai} \in G_a$ of a:

$$a = \{a_1, a_2, ..., a_k\}; a \in A. \tag{6.9}$$

Additionally, the description of an alternative $a \in A$ includes the action or set of actions defined with alternative a, after a is chosen in the decision making process.

6.3.3 Outcome

Implementing an alternative $a \in A$ over a state of the world $s \in S$ results in an outcome, exclusively related to a and s. The outcome refers to the time point $t + 1$, after the action or set of actions (defined with the chosen alternative) are performed. The outcome is represented with a function that maps a vector of attributes' values of a and s to an output value that can be of various types, depending on the kind of function used.

Definition 6.2 (Outcome). Let $s \in S$ be a defined state of the world and $a \in A$ a chosen alternative performed over s. An outcome is represented with the following function:

$$f : A \times S \mapsto \chi. \tag{6.10}$$

f can be considered to represent the implementation of alternative a over the state s, and χ is the set of all possible outcomes:

$$\chi = \{f(a, s) | \forall a \in A \wedge \forall s \in S\}. \tag{6.11}$$

6.3.4 Utility function and preference

A utility function u maps an outcome or consequence $x \in \chi$ to a utility value that is viewed as an individual's preference $pref$ of alternative $a \in A$:

$$u : \chi \mapsto C, \tag{6.12}$$

where C can be a set of real values $\mathbb{R}$ or a finite set of predefined nominal values.

In the simplest case, the utility function only uses the outcome values, but can be extended to consider states of the world:

$$u : \chi \times S \mapsto C. \tag{6.13}$$

Possible states of the world to be considered as well are states at time t' and $t+1$. Therefore, preference is expressed as a function of the time point: $pref(t)$ - if only the state of the world in time t is considered, $pref(t')$ - if the state of the world at time t' is considered, and $pref(t+1)$ - if preferences are expressed in accordance with the state of the world at time $t+1$.

To clarify, all utility functions consider the outcome of particular alternatives that refers to time $t+1$. However, the differentiation of preferences is done over possible states of the world at particular times: t, t' or $t+1$.

Additionally, a utility function can also consider the probability distribution of possible states of the world.

6.3.5 Model

A model in the following definition of the methodological framework is a description of a system or function that maps a given tuple of values (as input to the model) to an output value. In particular, a model can refer to a predictive or diagnostic model.

A predictive model (M) is a model that performs a predictive task of an unknown quantity. For the purpose of the methodological framework, predictive models are built from data using data mining and machine learning methodology.

A diagnostic model (D) is a decision model built from experts' knowledge using the DEX methodology. Diagnostic models are used for estimation tasks based on experts' knowledge, as well as for evaluation of alternatives with regards to possible outcomes.

Predictive and diagnostic models can be employed for prediction or estimation of numeric and nominal attributes.

6.4 Quasi Ex-post Risk Analysis

The proposed methodological framework is applicable over decision problems that have a temporal aspect. Namely, the given data strongly defines the state of the world $s_t \in S$ at time t, and the decision problem requires evaluation of the state of the world $s_{t'}, s_{t+1} \in S$ at future times t' and $t+1$.

The methodological framework is broadly based on decision table for decision making under risk and uncertainty (Table 2.2). Therefore, the temporal aspect of the decision table (2.2) will be reviewed first.

The decision table for decision making under risk and uncertainty (Table 2.2) assumes that the complete decision problem is described with the state of the world S, the set of alternatives A, the utility function u and the probability distributions for each state in S. Considering the course of time, we could write that an alternative $a_t \in A$, evaluated at time t, is evaluated over a state $s_t \in S$ also considered at time t with probability $p(s_t)$.

The evaluation is done using the utility function u that gives outcome $x_{t+1} \in \chi$ that expresses the utility that an individual will gain at time $t+1$ by the alternative chosen at t. Preferences $pref(t)$ are then expressed through the probability of s_t taking place and the possible utility gained from chosen alternative a_t:

$$x_{t+1} = f(a_t, s_t), \tag{6.14}$$

$$pref(t) = p(s_t)u(x_{t+1}). \tag{6.15}$$

This formulation does not allow consideration of the state that will take place upon implementation of the chosen alternative, i.e. the state of the world $s_{t+1} \in S$ that will take place at time $t+1$. The proposed methodological framework tries to consider s_{t+1} in the evaluation of alternatives, as well.

The state s_{t+1} is uncertain at time t and needs to be estimated or predicted as precisely as possible. For this purpose, we introduce a predictive model M built from empirical observations of the state of the world. The model M tries to predict the state of the world s_{t+1} when s_t is given:

$$s_{t+1} = M(s_t). \tag{6.16}$$

The predicted state s_{t+1} is assumed to be an almost certain event that will happen at time $t+1$. This holds if the state s_{t+1} has a set of only numeric uncertain attributes. Otherwise, when only nominal attributes are present, a probability distribution of possible states that can take place at time $t+1$ can be considered. The formalization of the methodological framework assumes that the predicted state s_{t+1} is almost certain, and therefore probability of 1 ($p(s_{t+1}) = 1$) is assigned.

Accordingly, the formulation in Equation 6.15 is updated as follows:

$$pref(t+1) = p(s_t)u(x_{t+1}, s_{t+1}) = u(x_{t+1}, s_{t+1}). \tag{6.17}$$

Visually, the set of performed actions on a time-line is described as in Figure 6.2. Input in the time-frame t to $t+1$ is the set of alternatives A and the set of states S. The output refers to the consequence x_{t+1} through implementation of alternative a_t. The time point $t+1$ occurs after alternative a_t is applied or performed.

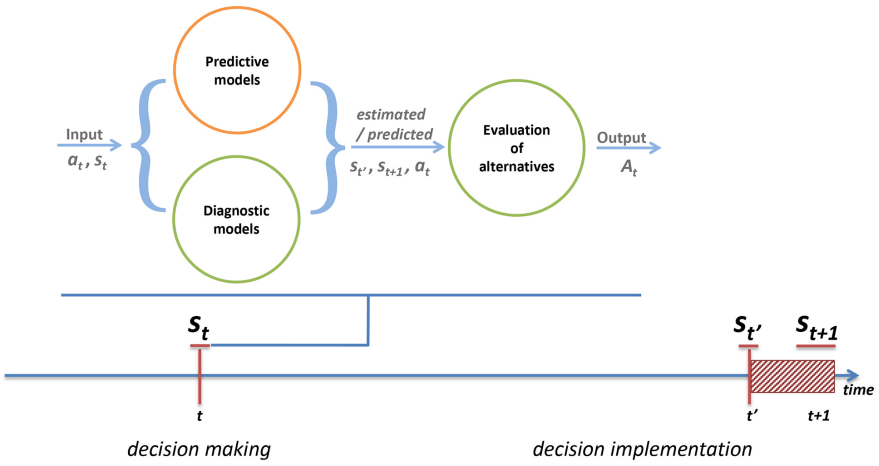


Figure 6.2: Set of actions performed over time.

When an individual is facing a decision problem in a fast-changing world, predicting the state of the world $s_{t'}$ that will take place at t' is a challenge. As in the case of predicting state s_{t+1}, the uncertain state $s_{t'}$ can be predicted using a predictive model M. Accordingly, preferences $pref(t')$ are then expressed with regard to $s_{t'}$, and the possible utility gained from a_t is expressed with utility function u':

$$s_{t'} = M(s_t). \tag{6.18}$$

The predicted state $s_{t'}$ is also assumed to be almost certain to happen at time t':

$$x_{t+1} = f(a_t, s_{t'}), \tag{6.19}$$

$$pref(t') = p(s_{t'})u'(x_{t+1}) = u'(x_{t+1}). \tag{6.20}$$

The Equation 6.20 can be updated so that the state s_{t+1} is considered in evaluating alternatives and their preferences:

$$pref(t', t+1) = u'(x_{t+1}, s_{t+1}). \tag{6.21}$$

Visually, the set of actions are described as in Figure 6.2. The time point t' is given before the chosen alternative a_t is applied or implemented.

In the case when data are not available for building a predictive model, it can be replaced by a diagnostic model D that relies on estimation based on expert knowledge. Using a predictive or diagnostic model is considered to be a part of risk analysis, since it helps to assess how a particular state of the world will behave in the future and how uncertain it is.

The essence of the proposed methodological framework is the identification of the actual states of the world at times t' and $t+1$ during the decision analysis process and evaluation of alternatives.

The implementation of the above contributions into a methodological framework uses the concept of risk analysis for organizing all tasks, i.e. the usage of predictive or descriptive models and the evaluation of alternatives. As described in Chapter 3, risk analysis consists of two important processes: risk assessment and risk management (the additional process of risk communication is left out of the formalization of the methodological framework).

In the context of risk assessment, whether the assessment is done ex-ante or ex-post, the contributions mentioned above are explained as follows. In the ex-ante approach to risk assessment a decision (choosing alternative a_t) is made at time t, when the state of the world s_t is given. Ex-post involves reviewing the decision of choosing a_t, when s_{t+1} is already known (at time $t+1$). The methodological framework is designed to improve the ex-ante approach with consideration of the state of the world (s_{t+1}) that will take place at time $t+1$. Such improvements of the ex-ante approach are called *quasi ex-post risk analysis*. Thus, the quasi ex-post makes a decision at time t when state s_t is given (optionally the state $s_{t'}$ is also known) by reviewing the outcome of a potential alternative a_t, given at time $t+1$.

Overall, the methodological framework is designed as a MCDA process that is wrapped within a process of risk analysis containing both risk assessment and risk management (Figure 6.3). In particular, the MCDA process is nested within the risk management process, where alternatives are evaluated in accordance with their outcomes, and optionally against the state of the world s_{t+1} that takes place upon their implementation.

The input in quasi ex-post risk analysis is a set of attributes that describes the state s_t at time t and a set of alternatives A. The output is a proposed alternative $a_t \in A$ or set of alternatives $a_{ti} \in A_t, i = 1, ..., n$, where $n = |A_t|$ and $A_t \subseteq A$. Green circles represent

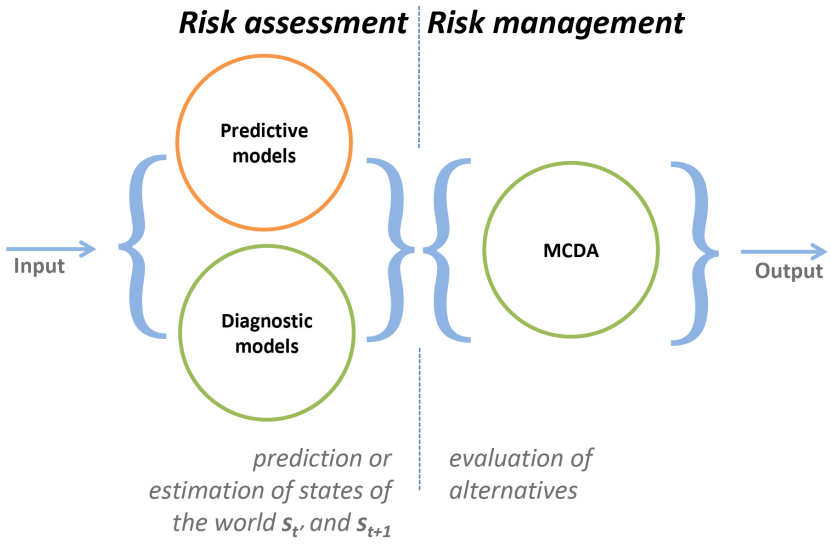


Figure 6.3: Conceptual design of the methodological framework: quasi ex-post risk analysis

models built using the DEX method, while the orange circle represents predictive models built using data mining and machine learning methods.

The following describes both risk assessment and risk management in more detail. Since both appear as parts of a quasi ex-post risk analysis, they are referred to as modules in the reminder of the thesis.

6.5 Risk Assessment

Theoretically, risk assessment, as stated in Chapter 3, provides the objective information needed for decision making, including a characterization of the relevant uncertainty that could influence the decision. It separates 'what is known' from 'what is unknown', which represents the uncertainty, and it focuses appropriate attention on the latter and how that might affect decision outcomes and, therefore, the decision itself.

The risk assessment module of the proposed quasi ex-post risk analysis deals with uncertainty due to lack of information about the probability of occurrence of a state of the world. In other words, 'what is unknown' is tightly related to states of the world and, in general, the task of risk assessment is how to describe it in order to be taken into account when decision is made. Final risk assessment is then done over 'what is known' accompanied with a description and characterization of 'what is unknown'.

Predictive models form a *predictive layer*, which hosts models for each element in $\nabla G_s \subseteq G_s$, qualified as uncertain or unknown. The *predictive layer* is a precursor of ex-ante risk assessment (Figure 6.4), supplementing the state of the world with predictions or estimations of values of the attributes that belongs to ∇G_s.

When data for attributes in ∇G_s are not available, the methodological framework allows integration of a *diagnostic layer*, which has the same role as the predictive layer, but instead of using predictive models, it considers diagnostic (decision) models. Such models are based on expert knowledge and do not introduce uncertainty that can be quantified.

At the input, the risk assessment module retrieves a description of the state of the world s_t at time t, and optionally an alternative a_t that is externally evaluated against the state s_t. According to the models specified, it predicts or estimates the values for

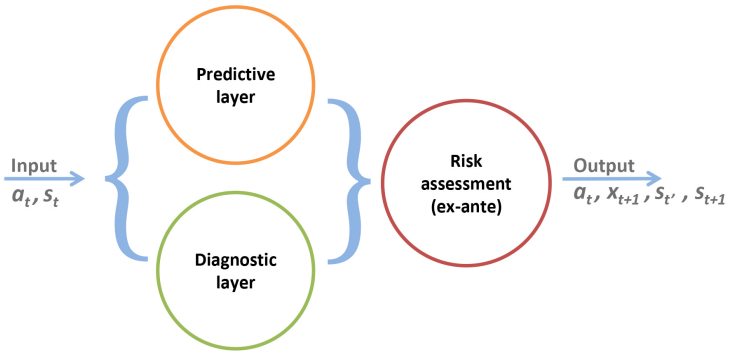


Figure 6.4: Conceptual design: the risk assessment module.

uncertain attributes of s_{t+1} or $s_{t'}$ that will take place at time $t+1$ or t', respectively. The predicted or estimated state of the world is then sent to the output for further use in the risk management module. Optionally, if an alternative a_t is provided at input and risk assessment models are defined, then this module can assess a risk profile (based on the risk assessment model) of a_t as applied on the predicted state of the world s_{t+1} or $s_{t'}$. Such risk assessment is performed with the ex-ante approach. In such a case, the quasi ex-post risk analysis behaves as a recommendation system, the output of which is shown in the following section.

As in Figure 6.4, throughout the thesis, predictive layers are represented with orange circles, and diagnostic ones with green circles.

6.6 Risk Management

The risk management module is part of the methodological framework associated with uncertainty derived from lack of information about the possible outcomes or consequences of decisions. It performs complete evaluation of the set of alternatives A over the state of the world predicted in the previous module. Evaluation of alternatives is performed by a pre-defined DEX decision model. This task is mandatory and the module must be provided with a DEX decision model for each implementation of the framework.

The risk management module gets as input the predicted state of the world s_{t+1} or $s_{t'}$, and optionally a risk profile of the alternative a_t that is supplied and externally evaluated over the state s_t.

The output of the module is designed to cover previously defined tasks of decision making (Section 2.3): choice, sorting and ranking (Figure 6.5). The decision task that will take place as output is defined in the implementation of the methodological framework. As a note, evaluation of alternatives is also a task within the risk management module, but it is not related to how the output should look.

Evaluation of alternatives refers to evaluating all alternatives in A over the predicted state of the world s_{t+1} or $s_{t'}$. The evaluation is done with a predefined DEX decision model that iterates over all alternatives. The evaluation defines the set of outcomes χ, from which gains or consequences can be recognized and utility values calculated, based on the utility functions u or u'.

Sorting is a task that assigns each alternative from A to a category from a predefined set of categories. This task is performed using a pre-defined function *cat* (referred to as a

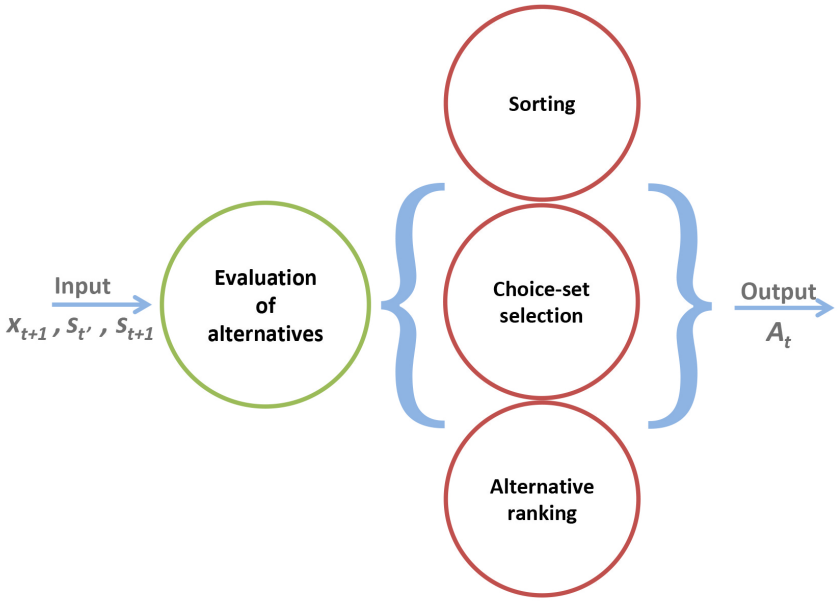


Figure 6.5: Conceptual design: the risk management module.

model) that can consider only the outcome $x \in \chi$, or both the outcome x and the predicted state of the world s_{t+1}. This model can be pre-defined or integrated into the model for evaluation of alternatives. The set of categories should be provided when the framework is designed. The output of this task is a categorization of alternatives into a predefined set of categories.

Choice set selection is a task within the methodological framework that is used to select most preferable alternatives from all available. Formally, this task uses the alternative sorting task as a precursor and selects only those alternatives that are categorized in the most preferable category. The output ($C_{\succeq}$) is the set of all alternatives that belong to the most preferable category. The most preferable category is pre-defined, i.e. supplied when the framework is implemented.

Formally, the choice set $C_{\succeq}$ is defined as:

$$C_{\succeq} = \{a : a \in A \wedge x = f(a, s_{t+1}) \wedge pref(t+1) = u(x, s_{t+1}) \wedge cat(pref(t+1)) = c\}, \quad (6.22)$$

where c is a category that is defined as most preferable, u is the utility function and cat is the model used for alternative sorting. Optionally, utility can be considered as dependent only on the outcome x. Moreover, if a state of the world $s_{t'}$ is considered, then the utility function used is u'.

Alternative ranking is the task of ranking all evaluated alternatives in A. Comparison is done over utilities calculated with the utility function u or u' over all outcomes in χ. The ranking relation is defined as:

$$a_1 \succeq a_2 \iff u(f(a_1, s_{t+1})) \geq u(f(a_2, s_{t+1})), \forall (a_1, a_2) \in A \times A, \quad (6.23)$$

where f is the function that represents implementation of an alternative over the state of the world s_{t+1}. Optionally, the utility can be expressed only in regard to an outcome, excluding the state of the world s_{t+1}.

The choice-set selection and alternative ranking tasks can be combined so that only alternatives from $C_{\succeq}$ are ranked in accordance with their utility.

These preferences about what tasks are to be performed in the risk management module are provided in the implementation of the methodological framework.

Part II

Case-study

The previous part of the thesis introduced the basic theory and methodology used for developing the methodological framework. First, decision and risk analysis were introduced (Chapter 2 and Chapter 3), followed by the methodology of decision modeling (Chapter 4), data mining and machine learning (Chapter 5). Part I ended with the formalization of the methodological framework (Chapter 6).

The methodological framework for quasi ex-post risk analysis has been applied on a case-study that is given in the following part. The proposed quasi ex-post risk analysis is applied to a decision problem from the domain of agriculture. The case-study decision problem concerns the influence of agricultural practices on surface and ground water quality and water protection.

Part II starts with a description of the problem that is reviewed in the case-study, along with related work (Chapter 7). Then, in Chapter 8 the implementation of the methodological framework is given. Finally, part II concludes with its results and evaluation (Chapter 9).

Chapter 7

Problem Formulation

Industry and agriculture, as the main water polluters, affect water quality through both point and diffuse-source pollution. Point-source pollution mainly refers to industrial or sewage treatment plants, while diffuse-source pollution comes from agricultural fertilization and plant protection via many diffuse sources (e.g., surface runoff and discharge through sub-surface drainage systems for surface water, and infiltration for ground water). Furthermore, several studies have shown that agriculture acts as the main diffuse-source polluter because of the use of plant protection products (referred to as pollutants in the remainder of the thesis). These products are applied on a field scale in accordance with conventional agricultural management practices (Capel, Larson, & Winterstein, 2001; Holvoet, Seuntjens, & Vanrolleghem, 2007).

Conventional agricultural management and production are based on traditional economics. They view capital as simply being cash, investments and economic instruments. However, sustainable development is now seen to rely on four types of capital: the traditional financial capital, the manufactured capital of infrastructure, human capital in the form of intelligence, culture and organization, and the natural capital of renewable and non-renewable stocks of natural resources that support life and economic activities (Hawken, Lovins, & Lovins, 2010). There is therefore a need to develop an integrated and accepted system of valuing or measuring natural capital and ecosystem services. Furthermore, Fenech, Foster, Hamilton, and Hansell (2003) point out that turning the idea of natural capital into a practical means of measuring or modeling both economic and ecological systems requires considerable study and innovation.

The pollution of surface and ground water with pollutants in agricultural areas occurs when pollutants (herbicides and/or pesticides) are discharged directly or indirectly into surface or ground water bodies due to the absence of adequate treatment that would protect the environment from harmful compounds. A recent overview of the US Geological Survey National Water-Quality Assessment programme and the National Stream Quality Accounting Network concerning pesticide occurrence in US streams and rivers over two decades (1992–2001, 2002–2011) shows that one or more pesticides or pesticide degradation were detected more than 90% of the time in streams across all land uses during both decades (Stone, Gilliom, & Martin, 2014). These pesticide effects could take place in a very short time after their release in the environment, either as agricultural applications in the fields or as spillages due to bad management practices.

The main pathways of diffuse pollution at the field scale are surface runoff, discharge through subsurface drainage systems, and lateral seepage (lateral hypodermic flow on a non-permeable soil substratum), while infiltration is identified as a direct pollutant transfer path in groundwater (Holvoet et al., 2007; Brown & van Beinum, 2009). The results of a review study by Brown and van Beinum (2009) have shown that surface runoff and

drainage make a significant contribution to the pollution of surface waters with pollutants as well. Drainage has been considered a relevant route for transport of pollutants in 6 out of 10 environmental scenarios representative of agricultural conditions across Europe (FOCUS, 2001).

At a general level, it is often a question whether conventional agricultural management practices concerning the application of plant protection products deliver expected and favourable results with accounted environmental protection, or whether they need to be further tuned to specific local conditions in order to achieve the required efficiency and environmental protection. The decision problem that is of interest in the domain of water protection from agriculture is formulated in two steps:

- Assess the risk of water pollution for the planned practice of applying plant protection products, with known efficiency in crop protection.
- If the planned agricultural practice is assessed to have a risk of water pollution, find a possible solution for keeping the water quality and environmental protection at a safe level.

The given decision problem requires definition of all relevant possible states of the world S. The state of the world S should encompass all possible contributing factors to water pollution (referred to as pollution factors). This task will be fitted in the risk assessment module. A set of mitigation measures per pollution factor (the alternative set A) is used in the risk management module, where potential solutions are proposed. A solution is considered satisfactory if it successfully reduces the ecological risk of pollutant transfer without reducing the efficiency of crop protection products applied on the field.

Considering the fact that there exists more than one water pathway for water pollution, the decision problem is extended to encompass control over all of them: surface runoff, discharge through sub-surface drainage systems, and infiltration. The following section describes these water pathways in detail.

7.1 Water Pathways

7.1.1 Discharge through sub-surface drainage systems

Discharge through sub-surface drainage systems (drainage outflow) denotes the discharge from tile drainage infrastructure installed on a field to enhance the moisture and aeration conditions of the soil and to lower the groundwater table (Zimmer, 1993). Tile drainage relies on subsurface drains with perforated plastic pipes. It shortens the residence time of water in biologically active root zones and aggravates the diffuse pollution of adjacent surface water with nutrients and pollutants (Tomer, Meek, Jaynes, & Hatfield, 2003). In our case-study, we focus on tile drainage water discharge and address the problem of estimating the time period when intensive drainage events occur in a tile-drained field, as well as the discharged quantity from a field.

European field studies of the transport of pollutants via tile drainage have identified four important factors that influence the concentration of pollutants in drainage outflow: (i) the time interval between application of pollutants and occurrence of the first subsequent drainage event; (ii) the strength of absorption of pollutants into the soil; (iii) the clay content of the soil; (iv) the degradation half-life of pollutants in soil (Brown & van Beinum, 2009; Trajanov et al., 2015). According to Brown and van Beinum (2009), regulatory assessment of the pollution of surface waters via drainage outflow could rely on two mitigation measures: (i) decreasing the permitted application rate, resulting in a proportional decrease of the pollution of drained water, which decreases the exposure of

surface waters; (ii) restricting the time period during which applications of pollutants may be made. Since losses of pollutants to drains are closely controlled by the time between the application and initiation of drainage (Jones et al., 2000; Renaud, Brown, Fryer, & Walker, 2004), limiting the applications of pollutants to times with no drainage (e.g. early autumn or late spring) can be an effective mitigation option.

7.1.2 Surface runoff

Surface runoff is water coming from rain, snow-melt, irrigation, or other natural sources, that flows over a land surface, and is a major component of the water cycle. It appears when the soil water matrix is not able to absorb more water causing water to flow over the surface of the soil. The reasons that lead to inability of the soil water matrix to absorb water can be: saturation (soil is infiltrated to full capacity), texture of the soil surface layer (capping soil) and extreme events of water dropping on the soil surface layer (e.g., storm-water). In our study, all three reasons for surface runoff water are considered to be independent water pathways.

Surface runoff has the greatest capacity to carry pollutants into surface water basins because, on the surface, it is in contact with the highest amount of pollutants. Also, unlike subsurface and groundwater pathways, surface runoff does not undergo any filtering through soils (Dehotin et al., 2015).

As surface runoff flows, the amount of water may be reduced in a number of ways: a small portion may evapotranspire; water may become temporarily stored in micro-topographic depressions; and a portion of it may become run-on, which is the infiltration of runoff as it flows overland. Any remaining surface water eventually flows into a receiving water body such as a river, lake or sea.

The adverse impacts of surface runoff can be mitigated in several ways. The most preferred way is to change land and crop management on the field to minimize water flow. On a wider area or region, erosion and flood control techniques can be applied. Finally, short-term mitigation - measures that are effective after a short period of time - related to plant protection practices and not to the minimization of the quantity of water flow, can be applied. (Arnold & Gibbons, 1996).

7.1.3 Infiltration

Infiltration refers to the movement of water into the soil layer. Movement of water into the soil depends on gravity, capillary action, and soil porosity. Of these factors, soil porosity is the most important. A soil's porosity is determined by its texture, structure, and organic content. Coarse-textured soils have larger pores and fissures than fine-grained soils and therefore permit more water flow. Pores and fissures found in soils can be made larger through a number of factors that enhance internal soil structure (Guzha, 2004).

The capacity of infiltration to carry pollutants into water basins is similar to drainage outflow, since the infiltration process is of similar nature. Therefore, the reduction of the quantity of water flow requires long-term mitigation measures such as installing a tile-drainage network, which is a primary measure that can help with infiltration water flow control.

7.2 Data

A representation of a state of the world (agricultural field) at a particular moment in time requires a detailed analysis of history in order to mitigate uncertainty. We use the following data to reduce the uncertainty of a state of the world.

The experimental site, where data were collected, is located in western France. It is situated at the southern end of the Armorial massif, in the La Jaillière province. It is owned by ARVALIS - Institut du Végétal, France. The site has been dedicated to the study of the influence of agricultural management practices on water quality since 1987. It is a reference site for the European Commission FOCUS working group (FOCUS, 2001). The La Jaillière site is considered representative of agricultural regions in Europe with shallow silt clay soils. Soils are hydromorphic brown with a silt clayed texture, and shallow schistose bedrock situated at about 0.90 m below the surface. The average clay content is 22 %, but variations from 18 % to 30 % were observed depending on soil horizons (Arlot, 1999). Organic matter content was found to be 2 % on average in the superficial soil horizon (Madrigal, 2004).

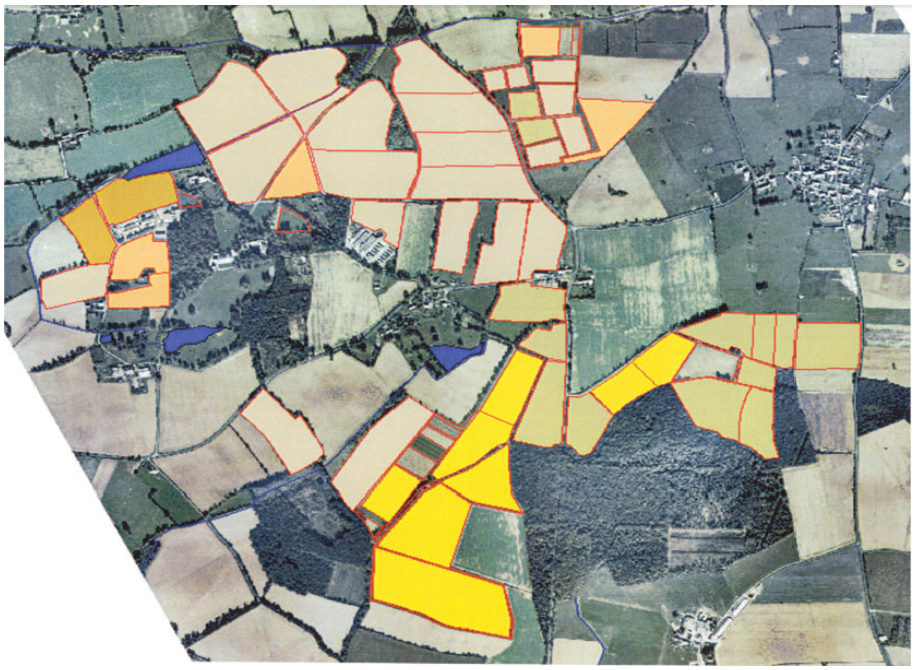


Figure 7.1: La Jaillière site. All fields on the site (AGRESTE, 2000; Branger, Debionne, Viallet, Braud, & Vauclin, 2006).

The climate at the site is of a oceanic type. The mean annual precipitation of 617 mm is evenly distributed throughout the year (monthly values between 40 and 62 mm). The mean annual potential evapotranspiration is 610 mm. The site contains many fields divided in north and south parts. Furthermore, each part contains blocks of fields (Figure 7.1). Each block is used for a different type of experimental analysis.

In our study, we include data from 11 fields. Each field is about, or less than, 1 ha of surface area and is cultivated following a traditional winter wheat and corn crop rotation. Fields are equipped with an independent tile-drainage system and surrounded by metal cuttings for hydraulic isolation from other farm fields, and with a collecting trap for surface runoff measurement (Figure 7.2). Tile drains are located at 0.9 m below the soil surface, with a spacing of 10 m (Branger, Debionne, Viallet, Braud, & Vauclin, 2006).

Three stations where water is collected are located on the site. Water is collected from drainage outflow and surface runoff separately for each field. Since 2005, a small meteorological station is installed on the site. This station gives information about the temperature, evaporation, and amount of rainfall. From the available meteorological data, the following quantities are derived: minimal, average and maximal temperature per day,

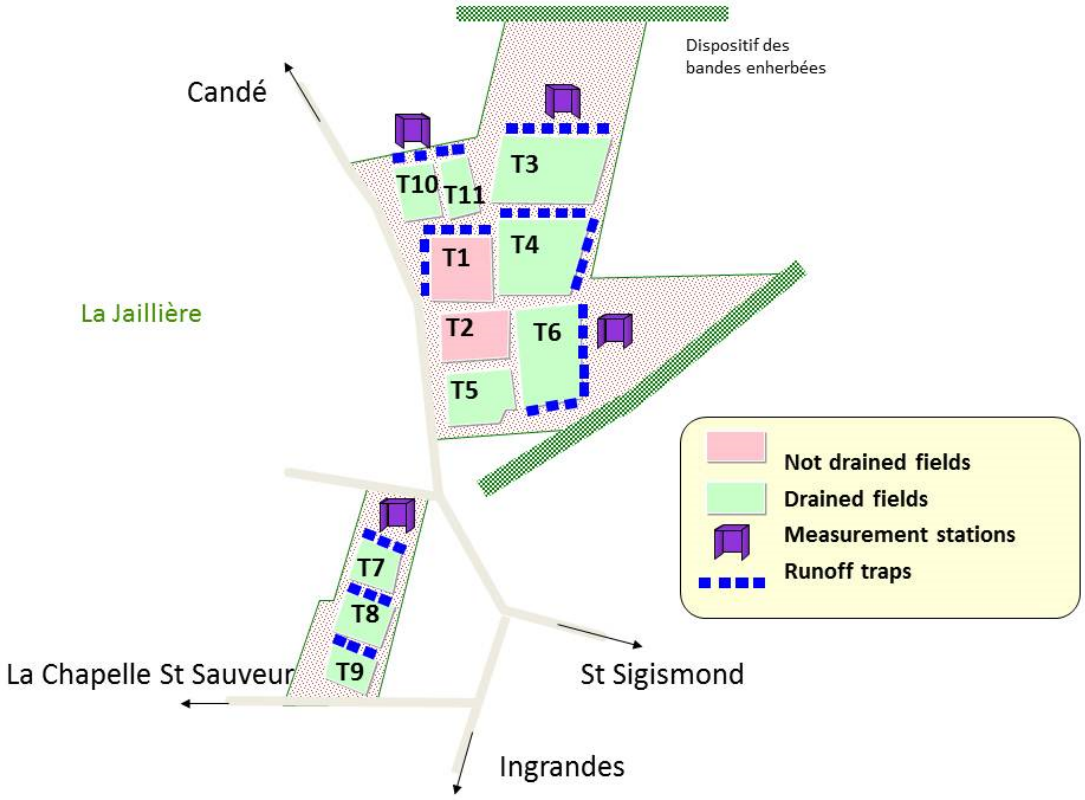


Figure 7.2: Layout of the fields with their names, surface runoff and drainage outflow systems' characteristics, and location of measurement stations where water is collected.

evapotranspiration per day, and amount of rainfall per day.

Our study is based on data for the various agricultural practices performed on the fields, together with the amount of water flowing out of the fields, as well as pollutants concentration in the flown water (the PCQE database - Pratiques Culturaleset Qualité des Eaux). We also consider a database of soil properties, and meteorological data provided by METEO France. Following is a description of each type of data collected at the La Jaillière experimental site.

Drainage and surface runoff rates are routinely monitored at hourly intervals, but the data recorded in the PCQE database are based on cumulative values per day. A day for water flow observations is defined as the time period that starts at 00:00 (midnight), lasts for 24 hours and has records for each day in a campaign. A campaign is defined as the time period that starts on September 1st, and finishes on August 31st. A total of 25 campaigns (1987 - 2012) are included in the study for each field where a drainage system is installed (Table 7.1). The observations for surface runoff are similar and are available for each field where runoff traps bound the field's edges (Table 7.1).

The meteorological data were collected from two sources. Starting from 1987, data were taken from Météo France, the French national meteorological agency. Météo France has a wide range of stations in France, some of them in the surroundings of La Jaillière. Therefore, the data were collected from the nearest meteorological station to La Jaillière, referenced with number 4499. Since January 1st, 2006, the data were collected from the ARVALIS meteorological station located at the site. Data are collected in a separate database and contain information about the minimal, mean and maximal temperature per

Table 7.1: Basic statistics of daily collected data for Surface runoff and Drainage outflow. *Std. Dev.* stands for standard deviation, *Tot. Records* stands for total number of records in the database.

Statistic	Surface Runoff	Drainage Outflow
Min (mm)	0	0
Max (mm)	37.32	46.83
Average (mm)	0.10	0.51
Median (mm)	0	0
Std. Dev. (mm)	0.78	1.88
Tot. Records	91320	91320
Missing Values	22964	17224
Years	1987-2012	1987-2012
Fields	9	9

day, cumulative evapotranspiration per day and cumulative rainfall per day. It is important to note that a day is defined here as the period that starts at 06:00 and lasts for 24 hours, which is different from a day in the PCQE database, described before, where it starts at 00:00.

The transfer of pollutants occurs only if the water in the soil exceeds the maximum (100%) soil water holding capacity; therefore, the concentration of pollutants in water outflow is measured only for time periods with actual water outflows from the fields (drainage periods). The amount and variety of collected data about pollutant transfer during the drainage periods of 18 campaigns (76 active ingredients and 4 metabolites in total) make the La Jaillière site a unique experimental site in Europe. Each monitored active ingredient from a water sample is labeled as risky or not risky, according to PNEC (Predicted Non-Effect Concentration) values of monitored active ingredients (EU directive 2008/105) (European Parliament & Council, 2008) and a threshold concentration of 2 μg/L, where the latter represents a threshold for raw water that could be used in a purification process for producing drinking water (EU directives 80/778 and 98/83) (European Parliament & Council, 1980, 1998). PNEC represents the concentration of an active ingredient which has no predicted effect on aquatic ecosystems. In other words, PNEC is the concentration below which exposure to an active ingredient is not expected to cause adverse effects on surface water.

The risk level of each measured concentration of an active ingredient in a water sample was assessed according to the following threshold criteria:

If PNEC of the active ingredient ($pnec(AS)$) is greater than or equal to 2 $\mu g/L$, the sample is considered risky or not risky according to the following criteria:

$$sample = \begin{cases} notrisky, & \text{if } c(AS) < 2\mu\text{g/L} \\ risky, & \text{if } c(AS) \geq 2\mu\text{g/L} \end{cases}, \tag{7.1}$$

otherwise ($pnec(AS) < 2\ \mu g/L$):

$$sample = \begin{cases} notrisky, & \text{if } c(AS) < pnec(AS) \\ risky, & \text{if } c(AS) \geq pnec(AS) \end{cases}, \tag{7.2}$$

where $c(AS)$ represents the measured concentration of a given active ingredient AS, and $pnec(AS)$ is the PNEC value of AS.

7.3 Expert Knowledge

Expert knowledge has been provided by experts from ARVALIS, and was given in the form of tables that contain decision rules. It is based on experiments, data collected from experimental stations across France and empirical analysis in accordance with farmer advisers. In addition, the expert knowledge provided is an integral part of the AQUANOUVAEU conceptual model, owned by ARVALIS. Decision rules are defined with a set of predicates, with which the set of states, or the world S is defined. In accordance with the decision rules, the following elements were considered as descriptors of a state of the world S:

- soil substratum (depth, level of permeability and texture),
- soil surface layer,
- soil cultivation,
- field landscape,
- crop rotation,
- crop protection (type of active ingredient, dose and time of application),
- weather conditions.

In addition, the provided decision rules normally define the scope of mitigation measures, that determines a set of alternatives A. The scope of mitigation measures leads to a formalization of the factors that are potentially crucial for mitigating potential ecological risks of pollutant transfer in a given situation. The factors that impact the natural behavior of pollutant transfer in water are:

- time of application,
- dose of application,
- selection of active ingredient,
- soil cultivation,
- in-field landscape management,
- near-field landscape management.

Overall, the provided expert knowledge helps in reducing the problem of uncertainty of state of the world definition, as well as the uncertainty related to possible consequences. The complete role of expert knowledge in building the decision support system is given in detail in subsequent chapters.

7.4 Related Work

Early work related to water quality dates back to the beginning of the 20^{th} century, when Moore (1901) carried out a study on water purification: "in undrained clay land, cracks of one and two inches wide and five feet deep are sometimes met, with the result that direct passage of sewage and surface water into them has occurred, so that the effluent is not purified as intended. It is thus very unsuitable for irrigation, unless the surface is specially prepared". Ever since, scientists and experts have studied the phenomena of water and solute movement along certain pathways, bypassing or going through fractions of the porous

matrix in the soil. First, they tried to understand the process and its characteristics. Then, they developed models for describing the process of movement using soil characteristics. In the next stage, some conceptual models were built, based on analytical and statistical observations. In the last twenty years, better mechanistic models were developed to incorporate water flow processes (Gerke & van Genuchten, 1993).

Conceptual and mechanistic models built in the previous century become of interest as support in the decision making process. However, such models did not express the possible uncertainty of their simulations or forecast, which causes uncertainty to be propagated to a decision making process. We consider the two most used models for supporting decision making processes in water protection: MACRO and Root Zone Water Quality Model (RZWQM) that deal with water pathways and pollutant transfer simulation. Performance of the decision support system based on quasi ex-post risk analysis is compared with both MACRO and RZWQM.

With the development of operational research as a scientific field, scientists and experts considered the idea of building expert systems that would support the process of decision making. In particular, in the domain of ecosystem protection many efforts have been made to plan water and farmland use, and build expert systems that would improve traditional practices (Liao, 2005). Many are publicly unavailable due to institutional or organizational policies. Here, we consider expert systems built by ARVALIS, access to which is available upon bilateral agreement. Those expert systems are AQUANOUVAEU and AQUAVALLEE, and will be used for performance evaluation and comparison with the built decision support system.

7.4.1 Modeling approach

Both state-of-the-art models are used in the thesis for the comparison of simulations with the proposed predictive layer of the framework. The MACRO model is compared with regard to drainage outflow, since it does not simulate surface runoff, while RZWQM is used with regard to both drainage outflow and surface runoff.

7.4.1.1 MACRO

MACRO (Jarvis, 1994; Larsbo & Jarvis, 2003, 2005) is a one-dimensional dual-porosity model that combines the Kinematic Wave (KW) equation (7.3) for describing water flow and solute convection for the macro-pore region with Richards' equation (7.4) for water flow and solute convection dispersion in the matrix. Water transfer into the matrix is treated as a first-order approximation of the water diffusion equation and is proportional to the difference between the actual and saturated matrix of water contents. The KW equation has the form:

$$\frac{dh}{dt} + C\frac{dh}{dx} = D\frac{d^2h}{dx^2}, \tag{7.3}$$

where h is the debris flow height, t is the time, x is the downstream channel position, C is the pressure gradient (depth dependent nonlinear variable wave speed) and D is a flow (height dependent variable diffusion term). Richards's equation states:

$$\frac{d\theta}{dt} = d[K(\theta)(\frac{d\Psi}{dz} + 1)], \tag{7.4}$$

where K is the hydraulic conductivity (cm/s), Ψ is static pressure head (m), z is elevation above a vertical datum (m) and θ is the water content of the soil.

7.4.1.2 RZWQM

The Root Zone Water Quality Model, RZWQM (Ahuja, Rojas, & Hanson, 2000) utilizes a dual-permeability/mobile-immobile (DP/MIM) description of one-dimensional vertical soil water flow and chemical movement. Three transport regions are assumed to exist in the soil: cylindrical macro-pores, the mobile soil matrix, and the immobile soil matrix. In macro-pores, water flow is calculated using the Poiseuille equation (7.5), and solutes are displaced by convection. The Poiseuille equation has following form:

$$\Delta P = \frac{8\mu LQ}{\pi r^4}, \tag{7.5}$$

where ΔP is the pressure drop, L is the length of pipe, μ is dynamic viscosity, Q is the volumetric flow rate, and r is the radius.

In the mobile matrix region, water flow during infiltration is described using the Green-Ampt equation (7.6), and Richards' equation (7.4) during redistribution, while solute moves by convection (Köhne, Köhne, & Šimůnek, 2009). The Green-Ampt approach equation is:

$$F = \frac{K_a S_w(\theta_a - \theta_i)}{i - K_a}, \tag{7.6}$$

where θ_a and θ_i are the saturated and initial volumetric water contents, respectively, S_w is the soil water suction at the wetting front, i is rainfall intensity and K_a is the saturated hydraulic conductivity.

7.4.2 Expert systems

The state-of-the-art expert systems presented below are used in the thesis partly for comparison with the implementation of the framework on the given problem, and partly for integrating parts of the expert knowledge presented in the form of decision rules. These expert systems are briefly explored in the following subsections.

7.4.2.1 AQUAVALLEE

AQUAVALLEE is a diagnostic tool with precision to a watershed scale. It is developed by experts from ARVALIS and based on a GIS (Geographical Information System) analysis that identifies homogeneous areas in accordance with the type of transfer of pesticides (Réal, Lellahi, Francois, & Lepoutre, 2005).

In essence, the diagnostic tool, based on input about watershed or catchment, uses GIS data to obtain a map that will be layered with heat-maps and shapes. Such layers show various soil and landscape functions regarding water and pollutant pathways. Diagnosis is based on soil, subsoil and landscape properties (slope, river system, landscape features that may act as a buffer or purification zone (woods, forests, marshes, etc.) and does not take into account the climatology or practices implemented. However, following a diagnostic report, advice on changing practices and developing the catchment is proposed by taking farmers' practices and climate into account.

Water pathways are characterized by decision rules based on a combination of the input data and the diagnostic method. The decision rules are linked to the GIS system that helps in generating digital and mapping data and produces a map of possible types of pesticide transfer according to the characterized water pathways. The following types of water pathways can be characterized and combined:

- fast and slow infiltration,

- drainage outflow,
- surface runoff (by saturation and erosive runoff),
- inter-flow,
- floods,
- alluvial blanket fluctuations,
- spray drift.

The decision rules are specific to the study area and can be adapted from one catchment or watershed to another, depending on the type of soil and regional climate characteristics.

The data required for diagnosis is divided into two groups: measurement data:

- content of the selected area (watershed or catchment), to distinguish arable from non-arable land,
- density of the river system that reflects the hydro-morphism of the studied area,
- closeness of arable land to the river system,
- soil types and characteristics (texture and coarse materials content),
- available water capacity levels,
- slope levels,
- type of substrate (permeable or impermeable),

and landscape maps:

- parcel plan map,
- map of the river system,
- digital terrain model (topography),
- map of the geological substrate,
- soil map with soil properties.

The time required for diagnosis mainly depends on the time needed to provide the measured (input) data and maps. A case in France usually takes several weeks to generate a geological map that is used in the final diagnosis of the selected area. For a larger area, it can take a bit longer due to GIS data processing.

Once the risk transfer map is drawn up, expert knowledge is used to propose mitigation measures so that risk in the studied area is reduced. The result has the form of an expert report that includes landscape characteristics, estimated ecological risks and description of proposed mitigation measures.

The accuracy and quality of the diagnostic tool is highly dependent on the accuracy of the provided input data.

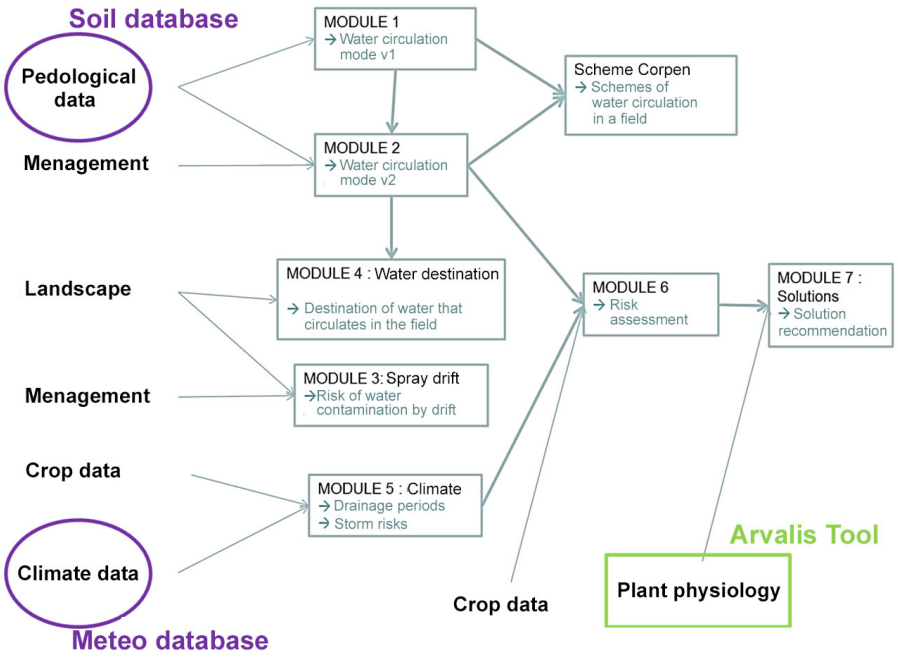


Figure 7.3: AQUANOUVAEU diagnostic tool: conceptual module organization

7.4.2.2 AQUANOUVAEU

AQUANOUVAEU is a conceptual tool consisting of decision rules presented in the form of tables (ARVALIS, 2015). It is a kind of simplification of the previously described tool AQUAVALLEE. It is composed of two parts: decision rules for pathways evaluation and diagnosis, and a system implemented in spreadsheet software that does calculations in order to feed the decision rules.

The decision rules are organized in 7 modules with different purposes (Figure 7.3). Starting with Module 1 and 2, AQUANOUVAEU asseses the various types of water pathway that may be present in the soil based on the specific characteristics of the soil. Modules 3 – 5 do assessment corrections in accordance with climate data and crop management practices. Module 6 estimates the overall ecological risk of pollutants transfer through diagnosed water pathways. Finally, Module 7 deals with mitigation measures of the estimated ecological risk of pollutants transfer.

The second part of AQUANOUVAEU can be linked to each module with decision rules, whenever they require input from a:

- soil properties database,
- pesticide properties database (PPDB),
- meteorological database,
- tool that simulates water content (SWHC) in the soil, and
- agricultural practices and crop management.

AQUANOUVAEU is also able to deal with outputs of various simulation models of water movement and pollutant transfer. As improvement over AQUAVALLEE, it estimates a period as a campaign with intensive water outflows (Module 5). Module 7 consists of decision rules that support an expert in proposing mitigation measures. This means that

the set of mitigation measures is not generated in an automatic manner but requires expert collaboration in generating the final report.

Unlike AQUAVALLEE, AQUANOUVAEU requires a somewhat smaller set of input data in order to make a preliminary risk assessment. However, such reduction influences the final accuracy. So far, the tool has only been evaluated on various real scenarios across Europe by experts from ARVALIS, as part of internal projects.

The result of AQUANOUVAEU has the form of an expert report, where landscape characteristics, estimation of water pathways and ecological risk of pollutant transfer are presented, and mitigation measures proposed in order to protect surface and ground water from pollutants, with crop protection products efficient as required.

Chapter 8

Quasi Ex-post Risk Analysis

In this chapter the implementation of the quasi ex-post risk analysis in the form of a decision support system (further referred to as a system) is described in detail. First, the overall structure of the system that consists of risk assessment and risk management modules is described. Then, the risk assessment module is presented with all components and models, followed by the implementation of the risk management module. This chapter concludes with a description of the graphical user interface built over the system.

8.1 Structure of the System

The overall structure of the implementation of quasi ex-post risk analysis consists of risk assessment and risk management modules (Figure 8.1). The input and output of the system are defined in accordance with the requirements of the defined decision model.

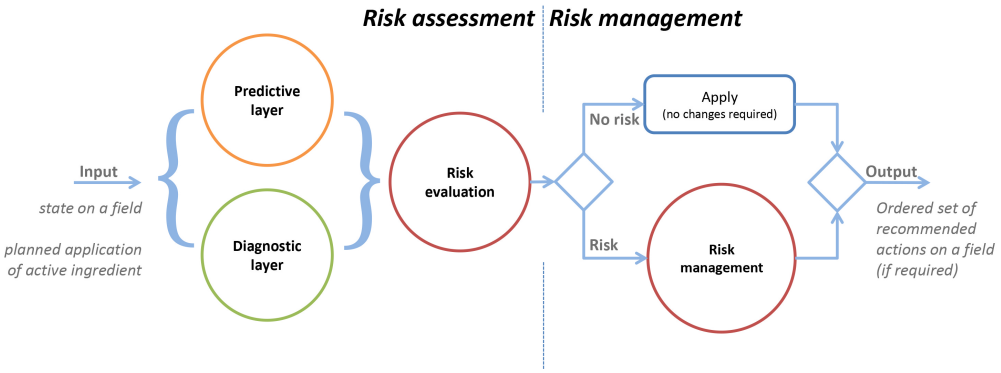


Figure 8.1: Implementation of the quasi ex-post risk analysis. Conceptual design.

The decision problem concerns the application of active substances on an agricultural field. The application of an active substance should be evaluated in advance. The state of the field at the time of application is generally not completely known, i.e. some descriptors are uncertain. In the context of quasi ex-post risk analysis, a state of the agricultural field is a state of the world, and the application of an active substance is an alternative. Therefore, the decision problem in the context of quasi ex-post risk analysis differentiates between the time of decision making t and time of application of chosen alternative t'. Our interest is evaluating alternatives at time t against the state of the world at the time of their application t'.

The input consists of a description of the current state of the agricultural field (a state of the world at time t) and an alternative that is represented as the planned application of an active substance to the field. This narrowly defines the scope of the system as a recommendation system to evaluate the provided alternative against the state of the world that would potentially take place at the time of application (at time t'). If the result of the evaluation does not satisfy the criteria of preventing water pollution and preserving efficiency of crop protection, then the system should propose or recommend a solution or solutions that would satisfy these criteria. Thus, the output is defined as a set of alternatives that satisfy the above criteria, from which an individual will make a choice. The time point $t + 1$ is defined as a time after an active instance is applied on a field. Therefore, the outcome is considered at time $t + 1$ when pollution can be quantified.

The risk assessment module has to (1) predict or estimate the state of the world that would potentially take place at time t' and (2) evaluate the ecological risk of the provided alternative against the predicted state of the world (at time t') - referred to as initial risk.

The risk management module takes as input both the predicted (estimated) state of the world and the result of the evaluation. If the result of the evaluation satisfies the above criteria, the risk management module outputs the given alternative as the only valid solution. Otherwise, it performs a search through the set of alternatives and tries to find those whose evaluation satisfies the criteria. These alternatives are then given as output of the system.

Evaluation of the alternatives is done separately for all five water pathways identified in Chapter 7. Thus, the exchange of information between risk assessment and risk management modules contain a vector of evaluations across all pathways.

8.2 Definitions

Following the definitions of basic elements or components, in Chapter 6, the specification of a state of the world, alternative and outcome are given here.

The world S of the given decision problem is defined as everything that happens on a field. A state of the world $s \in S$ is a state that describes the world S at a certain time point using a set of attributes. For the purpose of the case-study, this set of attributes consists of the following:

- depth of substratum,
- substratum texture,
- permeability of substratum,
- depth of permeability disruption,
- presence and efficiency of tile-drainage network system,
- soil water holding capacity (SWHC),
- cracks in the soil,
- permeability of surface soil layer,
- presence of capping layer,
- average slope of the field,
- slope disruptions,

- presence of thalweg on the field,
- presence of cultivated buffers,
- presence of access area issues,
- presence of corner issues,
- presence of downhill issues,
- crop present on the field,
- amount of water outflow,
- period of intensive flows,
- weather season (autumn-winter, spring or summer).

The description of a state s is a vector of values that correspond to the set of attributes.

The state of the world that obtains in a field at the time t of making decision is written as the current state of the world s_t. A state of the world that will take place at the time of application of an active substance (t') is written as $s_{t'}$.

The amount of water outflow and the period of intensive flows are two attributes from the state of the world that are considered uncertain, i.e. unknown at time t'. Others attributes are considered certain, since they do not change values over time and are part of agricultural practices. The set of uncertain attributes is thus $\nabla G_s = \{amount\ of\ water\ outflow, period\ of\ i$ and these attributes need to be predicted or estimated in order to get the description of the state of the world at time t'.

A set of alternatives A is a set of actions (practices) that can be performed on a field. In accordance with the defined decision problem, such actions belong to the scope of planned application of crop protection products, or the scope of landscape management that influences application of crop protection products (further referred to as application). An alternative $a \in A$ is defined with the following attributes:

- changing crop (g_{a_crop})
- time of application (g_{a_time}),
- dose to be applied of active ingredients found in crop protection products (g_{a_dose}),
- selection of active ingredients to be applied (selection of crop protection products) ($g_{a\_ingredient}$),
- tillage before application ($g_{a\_tillage}$),
- crop double sowing technique (g_{a_double}),
- setup cultivated buffers ($g_{a\_b\_cultivated}$),
- dammer inter-row soil cultivation (g_{a_dammer}),
- roughness of seed bed soil cultivation ($g_{a\_seed\_bed}$),
- tramlines management ($g_{a\_tramline}$),
- talweg buffers size ($g_{a\_b\_talweg}$),
- infield buffers size ($g_{a\_b\_infield}$),

- downhill buffers size ($g_{a\_b\_downhill}$),
- access area management (g_{a_access}),
- corners management (g_{a_corner}),
- edge management (g_{a_edge}),
- setup retention and dispersion facilities ($g_{a\_retention}$),
- setup fascine ($g_{a\_fascine}$).

The description of an alternative $a \in A$ is a vector of values that correspond to the set of these attributes. Since alternatives will be evaluated at time t, the notation that will be used in the remainder of the thesis is $a_t \in A$.

The set of attributes given above is the complete set. However, short-term and long-term mitigation measures are represented with different sub-sets. An alternative that represents a short-term mitigation measure is defined with: $\{g_{a\_crop}, g_{a\_time}, g_{a\_dose}, g_{a\_ingredient}, g_{a\_tillage}\}$, while long-term mitigation measures are represented with the following set: $\{g_{a\_tillage}, g_{a\_double}, g_{a\_b\_cultivated}, g_{a\_dammer}, g_{a\_seed\_bed}, g_{a\_tramline}, g_{a\_b\_talweg}, g_{a\_b\_infield}, g_{a\_b\_downhill}, g_{a\_access}, g_{a\_corner}, g_{a\_edge}, g_{a\_retention}, g_{a\_fascine}\}$.

The implementation or application f of alternative a_t over the state of the world $s_{t'}$ at time t' results in an outcome that occurs at time $t+1$, related exclusively to the alternative applied:

$$x = f(a_t, s_{t'}), x \in \chi. \tag{8.1}$$

As noted before, the risk assessment module evaluates the ecological risk of an alternative. Therefore, the domain of an outcome is tied to a value that expresses an increasing or decreasing pollutant transfer in water bodies, and is mapped to a two-value set $\chi = \{RISKY, NOT\_RISKY\}$.

Utility is estimated with a utility function u' that compares the outcome x and the state of the world s_{t+1} that would potentially take place at time $t+1$:

$$pref(t+1) = u'(x, s_{t+1}). \tag{8.2}$$

The utility has two possible values and expresses the preferences as to whether the alternative is accepted or not.

An alternative a_t, composed of the set of the attributes given above, represents a set of actions that can be performed on an agricultural field. Each of these actions are related to an explanatory complexity that is defined as the complexity of a particular action (represented with an attribute) to be performed on a field. Actions' complexities are defined in advance, by an expert. The complexity of a single action is referred to as partial complexity $c_{partial}$, while the aggregated complexity of an alternative across all attributes is referred to as total complexity c_{total} (Equation 8.4). The set of all partial complexities is C and corresponds to the attributes G_a that define an alternative $a \in A$:

$$C = \{c_{partial}(g_a) : g_a \in G_a\}. \tag{8.3}$$

$$c_{total} = \sum_{g_a \in G_a} c_{partial}(g_a). \tag{8.4}$$

8.3 Risk Assessment

The risk assessment module aims to improve the estimation of the state of the world ($s_{t'}$) at time t' and to evaluate the provided alternative a_t. It consists of two parts: predicting or estimating $s_{t'}$ and evaluating a_t. The first part (predictive part) is implemented separately for all five water pathways; the second part (evaluation part) has two different implementations: evaluation of ecological risk based on predictive models or on diagnostic models.

Prediction or estimation of $s_{t'}$ is done with predictive models M that can predict accurately water quantity flowed from a field, as well as intensive flow periods during the crop growing season, either winter or spring. Such predictions allow close description of the state of a field at the time of application (t'), which does bring concise information that allows ex-ante assessment of potential ecological risks. This part is based on both expert knowledge and knowledge obtained from data collected on experimental sites.

Due to the limited data available, the drainage outflow water pathway is the only pathway that is described with a predictive model for the uncertain attributes of $s_{t'}$. Predictive models are built from data from La Jaillière for predicting water quantity that will flow out of a field, and models for predicting the start and end of intensive water flow (drainage period) within a campaign. In addition, this implementation uses a predictive model for risk assessment that has been learned on data from La Jaillìre about previous applications and pollutants transfer through drainage outflow; its assessment is further considered in the risk management module. Such an approach is referred to as predictive ex-ante risk assessment.

The schematic design of the risk assessment module for drainage outflow is given in Figure 8.2.

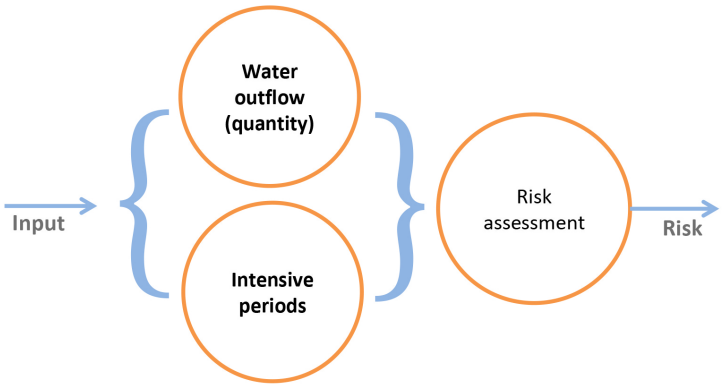


Figure 8.2: Risk assessment. Conceptual implementation design for drainage outflow.

The rest of the water pathways (simple surface runoff, surface runoff by saturation, surface runoff on capping soil and infiltration) are described with a diagnostic layer, where expert knowledge is used. The diagnostic layer consists of DEX decision models that cover expert knowledge of how water pathways are expected to behave in a given state of the field. The target of such diagnosis is the appearance and intensity of possible water pathways. The result of the diagnostic layer is an overall assessment of the ecological risk of pollutants transfer in water bodies; this is referred to as diagnostic ex-ante risk assessment (Figure 8.3).

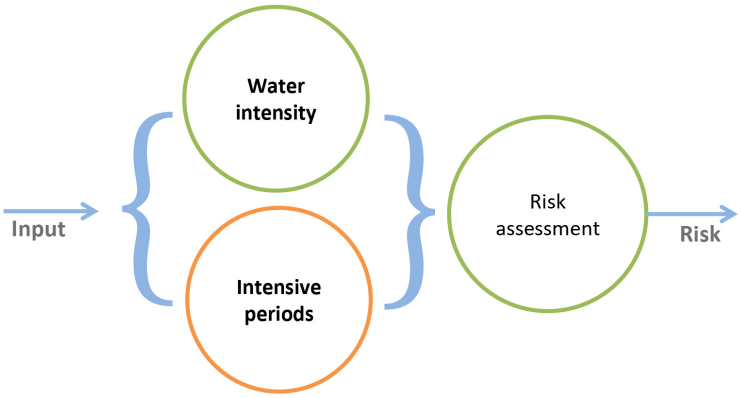


Figure 8.3: Risk assessment. Conceptual implementation design for other water pathways (surface runoff and infiltration).

8.3.1 Predictive layer

In the predictive layer we intend to model the water quantity that flows out of a field, as well as the period of time with intensive outflow within a campaign. The prediction layer includes three learned models from data collected on the experimental site La Jaillière: the models of drainage outflow and runoff by saturation water quantity, published in Kuzmanovski, Trajanov, Leprince, Džeroski, and Debeljak (2015) and the model of intensive flow period published in Trajanov et al. (2015).

We present the experimental setup in which the predictive models were built. First, building a model for predicting water quantity that flows out of a field is described. It includes pre-processing of the data, learning the models and choosing the best performing among them. Then, building a model for predicting a period of intensive outflows within a campaign is given, with details of how data are pre-processed and the model built.

8.3.1.1 Water quantity

First, we pre-processed the collected data and derived new input variables that could be used for better description of water outflow. Then, we established an experimental setup based on two regression problems and six methods. The two regression problems correspond to the two water outflow types (drainage outflow and runoff by saturation on fields with installed drainage systems). Finally, for each of the twelve modeling tasks, parameter tuning of the machine learning algorithms (linear regression, polynomial regression, regression trees, model trees, and bootstrap sampled ensembles of regression and model trees) was performed, resulting in over 2000 experiments (runs of the algorithms).

For the purpose of our data analysis, we assembled the dataset on water outflow, which yields one dataset for drainage outflow and one for runoff by saturation water outflow on fields with drainage systems. The independent variable set is the same for both regression problems: runoff by saturation and drainage outflow (Table 8.1).

The datasets comprise meteorological measurements, agricultural practices and crop management, and water outflows records. All data has been collected on a daily basis. From this, we have expanded the range of independent variables to be used for better description of the outflow process, as described below. The datasets do not include data about the soil content and texture, since we aim to learn models which perform well and best predict water outflows only from data that are permanently monitored (e.g., weather

Variable	Description
Temp	Average air temperature for the day of measurement [°C]
TempA$\boldsymbol{x}$	Average air temperature for the day of measurement and $\boldsymbol{x}$ days before, where $\boldsymbol{x}$={1, 2, 3, 4, 5} [°C]
TempN$\boldsymbol{x}$	Average air temperature for the $\boldsymbol{x}$-th day before the measurement, where $\boldsymbol{x}$={1, 2, 3, 4, 5} [°C]
Rainfall	Cumulative rainfall for the day of measurement [mm]
RainfallA$\boldsymbol{x}$	Cumulative rainfall for the day of measurement and $\boldsymbol{x}$ days before, where $\boldsymbol{x}$={1, 2, 3, 4, 5} [mm]
RainfallN$\boldsymbol{x}$	Cumulative rainfall for the $\boldsymbol{x}$-th day before the measurement, where $\boldsymbol{x}$={1, 2, 3, 4, 5} [mm]
Evp	Cumulative evapotranspiration for the day of measurement [mm]
EvpA$\boldsymbol{x}$	Cumulative evapotranspiration for the day of measurement and $\boldsymbol{x}$ days before, where $\boldsymbol{x}$={1, 2, 3, 4, 5} [mm]
EvpN$\boldsymbol{x}$	Cumulative evapotranspiration for the $\boldsymbol{x}$-th day before the measurement, where $\boldsymbol{x}$={1, 2, 3, 4, 5} [mm]
Irrigation	Cumulative irrigation for the day of measurement [mm]
IrrigationA$\boldsymbol{x}$	Cumulative irrigation for the day of measurement and $\boldsymbol{x}$ days before, where $\boldsymbol{x}$={1, 2, 3, 4, 5} [mm]
IrrigationN$\boldsymbol{x}$	Cumulative irrigation for the $\boldsymbol{x}$-th day before the measurement, where $\boldsymbol{x}$={1, 2, 3, 4, 5} [mm]
Crop	Crop present on the field at the day of measurement
CDCoef	Crop development coefficient for the day of measurement
Season	Weather season {*Autumn-winter, spring or summer*}
Days	Num. of days since the beginning of the campaign (*1st September*)

Table 8.1: The variables for modeling drainage outflow and runoff by saturation outflow.

conditions and agricultural practices).

Meteorological measurements include daily cumulative amounts of rainfall and evapotranspiration and the daily average, lowest and highest air temperature. We expanded this range of variables by including a history of up to 5 days (from the day under consideration), with both daily and cumulative values for rainfall and evapotranspiration (Figure 8.4). Similarly, we considered the average and daily averages for temperature. These are described in the first six rows of Table 8.1.

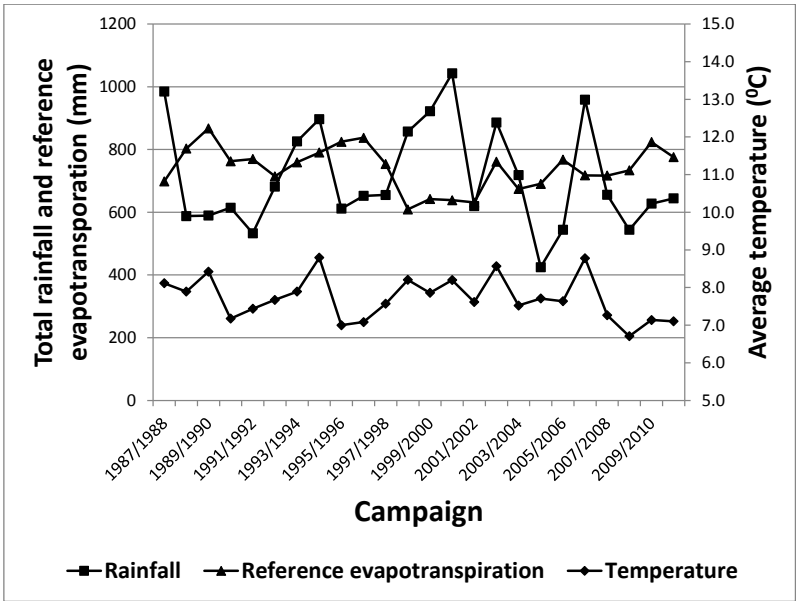


Figure 8.4: Annual variability of rainfall, reference evapotranspiration, and temperature within the selected case study for the study period (1987-2012).

The agricultural practices and crop management data cover the crop present on the field for each daily record. Crop management data were extended with the crop development coefficient, which incorporates crop characteristics and averaged effects of evaporation from the soil, and describes the crop development phase. It is represented as a numeric variable that takes values between 0.0 (initial phase under typical growing conditions) and 1.0 (late pre-harvesting phase). Furthermore, irrigation is represented with both daily records and a history of up to 5 days, as in meteorological measurements.

Weather seasons were described by one descriptive variable with values from the finite set of possible seasons (autumn–winter, spring, summer), and one numerical variable that represents the number of days since the start of the agricultural campaign (1st of September). A summary of the complete set of variables is given in Table 8.1. The total number of examples or instances in the dataset is approximately 90 000 with approximately 10 % of missing values in the target variable.

For the two modeling task (drainage outflow and runoff by saturation), we first perform preliminary data analysis to tune the parameters of linear regression, polynomial regression, regression trees, model trees, and bootstrap sampled ensembles of regression and model trees. Then, we compare the models learned with each tuned method in terms of their performance.

In linear regression, we tune the "Ridge" parameter, which regulates overfitting to the data by regularization and prevents unreasonably complex solutions/equations. In regression and model trees, we tune the parameter N_{min}. This parameter helps to keep the size of decision trees reasonable, which also prevents overfitting to the data. The

ensembles consist of unpruned decision trees that maximize variance in the predictions of the baseline models (regression and model trees) and overfit baseline models to a small portion of the instance space. We tune the parameter that controls the number of baseline models within an bootstrap sampled ensemble (N_{tree}). Summary of the parameter tuning experiments is given in Table 8.2.

	Parameter	**Range (step)**
Linear Regression	Ridge	$[10^{-10}, 10^{-3}]$ (10^{-1})
Polynomial Regression	Term Depth	[2-6] (1)
Regression Tree	Min. Number of Instances	[4-500] (1)
Model Tree	Min. Number of Instances	[4-500] (1)
Bagging (Regression T.)	Number of trees	5,10,25,50,75,100,250,500
Bagging (Model T.)	Number of trees	5,10,25,50,75,100,250,500

Table 8.2: Summary of parameter tuning experiments.

We evaluated the constructed models using separate pre-defined validation and test datasets, and randomly split train and test datasets by using 10-fold cross validation. The complete datasets are divided into three subsets: training, validation, and test data sets. The division was made in accordance with past campaigns. The training dataset consists of records from the campaigns 1987/1988–2004/2005, the validation dataset covers the campaigns 2005/2006–2007/2008, and the test dataset consists of the remaining campaigns, 2008/2009–2010/2011. The cross-validation is repeated ten times, due to the randomness included in the process of fold selection. The cross-validation does not consider the time component of the data, which can result in lower performance, but as shown later, in the next chapter, this does not influences overall performance. Such an approach results in a stable assessment of the expected performance of the models.

Performance is evaluated using three performance metrics: Root Mean Square Error (RMSE), Root Relative Square Error (RRSE) and Pearson's correlation coefficient (r).

8.3.1.2 Intensive periods

To build predictive models for the start and end of an intensive flow period, defined as the second task within the predictive layer, we used meteorological data and water outflow quantity. Data were labeled by experts from ARVALIS. The criteria used for estimating an intensive flow period for a drainage water pathway (further referred to as drainage period) are based on the quantity of cumulative drained water per campaign. In general, expert judgment of the start of a drainage period considers a threshold of the cumulative drainage outflow, which is not precisely specified but is in the range of 5–10 mm (Trajanov et al., 2015). In addition to the absolute cumulative drainage outflow, experts also take into account the temporal trend of the drainage outflow, which must be distinguished from the trend of the previous period. Therefore, we defined five different hypothetical thresholds of the cumulative drainage outflow: 5, 6, 7, 8, 9 and 10 mm, and used statistical measures to discover a rule from the available data regarding the possible thresholds of the cumulative drainage outflow since the start of a campaign (which influences the start of a drainage period). On the other hand, according to expert judgment, the drainage period ends when the weekly cumulative drainage outflow is below 1 mm and does not change in the next period. This work has been published in Trajanov et al. (2015).

In order to test the predefined hypothetical thresholds, we used the available measured data and calculated the cumulative drainage outflow since the start of a campaign, separately for each field and each year (1987–2012). Furthermore, we used the cumulative

drainage outflow to calculate the dates when the drainage period starts, according to the predefined hypothetical thresholds. These dates were later used for a statistical comparison with the dates provided by the experts.

First, we pre-processed the daily meteorological data, described above, for the period of 25 years (1987–2012). From these data, we calculated several new aggregated attributes and finally obtained a data set containing information for 9 fields over 25 years (two fields were excluded because they were not drained), resulting in 78 894 daily records (i.e. examples).

Attribute name	**Description**	**S1**	**S2**	**E**
Avg_ temp_ past_ 1-7_ days	For each day, the average air temperature in the past 7 days	A	A	A
Avg_ temp_ past_ 8-14_ days	For each day, the average air temperature in the week before	A	A	A
Avg_ temp_ next_ 1-7_ days	For each day, the average air temperature forecast for the next 7 days	A	A	A
Rainfall_ cumul	For each day, the cumulative rainfall from the beginning of the campaign	A	A	A
Tot_ rainfall_ past_ 1-7_ days	For each day, the total rainfall in the past 7 days	A	A	A
Tot_ rainfall_ past_ 8-14_ days	For each day, the total rainfall in the week before the last one	A	A	A
Tot_ rainfall_ next_ 1-7_ days	For each day, the total rainfall forecast for the next 7 days	A	A	A
Drainage_ cumul_ total	For each day, the total cumulative drainage since the beginning of the campaign	A		
Provided_ start_ of_ drainage	The dates of the start of a drainage period provided by the experts	DV	DV	
End_ of_ drainage	The dates of the end of a drainage period provided by the experts, estimated ex-ante			DV

Table 8.3: Attributes (A) and dependent variables (DV) included in the analysis of: S—start of a drainage period, E—end of a drainage period. S1 and S2 denote analysis using total drainage and meteorological attributes, and only meteorological attributes, respectively.

The attributes used for estimating the start and end of a drainage period are given in Table 8.3. They include average temperature and total rainfall, measured for last two weeks and forecast for the following week. Additionally, in another scenario, cumulative drainage and rainfall were considered.

The dataset described above consisted of daily data for each field and each year in the period 1987–2012 (Table 8.3). To estimate the start of a drainage period, we filtered the dataset and chose only the data calculated before and during the drainage period. All data collected after the end of the drainage period in an agricultural campaign were excluded from the data set. To estimate the start of the drainage period, we used meteorological

data (rainfall and temperature) and the total cumulative drainage since the beginning of a campaign. Estimation was done on a daily basis, attempting to answer the question whether the day under consideration is in drainage period or not.

We used three dependent variables (attributes) for the estimation of the start of a drainage period: (i) dates of the start of a drainage period provided by the experts (*Provided_ start_ of_ drainage*); (ii) dates of the start of a drainage period at 5 mm total cumulative drainage threshold; (iii) dates of the start of a drainage period at 10 mm total cumulative drainage threshold. The dependent variables are labeled daily and have two possible values: *no_ drainage*, if the drainage period has not started yet, and *start_ drainage*, if the drainage period has already started.

The analyses were divided into two parts. In the first part, we used only meteorological data and assumed that the cumulative drainage for the fields is unknown. In the second part of the analyses, besides the meteorological data, we also used the cumulative drainage since the start of a campaign as an attribute, but only when the target attribute was the date provided for the start of a drainage period. Namely, the calculated dates for the start of a drainage period were calculated from the cumulative drainage since the start of a campaign, so that the cumulative drainage could not be used as an independent attribute predicting the calculated start of a drainage period.

Three sets of experiments were carried out for each of the target attributes (*Provided_ start_ of_ drainage* and *End_ of_ drainage*), using three sets of attributes:

- only past data about temperature and cumulative rainfall (plus one additional experiment including cumulative drainage for the prediction of the provided date for the start of a drainage period),
- past and future data about temperature and rainfall (plus one additional experiment including cumulative drainage for the prediction of the provided date for the start of a drainage period),
- past and future data for temperature and cumulative rainfall (plus one additional experiment including cumulative drainage for the prediction of the provided date for the start of a drainage period).

In total, we obtained 12 models with different sets of attributes, for each target attribute.

Estimation of the end of a drainage period also uses the list of attributes given in Table 8.3. The target variable is set to be *End_ of_ drainage*, with two labels: *drainage* denoting that the drainage period is still active, and *end_ drainage* that means that the drainage period is finished.

We obtained several predictive models for the end of a drainage period, using two different combinations of attributes. The first uses only meteorological data from the past and the second one, also considers forecast meteorological data (for upcoming days).

Predictive models for the drainage period are built with J48, decision trees for classification that is evaluated using cross validation. Performance is evaluated using two performance metrics: precision and recall.

Overall, the predictive layer consists of models that used forecast meteorological data. When forecasts from the official meteorological station (Mètèo France) were not available for a longer period, we introduced a simple method for estimating a weather profile for a given campaign. Profiling the weather within a campaign is done using the k-Nearest Neighbor lazy method over data from previous 25 campaigns, where $k = 5$. In other words, the system tries to find five most similar campaigns in regard to weather profiles, and do a simple average of the weather data (temperature, rainfall and evapotranspiration) on a

daily basis. In this way, we obtain a vector of values that represents the weather profile across the whole campaign, and is used in models that require a longer period of weather forecast.

8.3.2 Diagnostic layer

In the absence of available measured data for agricultural practices and water movement for a specific region, it was necessary to make risk assessment that provides estimations without models built on data, in order to preserve the full functionality of the system. Therefore, a new layer was introduced - a diagnostic layer - used to diagnose the potential intensity of water outflow. It is implemented with DEX decision models built in accordance with expert knowledge available in the AQUANOUVAEU expert system. DEX decision models were built in collaboration with the experts from ARVALIS.

As previously stated, all water pathways are considered in risk assessment. Here, DEX decision models evaluates water outflow intensity.

Drainage outflow is implemented with both layers predictive and diagnostic, since available data are limited to a specific region. Therefore, we introduce risk assessment for drainage outflow based on a diagnostic layer. The DEX decision model (Figure 8.5) is described below.

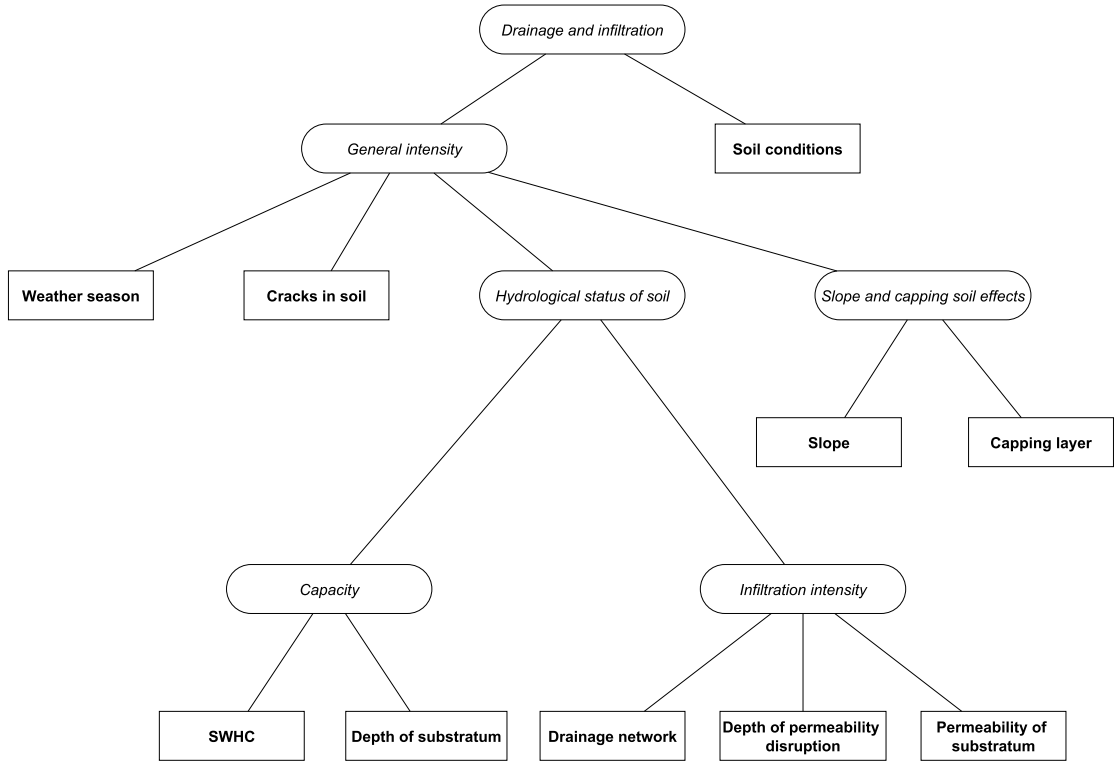


Figure 8.5: Structure of the drainage and infiltration outflow model. Bolded and non-bolded italic boxes represent basic and aggregated attributes, respectively.

The hierarchical structure of attributes (Figure 8.5) represents the breakdown of the process of drainage outflow intensity estimation into more and more specific factors that influence the estimation, represented by lower-level attributes. In total, there are 16 attributes, of which 10 are basic or input attributes and 6 are aggregated. Basic attributes appear as terminal nodes of the hierarchy and represent the input space of the model. Ag-

gregated attributes appear as internal nodes. They represent the intermediate or output space and depend strongly on lower-level basic and aggregated attributes.

Drainage outflow intensity is assessed on the basis of *general intensity* of water outflow that is tuned to local soil-specific conditions. *General intensity* of water outflow further depends on *hydrological status of the soil* and *effects by slope and capping layer*, which are tuned by season and the possibility of having cracks in the soil. In the model, this is reflected in the third level of the hierarchy, where two aggregated attributes are connected with two basic attributes that correspond to tuning to out of the box specifics that can influence the general intensity flow.

Hydrological status of the soil is composed of two factors: *capacity of the substratum* and qualification of the soil ability to allow *water infiltration* through the substratum, while *slope and capping layer effects* are affected by average field slope and the presence of a capping layer on top of the soil.

Capacity of substratum is based on decomposition into soil water holding capacity (SWHC) and depth of substratum, and *water infiltration* is again a composition of a presence and efficiency of a drainage system (network), depth of permeability of disruption and quantitatively described permeability of the substratum.

Attribute	Scale
Drainage and infiltration	**Very high**; High; Medium; Low; Very low; ***No***
General intensity	**Very high**; High; Medium; Low; Very low; ***No***
Weather season	**Autumn-Winter**; Spring; ***Summer***
Cracks in soil	**Yes**; ***No***
Hydrological status of soil	**Very high**; High; Medium; Low; Very low; ***No***
Capacity	**Low**; Medium; ***High***
SWHC	**<120**; ***>120***
Depth of substratum	**0-40**; 40-80; ***>80***
Infiltration intensity	**No**; Very low; Low; Medium; High; ***Very high***
Drainage network	**No**; Poor; Moderate; ***Well***
Depth of permeability disruption	**0-40**; 40-80; ***>80***
Permeability of substratum	**No**; ***Yes***
Slope and capping effects	**Very high**; High; Medium; Low; Very low; ***No***
Slope	**0-2%**; 2-5%; 5-10%; ***>10%***
Capping layerl	**No**; Very low; Low; Medium; ***High***
Soil conditions	**Sand, Gravel and Stones**; ***other***

Figure 8.6: Value scales of attributes in the DEX model for estimating drainage and infiltration outflow intensity.

Attribute value scales are different at different levels in the hierarchy, but all attributes can be described with nine different scales (Figure 8.6). Basic attributes differentiate eight value scales, while aggregated ones share one value scale. Each value scale (out of eight) represents appropriate description of basic attributes. The one that is shared among all aggregated attributes (including output) takes six values: *Very high*, *High*, *Medium*, *Low*, *Very low*, *No*. *Very high* takes place when the described attribute is at maximum level, while *No* is used when the setting is not observed or is quantitatively equal to 0.

The drainage outflow DEX model is the same as for the infiltration water pathway, since both pathways share the same properties and in fact are similar. Drainage outflow is considered artificial due to human intervention on the field, while infiltration is considered natural water pathway. The only difference among both pathways in regard to the model is the *Drainage network* attribute. If the value is *No*, the model estimates infiltration water pathway intensity, otherwise drainage outflow.

Istok and Kling (1983) stated that by introducing a tile-drainage system the water flow rates of runoff by saturation decreased by 70 %. Hence, runoff by saturation is assumed to

be complementary water pathway to drainage outflow (where applicable) and as a natural process is described with the same factors that influence its appearance. Therefore, the DEX model for runoff by saturation shares the same structure and hierarchy with drainage outflow, but differs in utility tables that describe aggregation decision rules among basic and aggregated attributes.

Surface runoff on capping soil and simple surface runoff are described as a similar water pathway that is caused by short-term rainfall events or storms. Surface runoff on capping soil is applicable only when the soil is characterized with a capping layer that reduces water infiltration, otherwise the experts characterize a flow as simple surface runoff. Both water pathways are applicable during spring and summer intensive rainfall events.

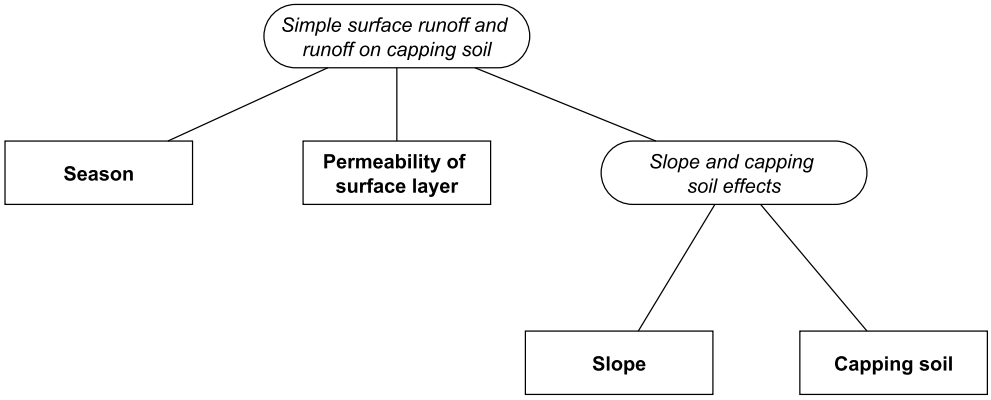


Figure 8.7: Structure of the simple surface runoff and runoff on capping soil model. Bolded and non-bolded italic boxes represent basic and aggregated attributes, respectively.

The hierarchical structure of attributes (Figure 8.7) is simpler here, indicating the breakdown of the process, which is influenced by several strong factors. In total, there are six attributes, of which four are basic or input attributes, one is an intermediate aggregated attribute and one an output aggregated attribute.

Simple surface runoff and runoff on capping soil intensity is assessed on the basis of *effects by slope and capping layer*, the value of which is corrected by weather season and level of permeability of the surface layer. Furthermore, *effects by slope and capping layer* is composed of two factors: slope and presence of capping layer, which theoretically define the capability of the soil to infiltrate a large amount of water. With reduced capability, surface runoff flow appears either by dominated slope or permeability disruption by the capping layer on the surface of the soil. Significant distinction between two types of surface runoff is made by the presence or absence of a capping layer on the surface of the soil.

Attribute value scales are different at different level in the hierarchy, but all attributes can be described with a total of five value scales (Figure 8.8). Basic attributes do not share the same value scale, but, as before, aggregated attributes share the same value scale. The former value scales represent appropriate description of the basic attribute, while the latter take six values: *Very high*, *High*, *Medium*, *Low*, *Very low*, *No*. With *Very high*, the model emphasizes the maximum level of the described factor's value, either intensity of surface runoff or effects by slope and capping layer. The *No* value emphasizes the opposite: total lack of water flow or no effects from slope and capping layer in regard to appearance of water flow.

Attribute	Scale
Simple surface runoff and runoff on capping soil	**No**; Very low; Low; Medium; High; ***Very high***
Season	**Spring**; Autumn-Winter; ***Summer***
Permeability of surface layer	**Low**; ***Medium and High***
Slope and capping effects	**Very high**; High; Medium; Low; Very low; ***No***
Slope	**0-2%**; 2-5%; 5-10%; ***>10%***
Capping soil	**No**; Very low; Low; Medium; ***High***

Figure 8.8: Value scales of attributes in the DEX model for estimating simple surface runoff and runoff on capping soil intensity.

8.3.3 Ex-ante risk assessment

Ex-ante risk assessment contains models that map a predicted or diagnosed state of the world $s_{t'}$ to the level of risk of pollutants' transfer in a water pathway. The type of model or function we used to do the mapping from the input to output space strongly depended on the kind of layer we used previously, for describing the state of the world $s_{t'}$. If a predictive layer was used, a predictive model was applied as well in order to assess the risk of pollutants' transfer; otherwise, a simple linear function was used to map the intensity of water outflow from input to output.

For the purpose of learning predictive models for ecological risk assessment, only data for outflows from the drainage system were considered. Comparing these data with data collected on surface runoff by saturation, they have much higher variability in terms of both occurrence and intensity and are, for this reason, much less suitable for further analysis.

For each application of an active ingredient in a field (one example in the dataset), a list of descriptive agro-environmental attributes were derived from a 12-month history and forecast, grouped into the following time periods: 1 week, 2 weeks, 1, 3, 6 and 12 months before and after the day of application. Attributes included are average temperature, cumulative rainfall and cumulative drainage. We also used data about the previous, current and next crop on the field, the chemical properties of the active substance applied, such as *PNEC*, *KOC* (soil adsorption coefficient), and *DT50* (a measure of the amount of time it takes for 50 percent of the compound to disappear from the soil or water by degradation), and the number of months between the application of the active substance on a field and the first sampling of drainage water from that field. Cumulative drainage and first sampled drainage outflow are later provided from the previously described predictive layer which improves the knowledge about possible outflow, as well as estimated dates of intensive flow periods.

At first, the input space was limited to a small number of active ingredients, namely, four chemical compounds: diflufénical, isoproturon, glyphosate and bentazone. Later, all available data were used, which include 24 active ingredients (Figure 8.9).

For this task, a random forest with classification trees was employed with a precedence step of parameter tuning. Different combinations of agricultural and climatic variables and different settings of model parameters (number and depth of trees in the random forest and cost functions defining the cost of misclassifying a 'RISKY' example) were considered. The different combinations of attributes and parameter settings resulted in a total number of 1400 experiments.

The experimental setup yields a multi-dimensional matrix of model performance, providing a wide range of accurate models, and possible trade-offs as well. Relying on expert judgment, the set of independent variables has been limited to the following:

- dose of the active ingredient applied on the field (g/ha),

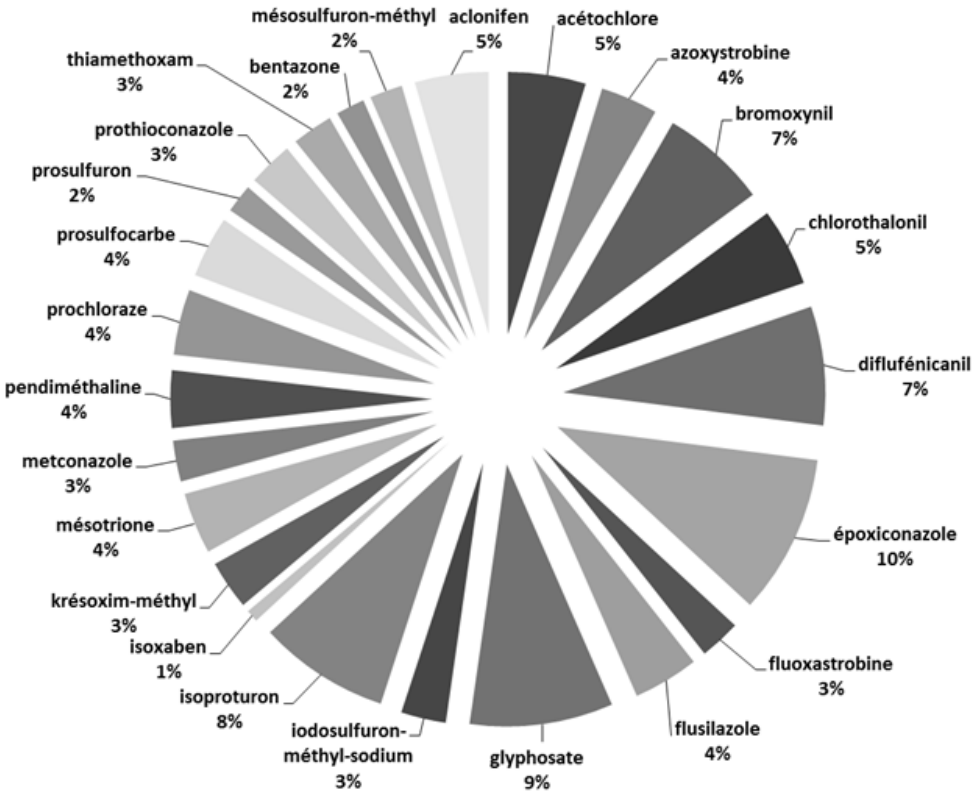


Figure 8.9: Data distribution by active ingredients. Total of 24 active ingredients considered.

- DT50 of the active ingredient (a measure of the time it takes for 50 % of the parent compound to disappear from the soil or water by degradation),
- number of weeks between the application of an active ingredient and the first sampling of drainage water,
- qualitative closeness of intensive flow periods after application of the active ingredient,
- current crop on the field,
- previous crop grown on the field,
- next crop that is planned in crop rotation,
- cumulative rainfall in the past week, two weeks, one month and three months (mm),
- cumulative rainfall forecast for the next one and two weeks (mm),
- risk of water pollution after application of an active substance as a target variable ($RISKY$ or NOT_RISKY).

The data available for training a model are imbalanced in favor of the NOT_RISKY class (Figure 8.10). Therefore, the learning process was wrapped with cost-sensitive learning by introducing a cost matrix, where the minority ($RISKY$) class has been penalized by increasing the number of its examples with random sampling, as described in Section 5.1.5. This approach forces the learning process to be fully focused on the $RISKY$ class and minimize wrong classification into it, as much as possible. The cost matrix has been tuned starting with arbitrary lower costs.

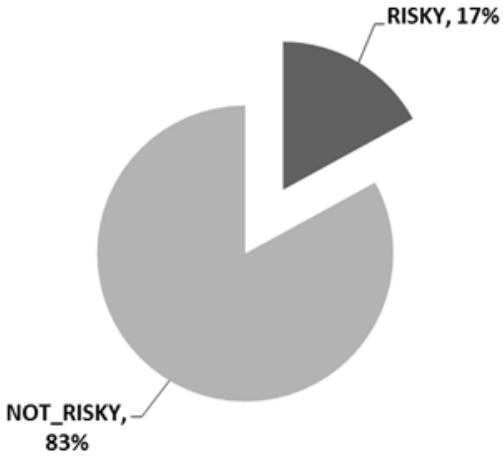


Figure 8.10: Class attribute distribution.

With the defined set of descriptive attributes and varying model parameter settings: number of trees (5, 10, 20, 50 and 100), depth of trees (3,4,5 and unpruned) and cost matrix values (5 %,10 %,15 %,20 % and 30 %), the experimental setup limited the number of output models to a hundred.

Evaluation of the models learned was done with precision and recall performance measures, where recall of the $RISKY$ class has been pushed to the maximum possible bounds, without significant degradation of precision for the same class. In other words, the goal was

to correctly predict as many of the risky applications of active ingredients (best possible recall for the RISKY class) without increasing the number of misclassified examples from the NOT_RISKY class (obtain a good enough precision for the $RISKY$ class, and recall and precision for the NOT_RISKY class). This was done by reviewing a precision-recall curve and a ROC curve and finding the trade-off point that satisfies the level of both precision and recall, as explained in the results.

Ex-ante risk assessment with a diagnostic layer is a simple function that maps estimated intensity values without any transformations. The set of possible outputs χ is a discrete finite-valued set:

$$\chi = \{Very\ high,\ High,\ Medium,\ Low,\ Very\ low,\ No\}. \tag{8.5}$$

8.4 Risk Management

The goal of the risk management module is to evaluate and compare the various alternative mitigation measures that can reduce the risk of pollution assessed in the previous step, to the accepted level defined in EU Directives and Regulations. The methodological framework employs alternative evaluation and sorting of alternatives, choice set selection and alternative ranking (Figure 8.11).

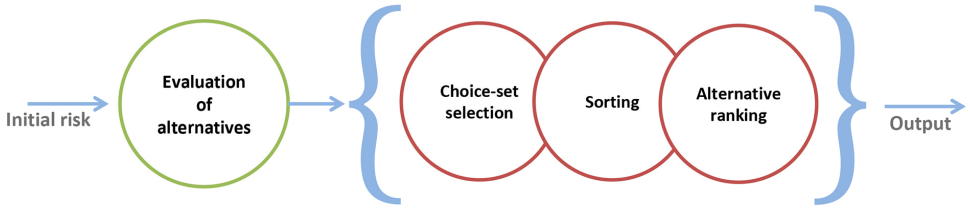


Figure 8.11: Risk management. Conceptual implementation design.

Evaluation and sorting of alternatives is implemented in one task using DEX decision models that map an alternative (mitigation measure) to a predefined class of $RISKY$ or NOT_RISKY. Such evaluated alternatives go through a selection process of a set containing only alternatives classified as NOT_RISKY, which are considered to reduce the assessed ecological risk. Finally, the choice set is ranked in accordance with complexity of mitigation measures, which results in an ordered set of mitigation measures, representing alternatives that may be used to protect water from pesticides applied for crop management purposes.

Preferences of evaluated alternatives are expressed with regard to the utility gained (i.e., whether the ecological risk is reduced or not), and the state of the world s_{t+1} that will take place at time $t+1$, upon implementation of the corresponding alternative over the state of the world $s_{t'}$.

The following is a description of each task that takes place within the risk management module.

8.4.1 Alternative evaluation and sorting

Evaluation of alternatives and their sorting consist of a total of 28 DEX decision models based on four different hierarchical structures. The difference between DEX decision

models that share the same structure lies in utility tables, where a combination of water pathway, crop and group of active ingredients defines the set of decision rules. The hierarchical structures, on the other hand, distinguish two types of mitigation measures with different sets of actions that can be performed on a field, per type of initially assessed ecological risk (whether the ecological risk is assessed using a predictive or diagnostic layer within the risk assessment). All models have the same output that sorts alternatives (mitigation measures) in two predefined classes: $RISKY$ and NOT_RISKY. The detailed presentation of all structures and utility functions (tables) is excluded from the thesis due to the confidentiality of the work, the rights to which belong to the ARVALIS institute.

The hierarchical structure of the DEX decision model that covers simpler sets of actions that can be performed on a field (short-term mitigation models), represents short-term only mitigation measures that are applicable before, during or after an application of an active ingredient and improve the state of the world s_{t+1} for a particular application (evaluated at time $t+1$). Such mitigation measures are applicable for the drainage discharge, infiltration and runoff by saturation water pathways.

The hierarchical structure of the attributes of short-term mitigation models (Figure 8.12) represents a breakdown of the mitigation factors into two branches: initially assessed ecological risk and influence of actions that define a mitigation measure. In total, there are 8 attributes, of which 6 are input and two are aggregated, including the output attribute. Input attributes appear as input nodes in the structure, including: *Initial risk*, *Crop* present on the field at time of application (t'), *Tillage* performed on the field, *Active ingredient*, *Dose* of the active ingredient planned to be applied, and *Time of application* (relative to the estimated or forecast intensive flow period). The aggregated attributes appear as internal nodes within the structure. There is one intermediate aggregated attribute *Effect*, which describes the possible effects of a combination of actions that can be performed. Such defined effect in combination with the initially estimated risk is propagated to the output where the overall efficiency of a mitigation measure is sorted in one of two predefined classes: $RISKY$ or NOT_RISKY.

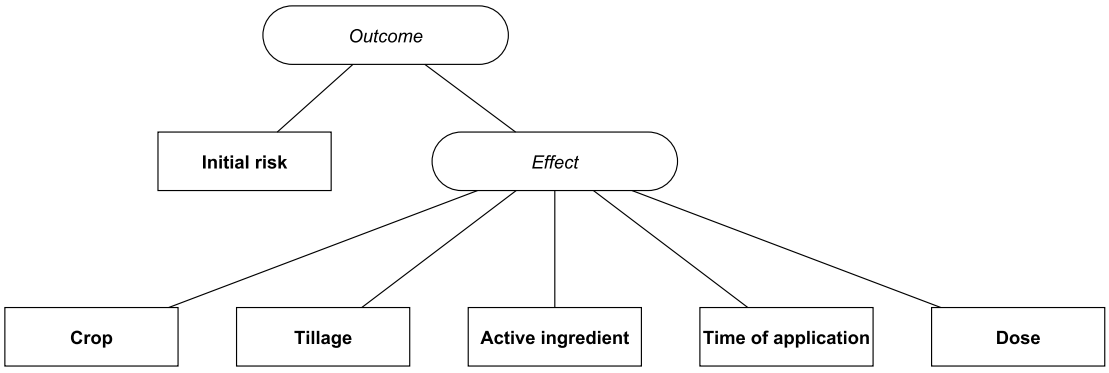


Figure 8.12: Structure of the short-term model. Bolded and non-bolded italic boxes represent input and aggregated attributes, respectively.

To summarize, the hierarchical structure of short-term mitigation models defines mitigation measures (as sets of actions - attributes) and expresses the potential influence that each mitigation measure has over initially estimated ecological risk (that represents the outcome of an implementation of the corresponding alternative a_t over the state of the world $s_{t'}$). In this structure (Figure 8.12), in the decomposition on the right (*Effect*), basic attributes explain the state of the world under consideration $s_{t'}$, while the input attribute

Initial risk, on the left lower-level, expresses the evaluation of the initial ecological risk. Furthermore, the right lower-level decomposition represents a mitigation measure (set of actions on a field). A subset of the input attributes is used for both describing the state of the world $s_{t'}$ and defining the set of actions (mitigation measure).

Attribute value scales are different at different levels in the hierarchy and for different combinations of crops and active ingredients (Figure 8.13, Figure 8.14). The *Tillage* and *Dose* input attributes have the same value scale in both types of hierarchical structure. The former is described with a binary scale that indicates whether tillage has been performed on the field or not $\{Yes, No\}$, while the latter has three values that qualitatively describe the dose of the active ingredient to be applied: *ARVALIS recommendation*, *Producer recommendation* or *Above producer recommendation*. The first one is provided by experts and is usually lower or equal to the producer's recommendation. Above producer's recommendation indicates overuse of an active ingredient, and such application is always evaluated as risky.

Attribute	Scale
Outcome	RISKY; *NOT_RISKY*
Initial risk	RISKY; *NOT_RISKY*
Effect	Increase transfer; *Decrease transfer*
Crop	
Tillage	No; *Yes*
Active ingredient	
Time of application	Close_WDP; During_WDP; *Before_WDP*
Dose	Producer recommendation; Above producer recommendation; *ARVALIS recommendation*

Figure 8.13: Value scales of attributes. Short-term model for predicted initial risk (output from predictive layer).

Attribute	Scale
Outcome	RISKY; *NOT_RISKY*
Flow intensity	Very high; High; Medium; Low; Very low; *No*
Effect	Increase transfer; *Decrease transfer*
Crop	
Tillage	No; *Yes*
Active ingredient	
Time of application	Close_WDP; During_WDP; *Before_WDP*
Dose	Producer recommendation; Above producer recommendation; *ARVALIS recommendation*

Figure 8.14: Value scales of attributes. Short-term model for flow intensity as initial risk (output from diagnostic layer).

Similarly, *Time of application* shares the same attribute value scale, but is further constrained by a combination of *Crop* and *Active ingredient*, since some are strictly limited to the winter or spring season, while others are applicable in both seasons. Again, the qualitative values expressed in the scales are relative to the observed or forecast intensive flow periods. During the winter season, possible values are *before winter flow period*, *during winter flow period* or *close to winter flow period*. Spring season water flows are characterized by *presence of spring flow period* or *absence of spring flow period*. Depending on the type of water pathway analyzed, drainage outflow/infiltration or surface runoff by saturation, the corresponding flow period is considered.

Initially assessed risk, as previously stated, can be derived from the predictive layer or the diagnostic layer of the risk assessment module. Therefore, two different scales are used in short-term models for the basic attribute: *Initial risk* or *Flow intensity*. The former has a scale defined as $\{RISKY, NOT\_RISKY\}$, while the latter coincides with the intensity of the estimated water outflow, $\{Very\ high, High, Medium, Low, Very\ low, No\}$.

Attribute value scales for crop and active ingredients differ with regard to their combination (Figure 8.15). The combination of these two input attributes may include a combination of a group of crops versus a group of active ingredients or a single crop versus a group of active ingredients. In both cases, active ingredients that belong to the same scale are considered possible replacements, and are applicable to the crop or group of crops in question.

In Figure 8.15, the matrix represents the possible combinations of crops and active ingredients. Active ingredients marked with a gray box for a particular crop (row of the matrix) belong to the single value scale in a short-term model. Crops that have the same *Active ingredient* attribute value scale are considered in the same short-term model and represent the *Crop* attribute value scale for the particular short-term model.

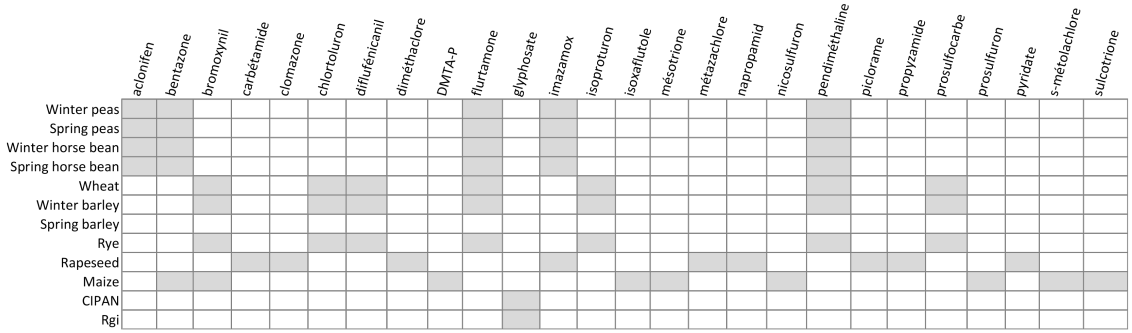


Figure 8.15: Value scales of attributes. Combinations of crops and active ingredients that appear as value scales in the short-term model.

The hierarchical structure of the DEX decision model that covers the remaining two water pathways covers medium- and long-term mitigation measures (further referred to as long-term mitigation models). Medium- and long-term mitigation measures provide actions, whose results are visible and effective in a longer time period. For example, the installment of buffer zones requires a longer time in order to become effective, an the same applies to retention and dispersion facilities on the edges of a field. Long-term mitigation models are valid for surface runoff on capping soil and simple surface runoff.

The hierarchical structure of the attributes of long-term mitigation models (Figure 8.16) describes the breakdown of mitigation factors into more and more partial factors that influence overall mitigation outcome going down through the lower-levels of the structure. In total, there are 35 attributes, of which 21 are input attributes, 12 are aggregated attributes (including the outcome) and 2 are linked attributes that inherit their value from the same input attributes.

On the first level, the structure is divided into two aggregated attributes: estimated ecological risk under effect of in-field management (*In-field management effects*) and possible mitigation with out-of-field management (*Out-of-field mitigation effects*). *In-field management effects* depends on two aggregated attributes that represent the effects of agronomic practices and in-field mitigation (*Agronomic effects* and *In-field mitigation effects*, respectively), accompanied with the estimated ecological risk from the previous module (*Flow intensity*). Aggregation at this level describes the general efficiency of in-field mitigation over different agronomic practices, which is limited to the ecological risk under consideration by the basic attribute *Flow intensity*.

Traversing the structure to the left, *Agronomic effects* is further broken down into the effects of a cultivated buffer and a double sowing practice, represented by an aggregated attribute *Cultivated buffers & double sowing effects*, and three input attributes: *Tillage*,

Roughness of seed bed and *Tramline management* that are binary-valued attributes corresponding to the presence or absence of a particular agronomic practice. Furthermore, *Cultivated buffers & double sowing effect* reflects the effects from sowing and crop related practices in the presence or absence of a landscape disruption.

In-field mitigation effects, on the other side, is decomposed into three types of issues and their effects on overall in-field mitigation: landscape disruptions and installed buffers related to such disruptions (*Overall buffer effects*), access area issues (*Access area effects*) and corner issues (*Corner effects*). Each of these issues and their effects is further decomposed into the presence of such issues and possible management measures regarding them, except for *Overall buffer effects*, which is decomposed recursively, in the same manner as before. It is dependent on slope disruption, thalweg disruption and downhill disruption. Accordingly, *Slope effect* is decomposed into presence or absence of such issues and the effect of different sizes of the infield buffer, *Thalweg effect* into presence or absence of a particular issue and effects of different sizes of the thalweg buffer, and *Downhill effect* into presence or absence of a downhill issue with effects of different sizes of the downhill buffer.

Out-of-field mitigation effects is a small decomposition that overall tunes the outcome when facilities are installed next to or near the edges of a field. It is composed of binary-valued basic attributes that indicate the presence or absence of edge works, retention and dispersion facilities and fascines.

Attribute value scales are different for the different types of attributes and their roles in the model (Figure 8.17). There are eight different qualitative scales. The simplest are the scales that describe the presence or absence of a particular subject, where presence is qualified as *Yes* and absence as *No*. Such a scale is assigned to the following input attributes: *Slope disruption*, *Thalweg*, *Double sowing*, *Cultivated buffers*, *Dammer inter row*, *Tillage*, *Roughness of seed bed*, *Tramline management*, *Downhill*, *Access area issues*, *Access area management*, *Corner issues*, *Corner management*, *Edge*, *Retention and dispersion facilities* and *Fascine*. Similarly, a binary-valued scale is assigned to the *Out-of-field mitigation effects* aggregated attribute (*Present*, *Not present*), with self-explanatory values. Aggregated attributes that express the effects of a particular action or issue are assigned the following three-valued scale: $\{Increase, No, Decrease\}$, except *Agronomic effects*, *In-field mitigation effects* and *Overall buffer effects*, which are expressed with $\{Increase, No, Low\ decrease, Medium\ decrease, High\ decrease\}$. Input attributes that specify the size of a particular buffer are expressed with $\{0\ m, 3\ m, 5\ m, 10\ m, 20\ m\}$. *In-field management effects* and *Flow intensity* are described with the following scale: $\{Very\ high, High, Medium, Low, Very\ low, No\}$, which expresses the level of an ecological risk estimated strictly with in-field management, and previously by the risk assessment module, respectively. Finally, the *Outcome* is expressed with a two-valued scale ($\{RISKY, NOT\_RISKY\}$) which estimates the ecological risk of actions performed as part of the mitigation measures.

Unlike the short-term mitigation model which considers all input attributes in the alternative construction, the long-term mitigation model considers a subset of the input attributes in order to construct a mitigation measure (alternative), while the rest are used to describe the state of the world $s_{t'}$. Thus, input attributes that express some part of the state of the world and cannot be changed are excluded from finding a new alternative. This subset consists of:

- slope disruption,
- thalweg,
- crop group,

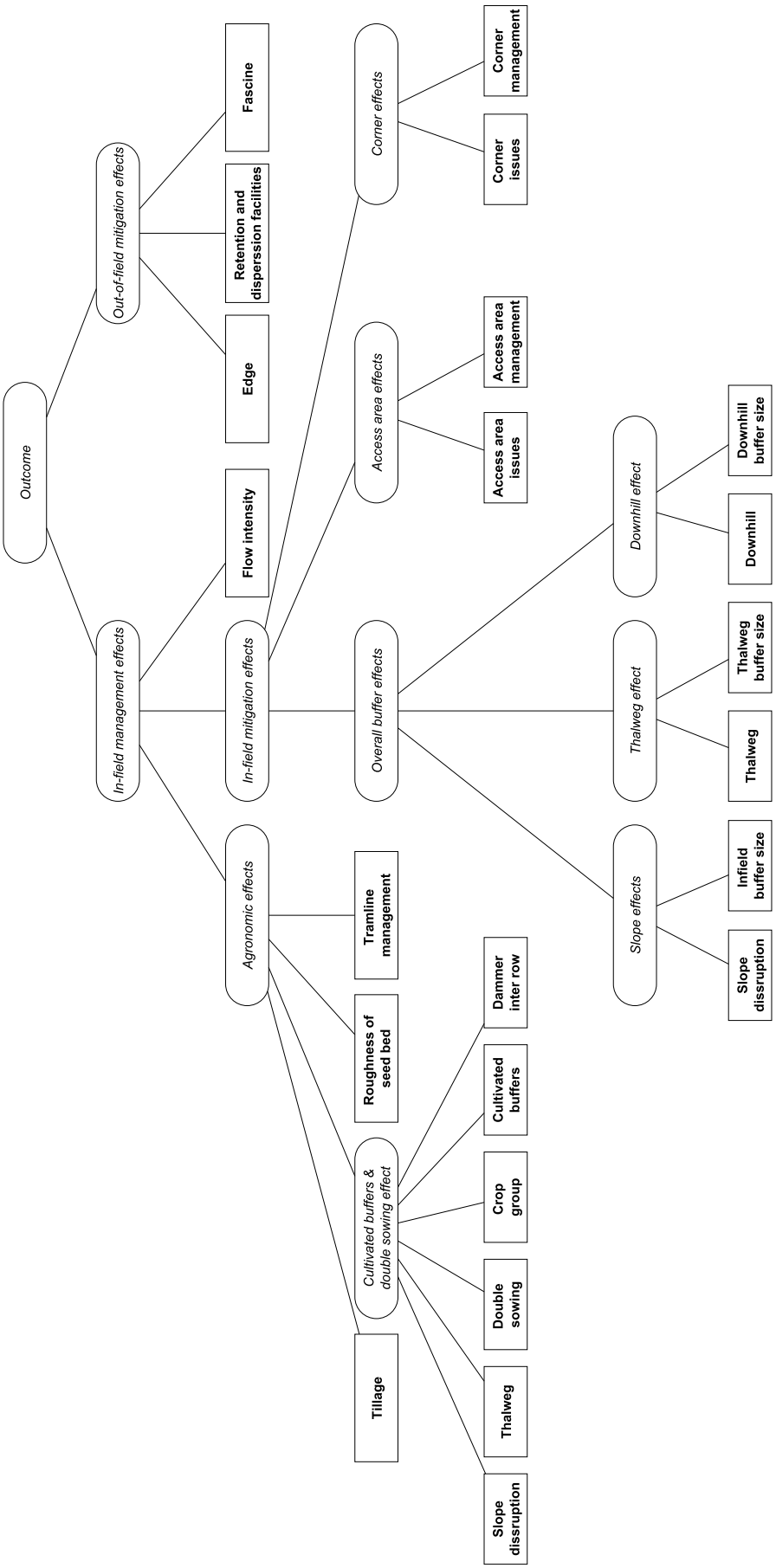


Figure 8.16: Structure of the long-term model. Bolded and non-bolded italic boxes represent input and aggregated attributes, respectively.

Attribute	Scale
Outcome	RISKY; *NOT_RISKY*
In-field management effects	Very high; High; Medium; Low; *Very low*; *No*
Agronomic effects	Increase; No; Low decrease; Medium decrease; *High decrease*
Cultivated buffers & double sowing effect	Increase; No; *Decrease*
Slope dissruption	Yes; *No*
Thalweg	Yes; *No*
Double sowing	No; *Yes*
Crop Group	Other; Winter cereals; Spring crops; Perannual crops and patatoes
Cultivated buffers	No; *Yes*
Dammer inter row	No; *Yes*
Tillage	Yes; *No*
Roughness of seed bed	No; *Yes*
Tramline management	No; *Yes*
In-field mitigation effects	Increase; No; Low decrease; Medium decrease; *High decrease*
Overall buffer effects	Increase; No; Low decrease; Medium decrease; *High decrease*
Slope effects	Increase; No; Low decrease; *High decrease*
Slope dissruption	Yes; *No*
Infield buffer size	0m; 3m; 5m; 10m; *20m*
Thalweg effect	Increase; No; Low decrease; *High decrease*
Thalweg	Yes; *No*
Thalweg buffer size	0m; 3m; 5m; 10m; *20m*
Downhill effect	Increase; No; Low decrease; *High decrease*
Downhill	Yes; *No*
Downhill buffer size	0m; 3m; 5m; 10m; *20m*
Access area effects	Increase; No; *Decrease*
Access area issues	Yes; *No*
Access area management	No; *Yes*
Corner effects	Increase; No; *Decrease*
Corner issues	Yes; *No*
Corner management	No; *Yes*
Flow intensity	Very high; High; Medium; Low; Very low; *No*
Out-of-field mitigation effects	Not present; *Present*
Edge	No; *Yes*
Retention and disperssion facilities	No; *Yes*
Fascine	No; *Yes*

Figure 8.17: Value scales of attributes. Decision model for long-term mitigation measures.

- downhill,
- access area issues,
- corner issues,
- flow intensity.

The rest of the input attributes are included in the subset, from which mitigation measures (alternatives) are constructed.

8.4.2 Choice set selection

Choice set selection is part of the risk management module of the methodological framework, used to select most preferable alternatives from all available. This step is mandatory for the case-study implementation of the framework. The decision problem requires finding a solution that will reduce the ecological risk of pollutant transfer in water bodies. The solution consists of a set of alternatives (mitigation measures) that are evaluated to successfully reduce ecological risk. We therefore look for the sub-set of all alternatives that are evaluated as not risky with regard to the state of the world $s_{t'}$.

The choice set $C_{\succeq}$, is thus the subset of all alternatives, the outcome of which is NOT_RISKY:

$$C_{\succeq} = \{a : a \in A \wedge f(a, s_{t'}) = NOT\_RISKY\}, \tag{8.6}$$

where $s_{t'}$ is the state of the world estimated to take place at the time of decision implementation.

In addition, this set can be filtered in accordance with individual preference. Preferences are expressed with regard to the outcome and state of the world s_{t+1} that would take place at time $t+1$. Thus, 8.6 can be updated to take preferences into account:

$$C_{\succeq} = \{a : a \in A \wedge f(a, s_{t'}) = NOT\_RISKY \wedge pref(t+1) = u'(f(a, s_{t'}), s_{t+1})\}, \quad (8.7)$$

The defined choice set $C_{\succeq}$ is an induced choice set, since the selection strongly depends on the predefined preference relation ($NOT\_RISKY \succeq RISKY$).

8.4.3 Alternative ranking

The alternative ranking task provides an ordered set of alternatives in accordance with their complexity. The complexity of an alternative is described as complexity of the mitigation measures to be applied on the field and their time frame of efficiency (whether short-term or long-term actions are proposed). In collaboration with experts from ARVALIS, the complexity of alternatives was modeled with a linear model, the outcome of which is considered in the final alternative ranking. The outcome of a linear model is a real number. This property guarantees that alternative ranking will result in a totally ordered set of alternatives, and that the preference relation ($\succeq$) will hold:

$$a_1 \succeq a_2 \iff \phi(a_1) \geq \phi(a_2), \forall (a_1, a_2) \in A \times A, \quad (8.8)$$

where ϕ is a linear model:

$$\phi : a \to \mathbb{R}, a \in A. \quad (8.9)$$

The general form of the model is defined as:

$$\phi(a) = \sum_{g_{ai} \in G_a} c_{partial}(g_{ai}), \quad (8.10)$$

where G_a is the set of attributes from which the alternative a is defined, and C is a set of parameters that express the complexity of each attribute g_{ai}. An attribute corresponds to an action that can be performed on an agricultural field.

Due to the existence of two different DEX decision models for alternative evaluation, the implementation of the framework differentiates two different models for calculating the complexity of a given alternative: short-term and long-term mitigation models.

In the former, an alternative $a \in A$ is defined with *Crop*, *Tillage*, *Active ingredient*, *Time of application* and *Dose* attributes, which corresponds to the following set of parameters C:

$$G_a = \{g_{a\_crop}, g_{a\_tillage}, g_{a\_ingredient}, g_{a\_time}, g_{a\_dose}\} \quad (8.11)$$

$$C = \{20, 10, 5, 1, 2\}. \quad (8.12)$$

The set of parameters reveals that changing the time of application is the least complex action on a field, while change of crop on the field is the most complex action.

The long term mitigation model defines an alternative $a \in A$ with *Double sowing*, *Cultivated buffers*, *Dammer inter row*, *Tillage*, *Roughness of seed bed*, *Tramline management*, *Infield buffer size*, *Thalweg buffer size*, *Downhill buffer size*, *Access area management*, *Corner management*, *Edge*, *Retention and dispersion facilities* and *Fascine* attributes, which corresponds to the following set of parameters C:

$$G_a = \{g_{a\_double}, g_{a\_b\_cultivated}, g_{a\_dammer}, g_{a\_tillage}, g_{a\_seed\_bed}, g_{a\_tramline}, g_{a\_b\_infield}, g_{a\_b\_thalweg}, g_{a\_b\_downhill}, g_{a\_access}, g_{a\_corner}, g_{a\_edge}, g_{a\_retention}, g_{a\_fascine}\} \quad (8.13)$$

$$C = \{3, 3, 3, 10, 3, 3, 20, 20, 20, 20, 20, 50, 50, 50\}. \quad (8.14)$$

The set of parameters reveals that the least complex are attributes that represent actions required in the domain of crop management and sowing, while the most complex are actions that need to be performed out of field.

In both mitigation models, parameters that express complexity are estimated in accordance with expert judgment.

8.5 Graphical User Interface

The graphical user interface (GUI) is built in order to support easy usage of the built decision support system. It is built over a multi-platform infrastructure, which allows scalability and fault-tolerance. The design guides individuals through the complete process of scenario evaluation, where a scenario is a planned application of an active ingredient on a field, and its evaluation is defined as the complete decision support process that includes quasi ex-post risk analysis.

The starting point is the input form, where individuals describe the state of the field at the time of planned application of an active ingredient (Figure 8.18). The description is limited to easily-observable information like location of the field, the crop that will be present at the time of application of an active ingredient, the active ingredient, the dose and time of application. This information is later used in automatically collecting details about the soil and substratum properties.

Each GUI field in the input form is accompanied with a "balloon", which explains what the field means and what kind of information is required. Some "balloons" are also equipped with an image that gives a visual description of what the GUI field stands for.

Once complete information is provided, the system continues the scenario evaluation, which can be sent in the background or the progress can be observed in the foreground. A mitigation report is then generated, which includes all the necessary information regarding the outputs of both modules (risk assessment and risk management), accompanied with a graphical visualization.

First, the outcome of risk assessment is given, including the description of the state of the world in accordance with the predictive or diagnostic layer and the risk assessed from the given state of the world (Figure 8.19).

If the pollution risk is assessed to be over the acceptable or the tolerable level, the risk management part of the report exposes all possible solutions, from which a decision is to be made. The possible solutions come from the ordered set of mitigation measures (alternatives), which appears as outcome from the alternative ranking step within the risk management module (Figure 8.20). Using different colors, the system clarifies whether the proposed change is a recommendation, a requirement or just a note. Recommendations are related to the dosage of the active ingredient, while notes are shown when change of the time of application is not required, but if it is done, this will have no effect on the assessed risk or outcome of the proposed mitigation measure.

initially, the system shows the important information without bothering the user with complete details. However, it allows reviewing of the complete process of scenario evaluation through a separate part of the GUI mitigation report (Figure 8.21 and Figure 8.22). Mainly, the details report has the same format, except when a predictive layer is employed in risk assessment. In such a case, the predictions of drainage quantities are visualized per day, and if measured data are available, the details part also shows them on the predictions chart. Figure 8.22 shows the components where outcome of the predictive layer is visualized.

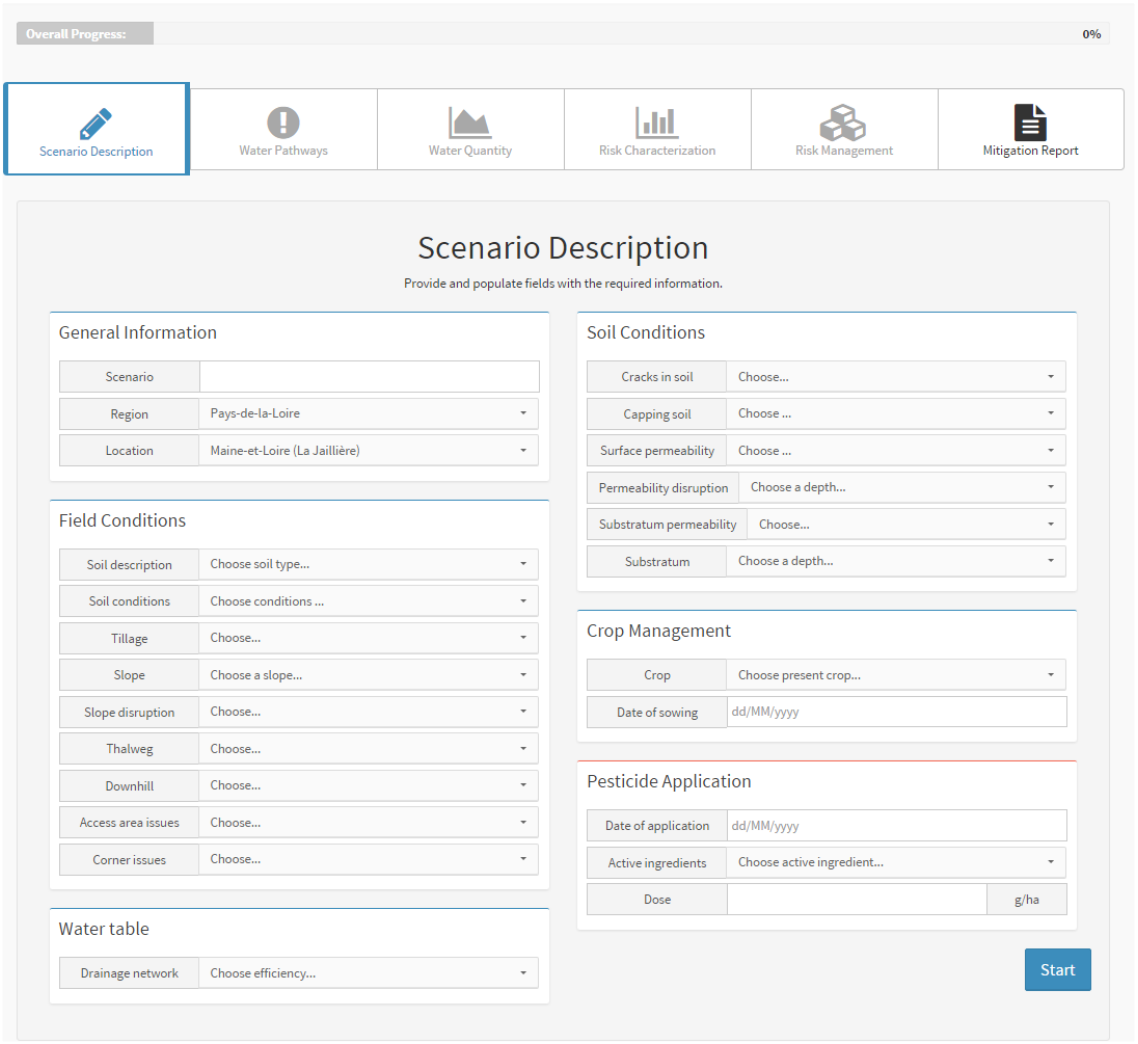


Figure 8.18: Graphical user interface. The input form where individuals describe the state of the field for planned application of active ingredients.

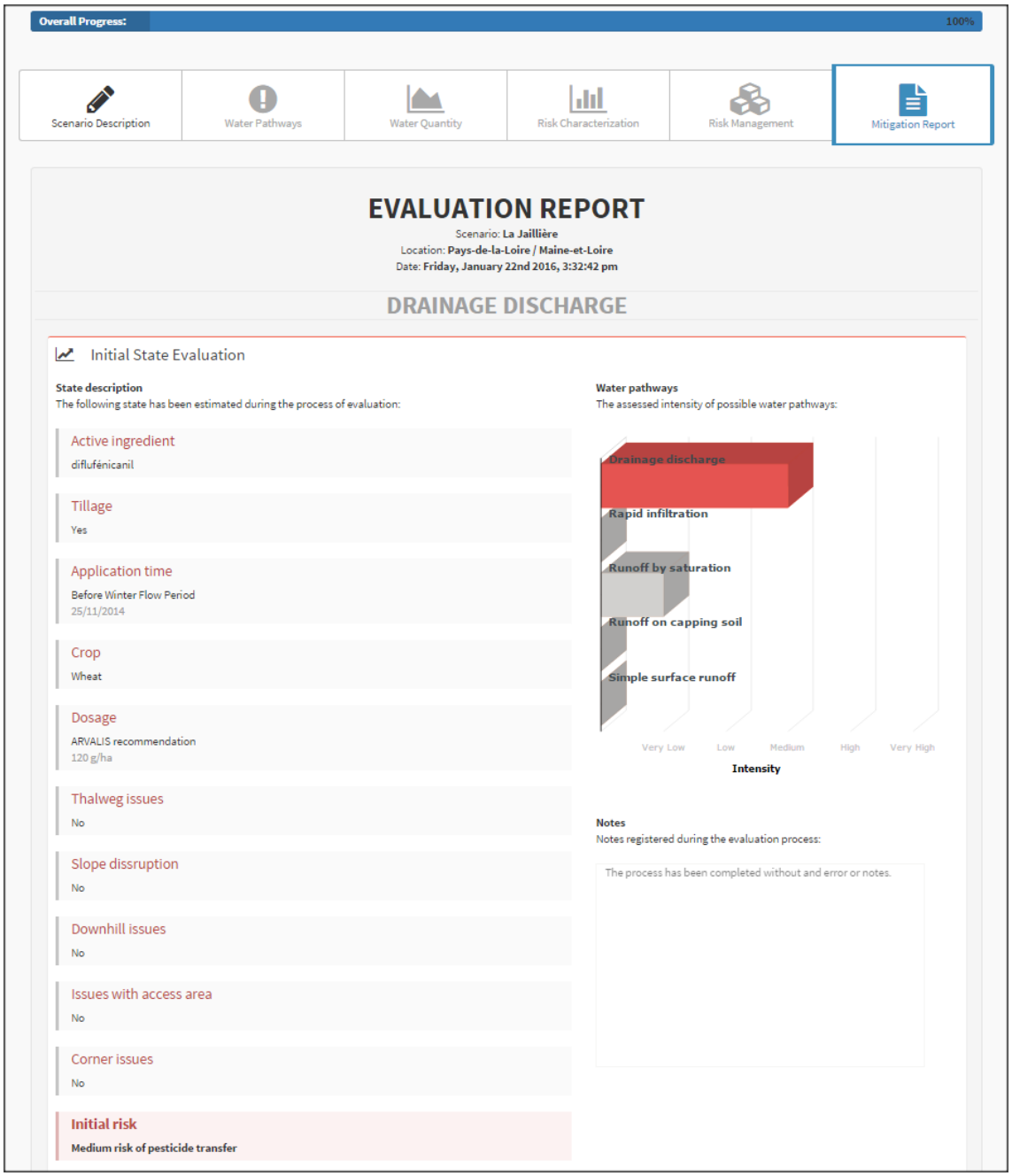


Figure 8.19: Graphical user interface. First part of the system's mitigation report, which presents the current state of the world and the outcome of risk assessment.

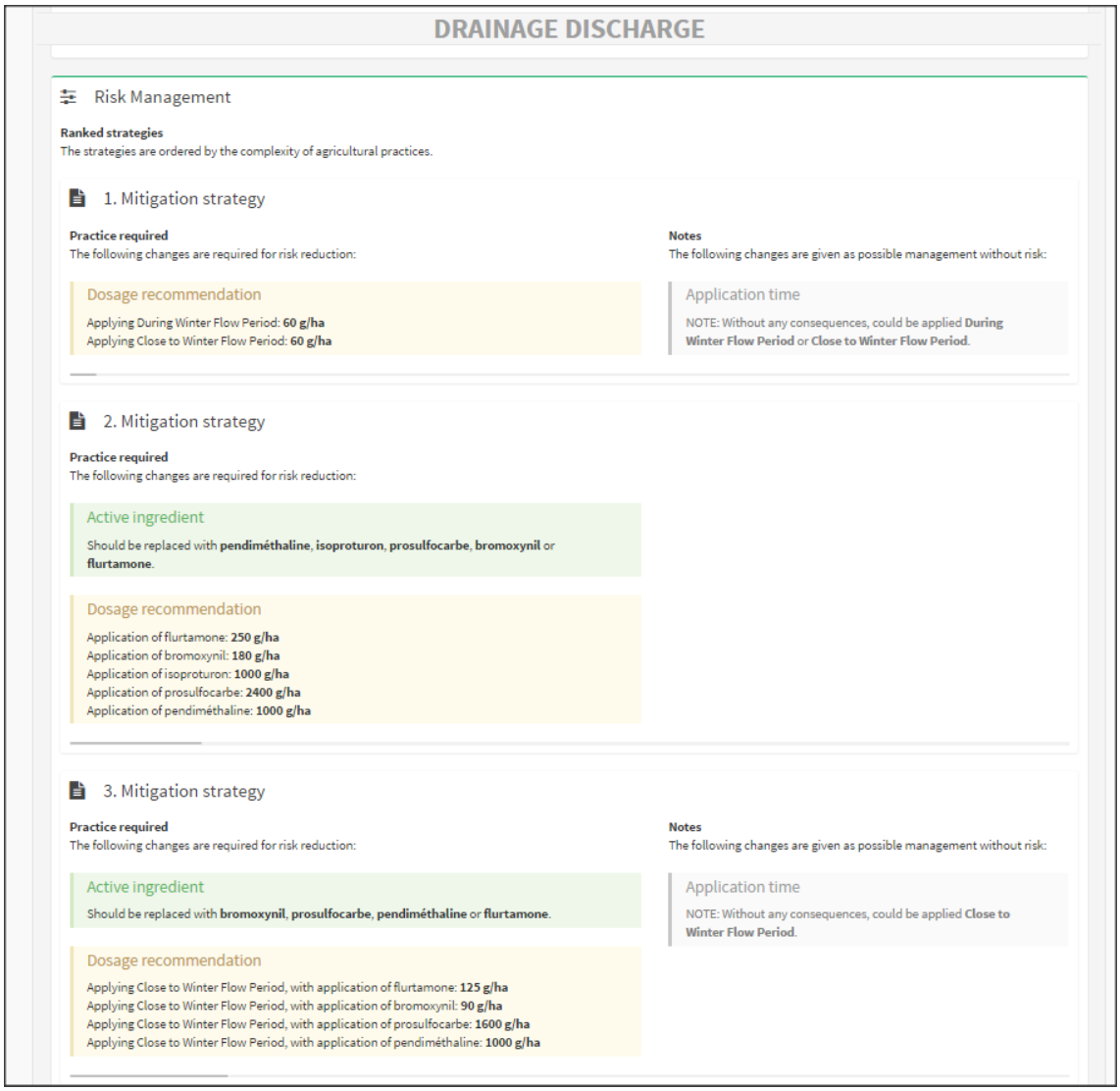


Figure 8.20: Graphical user interface. Risk management part of the system's mitigation report, which lists the ordered set of mitigation measures (outcome of the alternative ranking step within the risk management module).

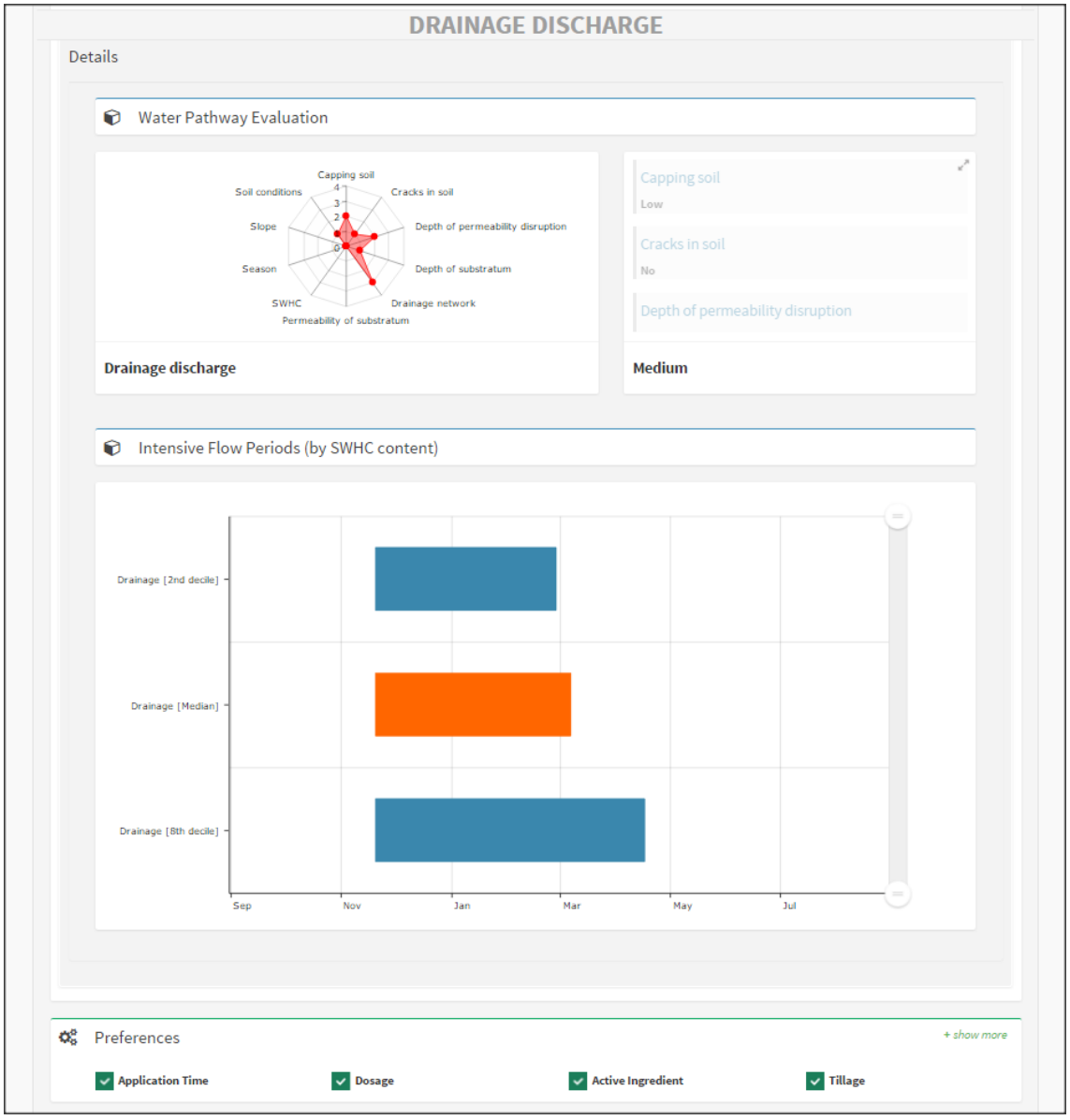


Figure 8.21: Graphical user interface. Detailed report of the steps performed with a diagnostic layer of the quasi ex-post risk analysis.

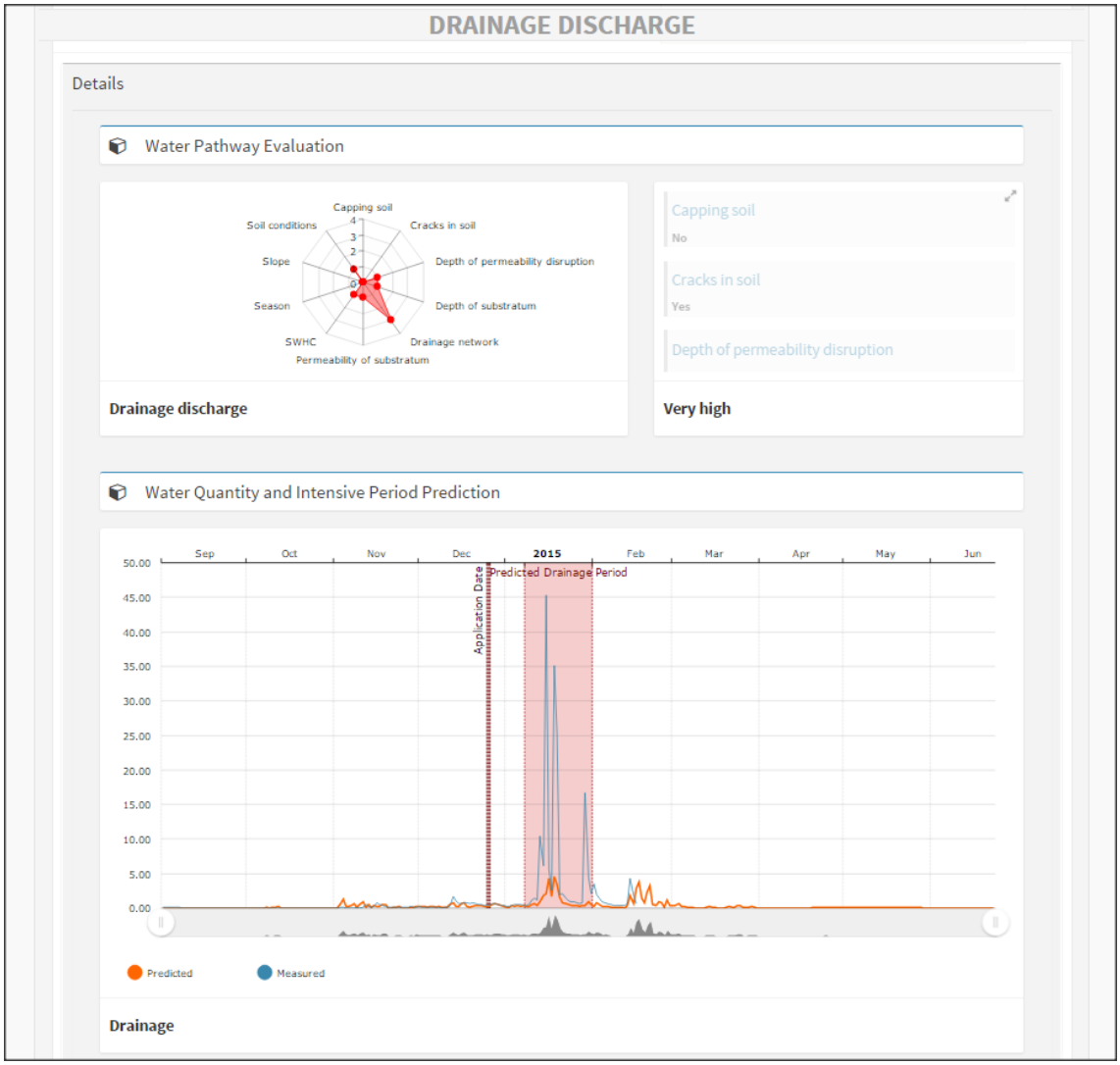


Figure 8.22: Graphical user interface. Detailed report of the steps performed with a predictive layer of the quasi ex-post risk analysis.

The described mitigation report is provided separately for the each water pathway. Mitigation measures are proposed for those pathways assessed as risky.

The system's integration with the GUI is a web-based software application, which is available on-line and can be accessed from anywhere. The evaluations are stored and can be later accessed for a performance evaluation or validation of the mitigation measures.

Chapter 9

Results and Evaluation

The effectiveness and efficiency of the framework implementation can be illustrated by a detailed analysis of performance of partial modules, as well as evaluation of the final results obtained with the implementation of quasi ex-post risk analysis. This chapter evaluates the performance of the built models, either predictive or decision models, and the results obtained from the system. First, risk assessment models are evaluated, including comparison with state-of-the-art models. Then, models from risk management are analyzed and, finally, the overall performance obtained with quasi ex-post risk analysis is presented.

9.1 Risk Assessment

As described in the previous chapter, the implementation of risk assessment includes a predictive layer, and risk assessment is then conducted ex-ante. This is applicable in scenarios that include analysis of drainage outflow and surface runoff by saturation in the regions where La Jaillière is representative of. Otherwise, the diagnostic layer is employed in order to improve the knowledge about the state on the field under consideration (state of the world).

9.1.1 Predictive layer

For the purpose of the predictive layer, we built predictive models for drainage outflow and surface runoff by saturation. Both are later compared with state-of-the-art models; drainage outflow is compared with the MACRO and the RZWQM model, while surface runoff by saturation is compared with the RZWQM only, since the MACRO model is not applicable for surface runoff water pathways. For the each type of water outflow, we first report the results of the step where the algorithms' parameters were tuned. Next, we compare the best performing models obtained by each of the methods described in the experimental design. Finally, we compare the best performing models with state-of-the-art models.

9.1.1.1 Drainage outflow

Each machine learning method has been used with various values of its parameters. With such a processing, we tuned the initial parameters of the methods, which improves the models' performance and handles the possible overfitting to the training data. Figure 9.1 shows the relation between parameter values and the performance of the models for each of the six types of models.

In the case of linear regression, values of the "Ridge" parameter smaller than 10^{-9} lead to models that are overfitted to the training data set and perform poorly on new, unseen

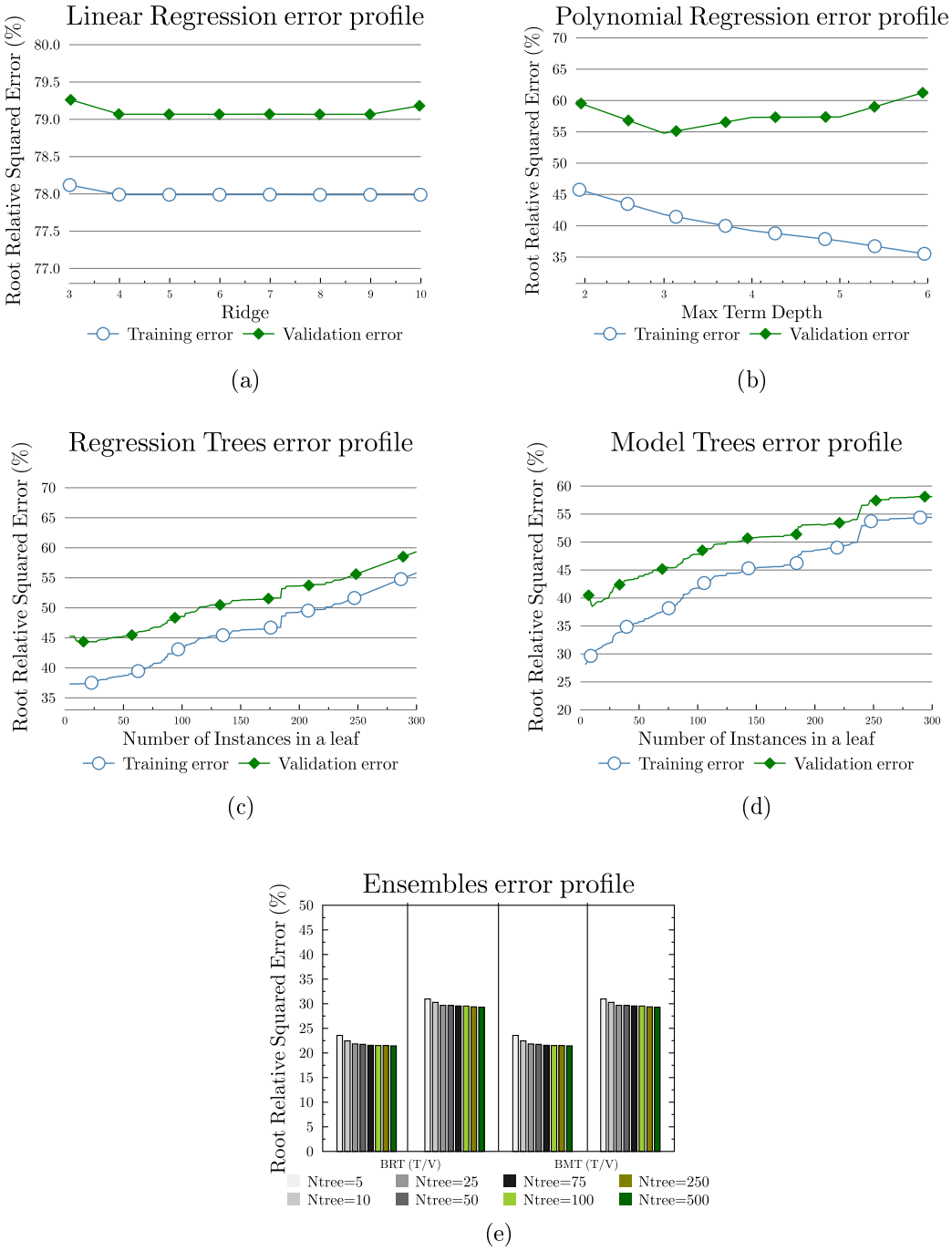


Figure 9.1: Error profiles resulting from tuning the parameters of each method used in the thesis, both for training and validation data: **a**) Linear regression performance for different values of the ridge parameter, i.e. 10^{-i}, where $i = \{3, 4, 5, 6, 7, 8, 9, 10\}$; **b**) Polynomial regression models with RRSE obtained by varying the term depth in the interval [2-6]; **c**) Regression tree performance for different values of the parameter N_{min}; **d**) Model trees performance for different values of the parameter N_{min}; **e**) Bagging ensembles of regression (BRT) and model trees (BMT) performance for different values of the N_{tree} parameter. T/V stands for Train and Validation data.

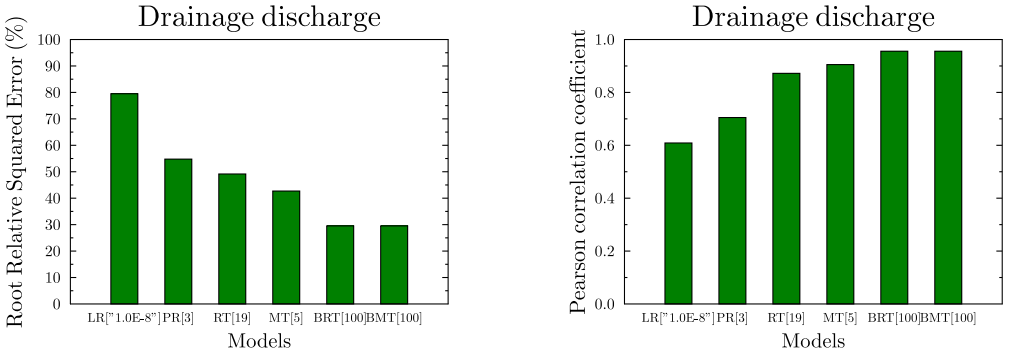


Figure 9.2: Performance of the best drainage outflow data mining models, over a validation dataset: **a**) Models' performances expressed with relative error (RRSE); **b**) Models' performances in terms of the Pearson correlation coefficient.

records. Values greater than 10^{-4} result in models that underfit the data. Therefore, the optimal range for the "Ridge" parameter is the interval $[10^{-4}, 10^{-9}]$, where the best value is 10^{-8} (Figure 9.1a).

Tuning the N_{min} parameter of the regression and model trees shows that the low values of 19 and 5 instances in the leaves are optimal for these methods, resulting in models with high performance (Figure 9.1c, 9.1d).

Tuning the ensembles, i.e. bagging of regression/model trees, includes tuning of the number of trees in ensembles of unpruned decision trees (N_{tree}). In such settings, we allowed each particular base model (regression or model tree) to overfit a particular sub-space of the instance space. On the other hand, by varying the N_{tree} parameter we estimate the optimal number of decision trees (base models) that correspond to the total of sub-spaces into which the instance space is divided. Figure 9.1e shows that the models learned with ensembles consisting of 100 regression or 100 model trees have best predictive performance, regarding performance and complexity. Namely, the performance of the models converges in a plateau which does not make significant improvements when the number of trees is further increased. Finally, the choice of the base model, regression or model trees, does not affect the performance of the ensembles.

Table 9.1 and Figure 9.2 show the RRSE, RMSE and Pearson correlation values for the best performing drainage outflow models. Figure 9.2 presents the overall performance over test data set, while Table 9.1 presents the model's performance for each data set, separately.

The ensembles learned with bagging of regression and model trees have the best performance (Figure 9.2). Furthermore, performance decreases slightly when applied on new, unseen data, as compared to performance on the training data set (Table 9.1). Namely, the RRSE shows that ensembles significantly improve the predictive performance of the learned models compared to the simple model, i.e. simple average of the target variable. The RMSE reveals the low deviation of the residual distribution (0.58 and 0.70 for validation and test set, respectively) compared to the standard deviation of the target variable (1.382 and 1.455 for the validation and test set, respectively). Finally, the correlation coefficient shows that the ensembles perform well in matching the trajectory of observed values for the target variable with the trajectory of predicted values.

The conclusions are further confirmed with the performance obtained by cross-validation,

		LR (10^{-8})	**PR** (*3*)	**RT** (*19*)	**MT** (*5*)	**BRT** (*100*)	**BMT** (*100*)
Training dataset	**Corr.**	0.63	0.76	0.93	0.96	0.98	0.98
	RMSE	1.62	1.56	0.78	0.59	0.45	0.45
	RRSE	77.99	41.79	37.46	28.30	21.50	21.50
Validation dataset	**Corr.**	0.61	0.77	0.89	0.93	0.96	0.96
	RMSE	1.57	1.05	0.88	0.74	0.58	0.58
	RRSE	79.07	54.77	44.32	37.43	29.50	29.50
Testing dataset	**Corr.**	0.61	0.75	0.87	0.90	0.93	0.93
	RMSE	1.56	0.99	0.94	0.82	0.70	0.70
	RRSE	79.50	46.9	49.15	42.7	36.60	36.60
Cross-validation	**Corr.**	0.61	0.76	0.90	0.93	0.95	0.95
	RMSE	1.52	1.51	0.85	0.70	0.61	0.61
	RRSE	79.14	41.79	44.21	36.46	32.01	31.97

Table 9.1: Summary of models' performance on each dataset for predicting drainage outflow. The values of the tuned parameters of the algorithms are given in brackets. *LR* stands for Linear Regression, *PR* for Polynomial Regression, *RT* for Regression trees, *MT* for Model trees, *BRT* for Bagging of Regression trees, and *BMT* for Bagging of Model trees.

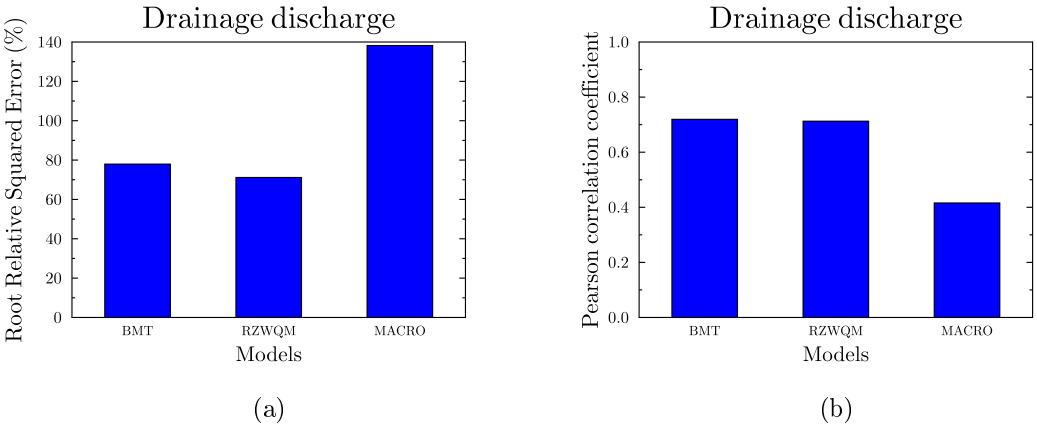


Figure 9.3: Comparison of the performances (RRSE and Pearson correlation) of the best data mining model (BMT - Bagging of Model Trees) for predicting drainage outflow with the performance of MACRO and RZWQM, over data collected in field T4 for the period 2008-2011.

the values of which do not differ from those obtained by time-based sampling of the training, validation and test sets (Table 9.1). Furthermore, the random sampling process reveals the difference among the best performing ensemble models. Bagging regression trees shows a higher variability in performance over ten different randomly sampled test datasets, compared to the bagging of model trees. Therefore, for further discussion we consider the model learned with bagging model trees as the best performing machine learning model.

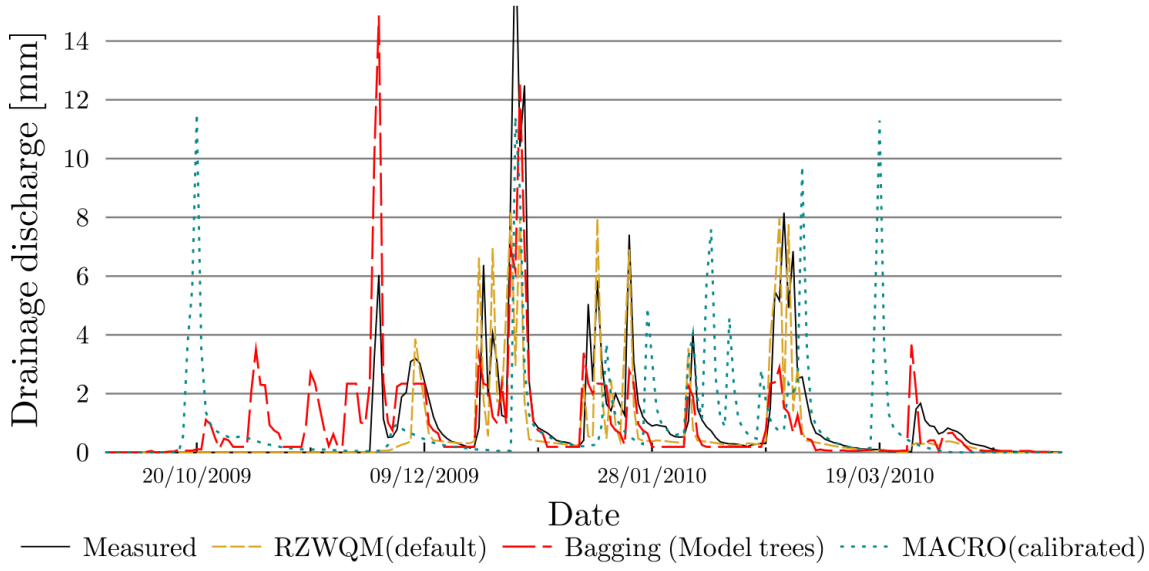


Figure 9.4: Simulations of the drainage outflow with the best data mining model, MACRO and RZWQM, and their comparison with measured data for field T4 during the campaign 2009/2010.

In order to strengthen the above findings a comparison with state-of-the-art models

was done. A comparison between the performance obtained from the best performing model (bagging of model trees) with commonly used state-of-the-art models MACRO and RZWQM for modeling drainage outflow (Figure 9.3) is conducted. The bagging of model trees and the RZWQM model with default parameter values show similar performance over the test data set. Namely, the RZWQM model performs slightly better in terms of root relative square error, while the correlations are effectively the same (Figure 9.3). The MACRO model exhibits far lower performance with a relative error of 130 %, which in fact means that it performs worse than the simple model that predicts the average of the target variable.

Figure 9.4 shows the simulation runs of these three models for the task of drainage outflow, along with measured data for the campaign 2009/2010 at field T4. A considerable difference in the curves is observed, and none of them present an exact match of the measured data. The RZWQM simulation performs very well in terms of timing the peak of outflows and, in some cases, their amplitudes. The data mining model predictions match the measured data within the period with many drainage events well, while roughly approximating the drainage outflow during the beginning of the campaign. On the other hand, the MACRO model, with calibrated parameters, only gives a rough approximation over the entire campaign, completely missing the main peaks of extreme drainage events.

9.1.1.2 Surface runoff by saturation

Modeling surface runoff by saturation has been done using the same methodology as for modeling drainage discharge, described in the previous subsection. Figure 9.5 shows the error profiles of data mining methods resulting from tuning algorithm parameters. High variability in the performance of regression and model trees can be observed as the N_{min} parameter is varied.

On the other hand, ensembles have a robust performance over the N_{tree} parameter range considered. The ridge parameter of linear regression was tuned to 10^{-9}, while regression and model trees performed best when the minimal numbers of instances in a leaf was set to 26 and 16, respectively.

The high variability of error in the case of regression and model trees gives a first insight into the quality of the collected data. The error variation for lower values of the parameter N_{min} emphasizes the presence of noise in the target variable and high variability among its values, observed under similar circumstances. This is further confirmed by the final performance of the models learned, which is bad and does not change much between the training and unseen data (Table 9.2).

Overall, the data mining models show lower predictive performance compared to those for the task of drainage outflow prediction. The difference is high for regression and model trees as well as for ensembles of regression and model trees. Linear and polynomial regressions show very poor performance, similar or even worse than the performance of average value predictors of surface runoff outflow.

The models learned with bagging regression and model trees have the lowest root relative squared error and the highest correlation coefficient (Figure 9.6). Therefore, we can conclude that these models outperform the rest. Cross-validation additionally strengthens the performance and confidence in behavior of bagging with model and regression trees and reveals the advantage of the latter when considering the variability in performance among the ten randomly sampled test data sets.

For the task of modeling surface runoff by saturation, a comparison between the performance of machine learning models and the performance of the RZWQM model was done. Figure 9.7a shows a considerable difference in the error of the two models, measured in terms of RRSE. This difference in RRSE values is directly visible as a qualitative difference

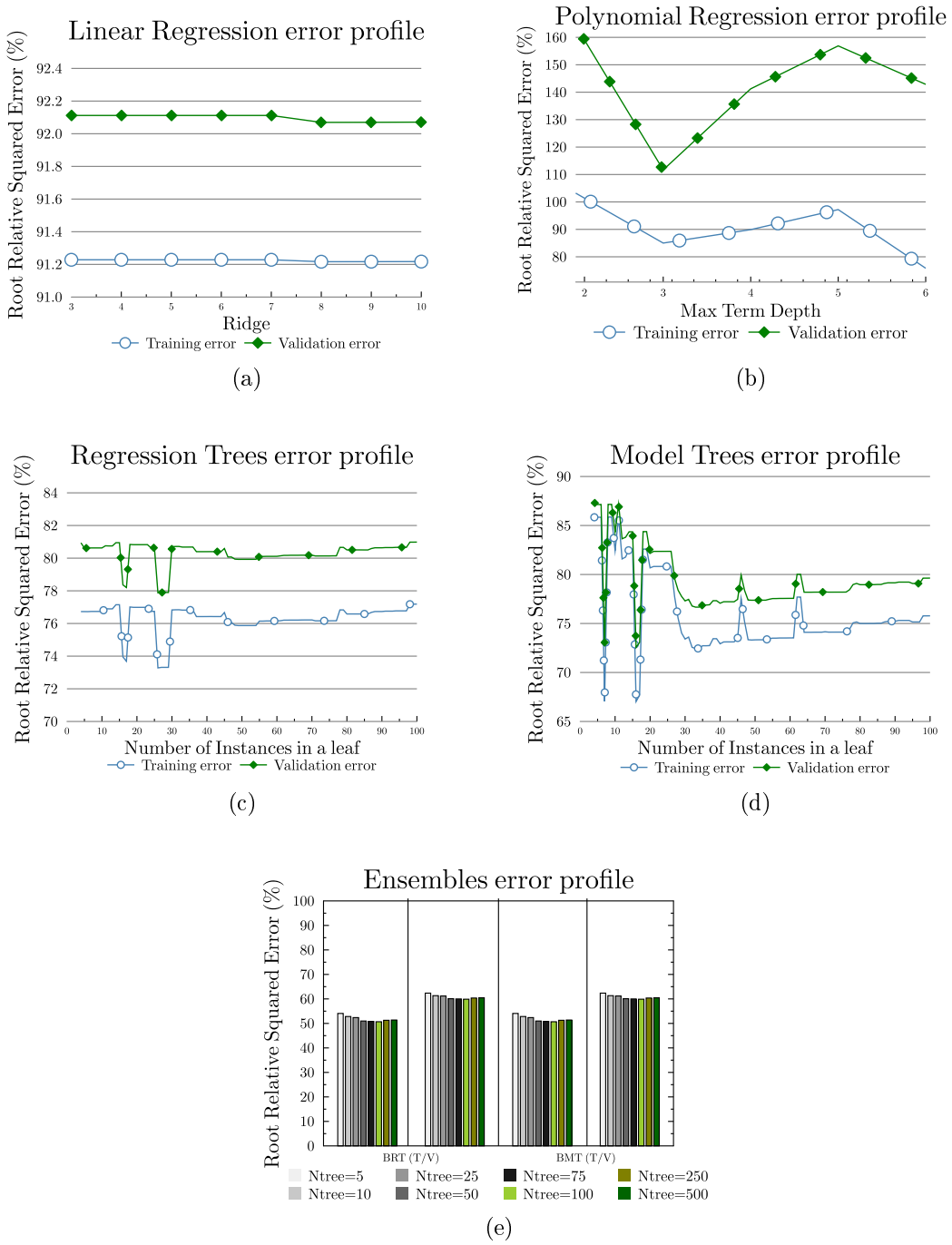


Figure 9.5: Error profiles resulting from tuning the parameters of each method used in the surface runoff outflow study, both for training and validation data: **a**) Linear regression performance for different values of the ridge parameter, i.e., 10^{-i}, where $i = \{3, 4, 5, 6, 7, 8, 9, 10\}$; **b**) Polynomial regression models with RRSE obtained by varying the depth of the right-hand terms in the interval [2,6]; **c**) Regression tree performance for different values of the parameter N_{min}; **d**) Model trees performance for different values of the parameter N_{min}; **e**) Bagging ensembles of regression (BRT) and model trees (BMT) performance in the case of varying N_{tree} parameter. T/V stands for Train and Validation data.

		LR (10^{-9})	PR (3)	RT (26)	MT (16)	BRT (100)	BMT (100)
Training dataset	**Corr.**	0.41	0.41	0.68	0.75	0.89	0.89
	RMSE	0.32	0.56	0.25	0.23	0.18	0.18
	RRSE	91.22	85.00	73.28	67.03	50.68	50.68
Validation dataset	**Corr.**	0.39	0.35	0.63	0.69	0.82	0.82
	RMSE	0.32	0.43	0.27	0.25	0.21	0.21
	RRSE	92.07	111.69	77.87	72.57	59.89	59.89
Testing dataset	**Corr.**	0.38	0.46	0.60	0.67	0.80	0.80
	RMSE	0.30	0.35	0.26	0.24	0.20	0.20
	RRSE	92.50	160.29	80.09	74.76	61.63	61.63
Cross-validation	**Corr.**	0.38	0.46	0.59	0.64	0.74	0.74
	RMSE	0.30	0.48	0.26	0.25	0.23	0.22
	RRSE	92.43	152.18	80.96	77.14	67.68	67.85

Table 9.2: Summary of models' performance on each dataset for the task of surface runoff water outflow prediction. The values of the tuned algorithm parameters are given in brackets. *LR* stands for Linear Regression, *PR* for Polynomial Regression, *RT* for Regression tree, *MT* for Model tree, *BRT* for Bagging of Regression trees, and *BMT* for Bagging of Model trees.

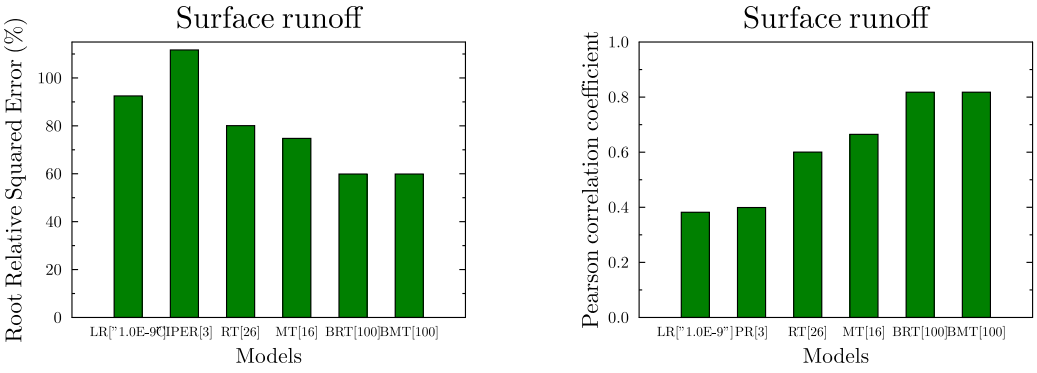


Figure 9.6: Performance summary of the best surface runoff data mining models, over validation dataset. **a**) Models' performances expressed with relative error (RRSE); **b**) Models' performances in terms of the Pearson correlation coefficient.

in the simulation shown in Figure 9.8, where the RZWQM model overestimates surface runoff during the winter period and predicts zeros in the rest of the campaign. On the other hand, the bagging ensemble of model trees makes good predictions for winter periods and overestimates surface runoff outflow at the beginning of campaigns. In general, it follows the dynamics of surface runoff outflow in most of the periods within the campaign.

The applicability of the models learned differs a lot from the applicability of state-of-the-art models. Namely, the MACRO and the RZWQM models are developed to cover a wider range of scenarios regarding soil and climate conditions, while our learned models are fitted to data available from the La Jaillière experimental site, which is a representative experimental site for one scenario (out of ten) defined by the FOCUS working group and covered by the MACRO model. Therefore, similar behavior can be observed if the models learned are applied on every other agricultural field that belongs to the defined scenario, for which the La Jaillière experimental site is representative.

The limited applicability of the learned models over a single region or similar regions can be considered a general limitation of the proposed approach when modeling environmental data. Namely, to cover all ten scenarios included in the MACRO model, data collected from each representative experimental site is required. That is the proposed approach cannot be applied to scenarios for which data are not available. In such cases, the system uses a diagnostic layer which is described in next section.

Finally, the value of the proposed modeling approach increases when the complexity of the input data for physically-based state-of-the-art models is considered. They require more specific data (besides the meteorological data and agricultural practices), such as organic carbon content, properties of each horizon in the soil, texture and bulk density for parameter estimation of thermal capacity, hydraulic conductivity and water retention, in order to produce reliable predictions.

9.1.1.3 Intensive flow period

Models learned for predicting intensive flow periods are limited to events related to drainage outflow only, since it is emphasized by the experts as most important in tile-drained fields.

As described previously, the experimental setup consists of learning models for estimating the beginning and ending of a drainage period. For the former, three different models

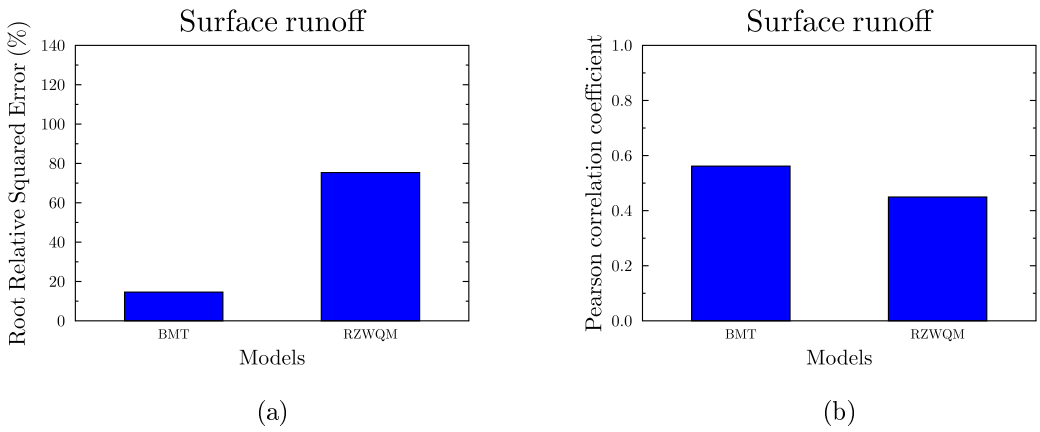


Figure 9.7: Comparison of the performances (RRSE and Pearson correlation) of the best learned models for predicting surface runoff by saturation with performance of RZWQM, over data collected in field T4 for the period 2008-2011.

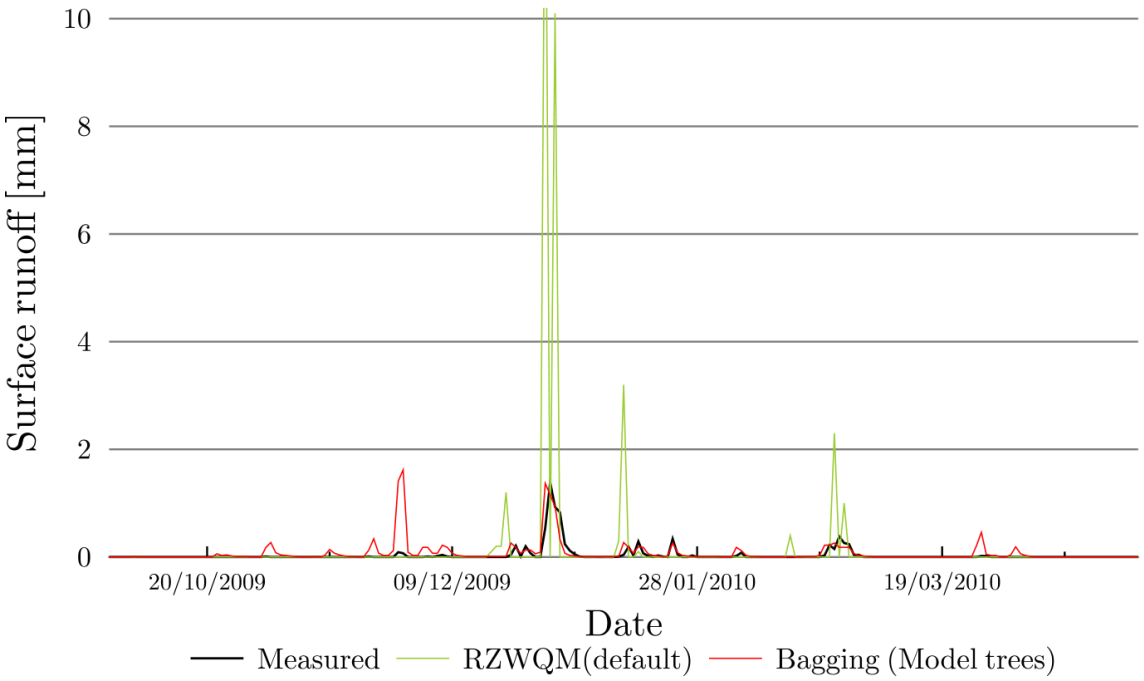


Figure 9.8: Simulation of surface runoff outflow with the best data mining model and RZWQM, and their comparison with measured data for the field T4 during the campaign 2009/2010.

have been learned based on input attributes: using only historic meteorological data, or historic and forecast meteorological data, or historic, forecast meteorological data and cumulative rainfall since the start of a campaign. The latter includes learning models based on historic meteorological data and models based on historic and forecast meteorological data. The complete study has been published in (Trajanov et al., 2015).

Table 9.3: Accuracy of the models predicting the start of a drainage period for different combinations of attributes, estimated with 10-fold cross-validation. The accuracy of models that consider cumulative drainage since the beginning of a campaign as an additional attribute are given in brackets.

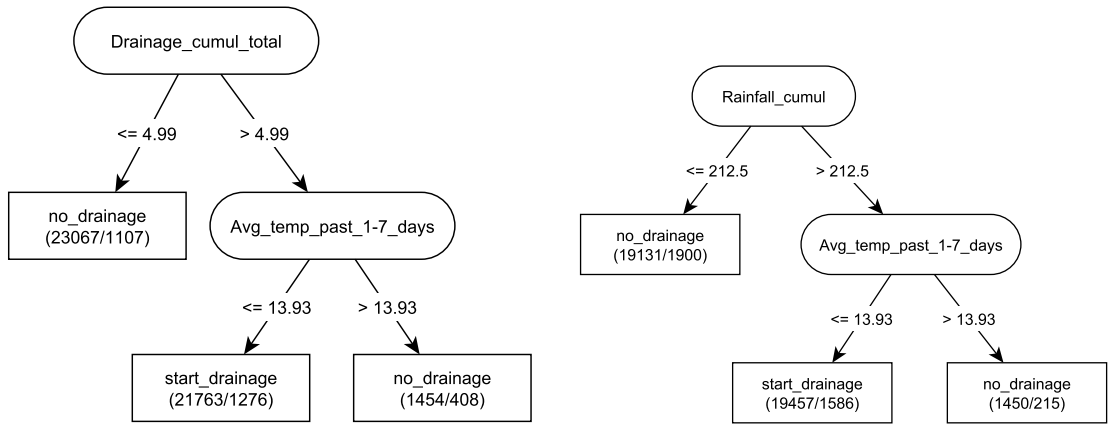
Attributes	Accuracy
Avg_ temp_ past_ 1-7_ days *Rainfall_ cumul* (*Drainage_ cumul_ total*)	89.9 % (94.5 %)
Avg_ temp_ past_ 1-7_ days *Avg_ temp_ past_ 8-14_ days* *Avg_ temp_ next_ 1-7_ days* *Tot_ rainfall_ past_ 1-7_ days* *Tot_ rainfall_ past_ 8-14_ days* *Tot_ rainfall_ next_ 1-7_ days* (*Drainage_ cumul_ total*)	74.6% (94.6 %)
Avg_ temp_ past_ 1-7_ days *Avg_ temp_ past_ 8-14_ days* *Avg_ temp_ next_ 1-7_ days* *Rainfall_ cumul* (*Drainage_ cumul_ total*)	89.8 % (94.1 %)

Table 9.4: Accuracy of models predicting the end of a drainage period for different combinations of attributes, estimated with 10-fold cross-validation.

Attributes	Accuracy
Avg_ temp_ past_ 1-7_ days *Avg_ temp_ past_ 8-14_ days* *Tot_ rainfall_ past_ 1-7_ days* *Tot_ rainfall_ past_ 8-14_ days*	85.9 %
Avg_ temp_ past_ 1-7_ days *Avg_ temp_ past_ 8-14_ days* *Avg_ temp_ next_ 1-7_ days* *Tot_ rainfall_ past_ 1-7_ days* *Tot_ rainfall_ past_ 8-14_ days* *Tot_ rainfall_ next_ 1-7_ days*	88.3 %

In Table 9.3, the accuracy of the learned predictive models for the start of a drainage period are presented. All scenarios were completed with and without *Drainage_ cumul_ total* as input attribute, and these results from models that cover cumulative drainage since the start of a campaign are given in brackets.

The predictive model built with the total cumulative drainage in the set of attributes (Figure 9.9a) has total cumulative drainage (*Drainage_ cumul_ total*) at the topmost po-



(a) (b)

Figure 9.9: Predictive models for the beginning of a drainage period using: **a**) dates provided by the expert for the start of a drainage period as a dependent variable, and past and future meteorological data and cumulative drainage as attributes (accuracy 94.56 %, TPR 0.946, FPR 0.06); **b**) 5mm threshold for the start of a drainage period as dependent variable and only past meteorological data and cumulative rainfall as attributes (accuracy 90.83 %,TPR 0.908, FPR 0.092).

sition in the model structure, and its crucial value that determines the starting date of a drainage period is 4.99 mm: this is in line with the hypothesis that 5 mm represents the threshold for assessing the beginning of a drainage period.

The best model (Figure 9.9a) uses meteorological data and cumulative drainage data. Models that do not cover cumulative drainage from the beginning of a campaign as input, but only use meteorological data, can still successfully estimate the beginning of a drainage period (Figure 9.9b). This leads to a solution that can be easily applied to an arbitrary field, where drainage is not measured but meteorological data are available.

Several predictive models were also obtained for the end of a drainage period, using two different combinations of attributes. The first uses only past meteorological data, and the second one, also uses future meteorological data. The attributes used for estimating the end of a drainage period and the accuracies obtained with the predictive models are presented in Table 9.4, while two models are presented in Figures 9.10a and Figures 9.10b.

9.1.2 Diagnostic layer

The diagnostic layer is evaluated using the data available from the La Jaillère experimental site. There are 10 fields available and for testing we used two different fields, one tile-drained field (*Field 4*) and another field without a drainage system installed (*Field 1*). Both share the same soil properties and climate conditions. Therefore, it seems appropriate to compare surface runoff by saturation on fields with and without a drainage system, and water outflows in different weather seasons within a campaign.

In order to compare the qualitative outcomes of DEX models with quantitative measured data, we use the total amount of rainfall per weather season or campaign as a reference value, from which measured data can be discretized in the case of surface runoff by saturation, while for drainage outflow, evaluation is done with the cumulative drainage outflow per campaign as a reference value. In total, data of 12 campaigns (2000/2001 -

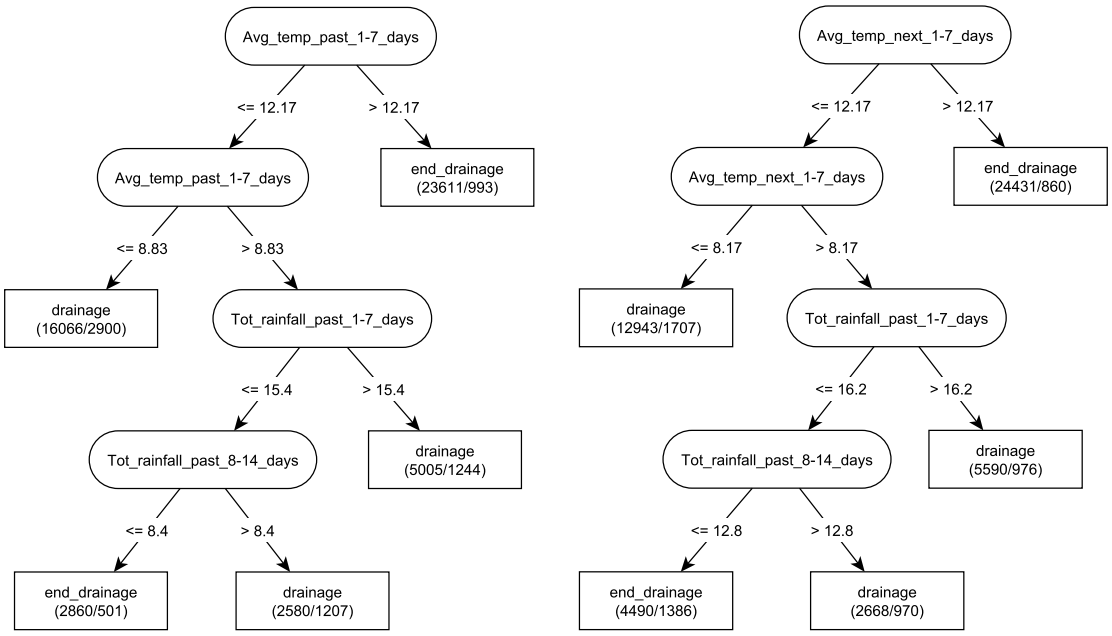


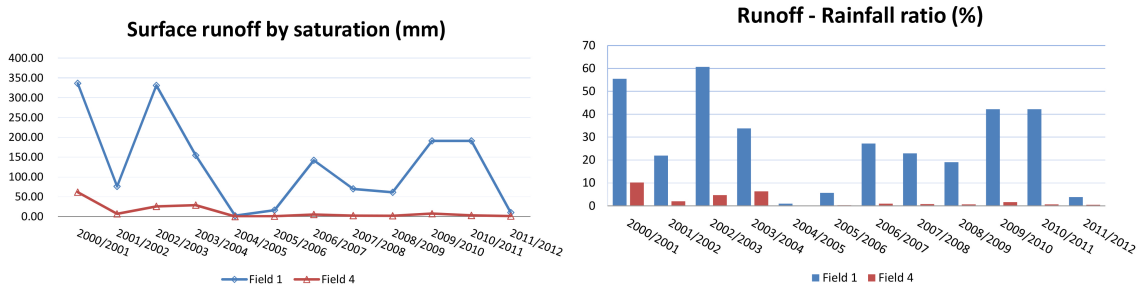
Figure 9.10: Predictive models for the end of a drainage period using: **a**) only past meteorological data (accuracy 85.94 %, TPR 0.859, FPR 0.135); **b**) past and future meteorological data (accuracy 88.28 %, TPR 0.883, FPR 0.133) as input attributes.

2011/2012) were used for the purpose of the evaluation.

Attribute	Field 1 (Winter)	Field 4 (Winter)	Field 1 (Spring)	Field 4 (Spring)
Runoff by saturation	**Very high**	Very low	***No***	***No***
Weather season	**Autumn-Winter**	**Autumn-Winter**	Spring	Spring
Hydrological status of soil	High	Very low	High	Very low
Capacity	Medium	Medium	Medium	Medium
SWHC	**<120**	**<120**	**<120**	**<120**
Depth of substratum	40-80	40-80	40-80	40-80
Infiltration intensity	Very low	***Very high***	Very low	***Very high***
Drainage network	**No**	***Well***	**No**	***Well***
Depth of permeability disruption	40-80	***>80***	40-80	***>80***
Permeability of substratum	**No**	**No**	**No**	**No**
Slope and capping effects	**Very high**	**Very high**	**Very high**	**Very high**
Slope	**0-2%**	**0-2%**	**0-2%**	**0-2%**
Capping soil	**No**	**No**	**No**	**No**

Figure 9.11: DEX decision model for evaluation of surface runoff by saturation.

In accordance with decision rules, the intensity of surface runoff by saturation during autumn and winter is estimated to be *Very high* and *Very low* for Field 1 and Field 4, respectively (Figure 9.11). Compared to the measured data for 12 campaigns (Figure 9.12a), in *Field 1*, the amount of water flow through surface runoff by saturation is far larger than the amount of water flow from *Field 4*. Furthermore, the ratio between the total amount of rainfall in autumn and winter, and water flow through surface runoff in the same period (Figure 9.12b) reveals that a portion of the water that flew out from *Field 1* through surface runoff is very high compared to the portion from *Field 4*.



(a) (b)

Figure 9.12: Measured data from *Field 1* and *Field 4* from the La Jaillière experimental site for surface runoff, represented: **(a)** with absolute values for 12 campaigns (2000/2001 - 2011/2012); **(b)** with runoff - rainfall ratio over 12 campaigns (2000/2001 - 2011/2012).

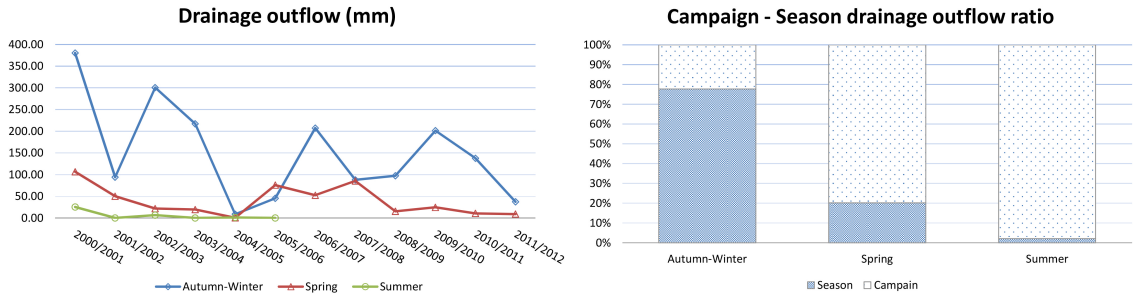
The evaluation of these two cases (*Field 1* and *Field 4*) by the DEX model shows the factors that influence most the intensity of surface runoff by saturation. Namely, it indicates that the presence of a drainage system on the field (*Field 4*), which produces a deeper level of permeability disruption, significantly improves the ability of the soil to infiltrate the water. *Infiltration intensity* is therefore *very high* for the case of *Field 4* and *very low* for the case of *Field 1*. It further influences the *hydrological status of soil*, by showing *very low* ability of appearance of surface runoff by saturation in *Field 4* and *high* in *Field 1*. Therefore, in autumn and winter, when a great amount of rainfall is expected, such *hydrological status of soil* produces *very high* intensity of surface runoff on *Field 1*, with no influence at all for *Field 4*. Due to the *very high* infiltration capacity, the latter will direct the water to the drainage network.

The same situation is observed in spring, but the lower rainfall and *very high* positive *Slope and capping effects* produce *no* surface runoff by saturation.

Attribute	Field 4 (winter)	Field 4 (Spring)	Field 4 (summer)
Drainage and infiltration	High	Very low	Very low
General intensity	High	Very low	Very low
Weather season	**Autumn-Winter**	Spring	***Summer***
Cracks in soil	***No***	***No***	***No***
Hydrological status of soil	High	High	High
Capacity	**Low**	**Low**	**Low**
SWHC	**<120**	**<120**	**<120**
Depth of substratum	40-80	40-80	40-80
Infiltration intensity	***Very high***	***Very high***	***Very high***
Drainage network	***Well***	***Well***	***Well***
Depth of permeability disruption	***>80***	***>80***	***>80***
Permeability of substratum	**No**	**No**	**No**
Slope and capping effects	***No***	***No***	***No***
Slope	**0-2%**	**0-2%**	**0-2%**
Capping layer	**No**	**No**	**No**
Soil conditions	***other***	***other***	***other***

Figure 9.13: DEX decision model for evaluation of drainage outflow.

Drainage outflow has been evaluated using the same 12 campaigns, and on the same field (*Field 4*). Unlike the evaluation of surface runoff by saturation, drainage outflow



(a) (b)

Figure 9.14: Measured data from *Field 4* in the La Jaillière experimental site for drainage outflow, represented: **(a)** with absolute values for 12 campaigns (2000/2001 - 2011/2012); **(b)** with drainage (per season) - cumulative drainage (per campaign) average ratio over 12 campaigns (2000/2001 - 2011/2012).

is evaluated by comparing weather seasons where the reference point is the cumulative drainage outflow across the whole campaign. Figure 9.13 shows the evaluation of three different scenarios: autumn-winter, spring and summer.

The scenarios are evaluated with *high* intensity during the winter period and *very low* intensity during the spring and the summer period. The difference is the weather season, which represents the amounts of rainfall that appear as input water into the ground. The structure of the model is the same as for surface runoff by saturation, but the decision rules differ, and exploit the estimation of drainage outflow intensity. Factors that positively influence the drainage outflow are *infiltration intensity* and *capacity* of the soil, which shows how fast water can move vertically through the soil. In all scenarios in Figure 9.13, *infiltration intensity* is *very high*, while *capacity* is *low*. Such settings describe fast movement of water through the soil and fast passage into the drainage network, which is assigned *well* efficiency. So, with more rainfall water (during the autumn and winter season), *high* intensity of drainage outflow is set, otherwise it is *very low*.

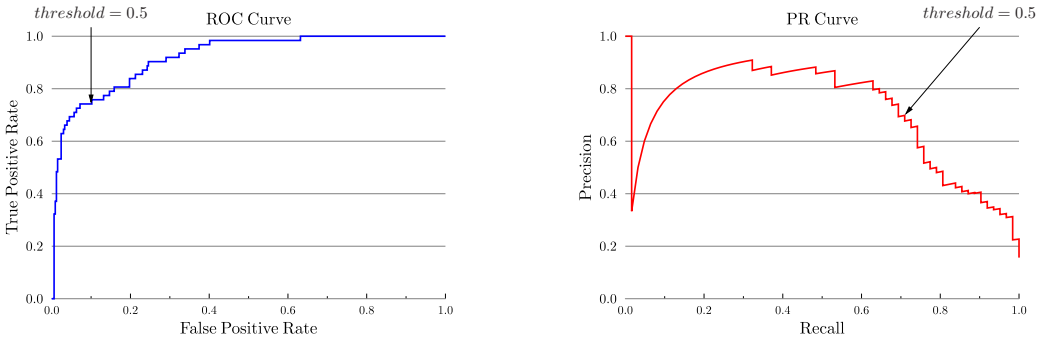
Outflow intensity is shown in Figure 9.14, where the left figure shows absolute drainage outflow quantities across 12 campaigns. Figure 9.14b reveals that the highest measured average drainage outflow per campaign is observed during autumn and winter (approx. 80 %), while the rest, approximately 20 % are measured during the spring and the summer seasons. Therefore, during the former, intensity is estimated as *high*, otherwise *very low*.

Since we do not have data collected for simple surface runoff and surface runoff on capping soil, the corresponding DEX models have been evaluated by the experts from ARVALIS. The evaluation was done in accordance with field observations, to a high degree of precision.

9.1.3 Ex-ante risk assessment

The selection of the best random forest model for predicting the risk of pollutant transfer in water from tile-drained fields resulted from an extensive process, where precision and recall measures, for the minority class ($RISKY$), were optimized. The highly skewed class attribute emphasizes dominance by the majority class (NOT_RISKY) and estimates an overall good performance for each model built. Therefore, an analysis of the models' performance for the minority class ($RISKY$) was conducted.

In the domain of environmental modeling, having a false alarm (*false positive*) regard-



(a) (b)

Figure 9.15: Model's performance curves: **(a)** ROC Curve; **(b)** Precision-Recall Curve.

ing issues with pollutant transfer in water bodies is accepted if it is limited to a few cases over some period of time. Otherwise, if the model fails to detect the issue (*false negative*), the consequence is catastrophic, even more so if it happens on a regular basis. Therefore, covering as many issues with water bodies contamination and accurately predicting them has a high interest for the given decision problem. Covering as many issues with contamination is described with the recall evaluation measure, while accurately predicting them is described with the precision evaluation measure.

Normally, precision and recall are inversely correlated measures. Increase in the recall of a class happens at the expense of its precision, and influences the recall and precision of the complementary class as well. These settings require a trade-off in minimizing *false positives* and *false negatives* in both classes.

The process evolved in the selection of a model, built with 50 unpruned classification trees with cost matrix (0.0; 1.0; 5.0; 0.0), which penalizes false negatives five times as severely as false positives. The performance of the model is shown in Table 9.5. Considering the NOT_RISKY class, high precision, recall and area under precision-recall are observed. On the other hand, the $RISKY$ class shows lower performance in all categories except the ROC area, which is a bit higher than the positive class, since the false positive rate is lower than in the other class. Overall, the selected method shows good performance.

Table 9.5: Model's performance described with: *TP Rate* - true positive rate, *FP Rate* - false positive rate, *Precision*, *Recall*, *ROC Area* - area under ROC curve, *PRC Area* - area under precision-recall curve.

	TP rate	FP Rate	Precision	Recall	ROC Area	PRC Area
NOT_RISKY	0,921	0,226	0,952	0,921	0,845	0,936
$RISKY$	0,774	0,079	0,667	0,774	0,933	0,723
Weighted Avg.	0,896	0,201	0,903	0,896	0,860	0,899

The performance described above is based on a boundary threshold of 0.5, above which instances are classified as positive, otherwise as negative. Based on this threshold, all models are evaluated and the best one is selected. Since the target is to maximize the recall and precision on a single class, threshold tuning is performed. Such analysis allows finding a better cut-off decision boundary that will behave better in separating the instance space into positive and negative instances.

However, as shown in Figure 9.15, further improvements by tuning the threshold are limited to few examples. Namely, if the threshold is set higher (approx. 0.6) then the false negative rate grows fast (close to half of the number of positive examples), while the false positive rate improves slowly. By setting the threshold below 0.5, precision decreases faster, while recall improves slowly (Figure 9.15b). Thus, the threshold of 0.5 is an optimal solution for the selected model.

9.2 Risk Management

Evaluation of the risk management module was performed on the test-case of ecological risk already estimated as *Very high* (or *RISKY* when using the predictive layer). The test-case was then reviewed and the changes of ecological risk were considered as a mitigation measure. In total nine different mitigation measures were taken into account, with various complexity.

The DEX decision model considered in the test-case is a model built for drainage outcome where one of the follow crops are presented: *Wheat*, *Barley (winter)* or *Rye*.

In Figure 9.16, the model that includes flow intensity (outcome from the diagnostic layer) and description of the state of the world $s_{t'}$ is presented.

Attribute	State	Mitigation 1	Mitigation 2	Mitigation 3	Mitigation 4
Outcome	RISKY	RISKY	RISKY	*NOT_RISKY*	*NOT_RISKY*
Flow intensity	Very high	Very high	Very high	Very high	Very high
Effect	Increase transfer	Increase transfer	Increase transfer	*Decrease transfer*	*Decrease transfer*
Crop	Wheat	Wheat	Wheat	Wheat	Wheat
Tillage	*Yes*	*Yes*	*Yes*	*Yes*	*Yes*
Active ingredient	diflufénicanil	diflufénicanil	isoproturon	diflufénicanil	pendiméthaline
Time of application	Close_WDP	*Before_WDP*	*Before_WDP*	Close_WDP	Close_WDP
Dose	Producer recommendation	Producer recommendation	Producer recommendation	*ARVALIS recommendation*	Producer recommendation

Attribute	Mitigation 5	Mitigation 6	Mitigation 7	Mitigation 8	Mitigation 9
Outcome	*NOT_RISKY*	*NOT_RISKY*	*NOT_RISKY*	*NOT_RISKY*	RISKY
Flow intensity	Very high	Very high	Very high	Very high	Very high
Effect	*Decrease transfer*	*Decrease transfer*	*Decrease transfer*	*Decrease transfer*	Increase transfer
Crop	Wheat	Barley(winter)	Barley(winter)	Barley(winter)	Rye
Tillage	*Yes*	*Yes*	*Yes*	No	*Yes*
Active ingredient	diflufénicanil	pendiméthaline	pendiméthaline	pendiméthaline	isoproturon
Time of application	*Before_WDP*	*Before_WDP*	*Before_WDP*	Close_WDP	Close_WDP
Dose	*ARVALIS recommendation*	*ARVALIS recommendation*	Producer recommendation	Producer recommendation	*ARVALIS recommendation*

Figure 9.16: State of the world and set of mitigation measures. Evaluation of mitigation measures using DEX decision model that consumes the flow intensity as an initial risk.

The option *State* describes the planned application of an active ingredient $a_t \in A$, described in Table 9.6. Its evaluation shows that its implementation over the "current" state of the world $s_{t'}$ at time t' is *RISKY* with regard to pollutants transfer into water bodies.

Table 9.6: Description of the planned application of an active ingredient. *Close_ WDP* stands for *close to winter drainage period*, defined as a week before the beginning of winter drainage period.

g_{a_crop}	=	*Wheat*
$g_{a\_tillage}$	=	*Yes*
$g_{a\_ingredient}$	=	*diflufenicanil*
g_{a_time}	=	*Close_ WDP*
g_{a_dose}	=	*Producer recommendation*

The task of alternative evaluation in the risk management module is to evaluate all possible changes over the state of the world or alternative, that are considered as mitigation

measures, given in model as alternatives. In Figure 9.16 a total of eight different mitigation measures are given, the evaluation of which is represented with the attribute *Outcome*. The evaluation of the alternatives is done using "what-if" analysis, as described below.

Mitigation 1 considers changing the time of application, from *Close* to *Before WDP*, which suggests that the planned application of the active ingredient is to be moved to the period more than a week before the estimated beginning of the winter drainage period. However, this mitigation measure does not improve the state of the world regarding the ecological risk of pollutants transfer into water bodies, since the outcome is still *RISKY*. The next proposed mitigation measure assumes change of the active ingredient to be applied (from *diflufenicanil* to *isoproturon*) and of the time of application, which again results in *RISKY* evaluation. The following mitigation measure represents change of the dose of active ingredient that is to be applied (from *Producer recommendation* to *ARVALIS recommendation*), the outcome of which evaluates the application to be *NOT_RISKY* at time $t + 1$, i.e., after the changes and the active ingredient are applied. Such evaluation suggests that the proposed changes (mitigation measure) are effective and will reduce the ecological risk considered. In a similar way, the rest of the proposed mitigation measures are evaluated, proposing one or more changes in the attributes that describe the alternatives. Namely, *Mitigation 4* proposes a change of the crop present on the field at the planned time of application t'. *Mitigation 5* proposes corrections regarding the dose of the active ingredient and the time of the application. *Mitigation 6* evaluates "what-if" the time of application is changed together with the active ingredient, dose and crop, while *Mitigation 7* considers changes of the time of application, active ingredient and crop. Finally, *Mitigation 8* investigates the influence of tillage and changes of active ingredient and crop, similar to *Mitigation 9*, which excludes changes related to the tillage of the field.

Attribute	State	Mititgation 1	Mitigation 2	Mitigation 3	Mitigation 4
Outcome	RISKY	RISKY	RISKY	*NOT_RISKY*	*NOT_RISKY*
Initial risk	RISKY	RISKY	RISKY	RISKY	RISKY
Effect	Increase transfer	Increase transfer	Increase transfer	*Decrease transfer*	*Decrease transfer*
Crop	Wheat	Wheat	Wheat	Wheat	Wheat
Tillage	*Yes*	*Yes*	*Yes*	*Yes*	*Yes*
Active ingredient	diflufénicanil	diflufénicanil	isoproturon	diflufénicanil	pendiméthaline
Time of application	Close_WDP	*Before_WDP*	*Before_WDP*	Close_WDP	Close_WDP
Dose	Producer recommendation	Producer recommendation	Producer recommendation	*ARVALIS recommendation*	Producer recommendation

Attribute	Mitigation 5	Mitigation 6	Mitigation 7	Mitigation 8	Mitigation 9
Outcome	*NOT_RISKY*	*NOT_RISKY*	*NOT_RISKY*	*NOT_RISKY*	RISKY
Initial risk	RISKY	RISKY	RISKY	RISKY	RISKY
Effect	*Decrease transfer*	*Decrease transfer*	*Decrease transfer*	*Decrease transfer*	Increase transfer
Crop	Wheat	Barley(winter)	Barley(winter)	Barley(winter)	Rye
Tillage	*Yes*	*Yes*	*Yes*	No	*Yes*
Active ingredient	diflufénicanil	pendiméthaline	pendiméthaline	pendiméthaline	isoproturon
Time of application	*Before_WDP*	*Before_WDP*	*Before_WDP*	Close_WDP	Close_WDP
Dose	*ARVALIS recommendation*	*ARVALIS recommendation*	Producer recommendation	Producer recommendation	*ARVALIS recommendation*

Figure 9.17: State of the world and set of mitigation measures. Evaluation of mitigation measures using the DEX decision model that takes the initial risk from the predictive layer.

Figure 9.17 shows the same alternatives applied to a model that also considers the drainage outflow pathway, but unlike previous one, this model considers as input the ecological risk assessed by the predictive layer. Therefore, this time instead of *Flow intensity*, the model is considering *Initial risk* as input.

As can be observed from both figures (Figure 9.16 and Figure 9.17), the evaluation is performed in the same way, and decision rules contained in both models evaluate to the same outcome for all mitigation measures. This indicates the consistency of the models in terms of the evaluation of mitigation measures, despite the different type of models used in the risk assessment module.

Once the alternatives are evaluated, the risk management module continues with a choice set selection. In the given test-case, all mitigation measures evaluated as *NOT_RISKY* will be selected (6 out of 9), a set of which is then input to the next task, alternative rank-

ing.

Alternative ranking is done using the linear model defined in 8.10. Partial complexities, represented as equation's parameters are given in 8.12. The full description of the registered actions (changes) per mitigation measure is given in Table 9.7.

Table 9.7: Description of possible changes of the state of the world $s_{t'}$ and alternative a_t, with partial and total complexity of a particular mitigation measure. Partial complexity is an array of complexities of actions $g_{ai} \in G_a$ where changes were identified (derived from 8.12). Total complexity is calculated using the model in 8.10.

Alternative	Changes	Partial complexity	Total complexity
Mitigation 3	g_{a_dose}	2	2
Mitigation 4	$g_{a\_ingredient}$	5	5
Mitigation 5	g_{a_time}, g_{a_dose}	1,2	3
Mitigation 6	g_{a_crop}, $g_{a\_ingredient}$, g_{a_time}, g_{a_dose}	20,5,1,2	28
Mitigation 7	g_{a_crop}, $g_{a\_ingredient}$, g_{a_time}	20,5,1	26
Mitigation 8	g_{a_crop}, $g_{a\_tillage}$, $g_{a\_ingredient}$	20,10,5	35

The outcome of the alternative ranking step is an ordered set of mitigation measures (alternatives). The order relation is a preference relation and is based on total complexities of the alternatives, derived from the actions' partial complexities. The ordered set for the given test-case is preference-based and described as follows:

$$Mit.\ 3 \succ Mit.\ 5 \succ Mit.\ 4 \succ Mit.\ 7 \succ Mit.\ 6 \succ Mit.\ 8 \tag{9.1}$$

The derived alternative ranking suggests that a single action is not always less complex and preferred than more complex actions. Such an example is observed with *Mitigation 4* and *Mitigation 5*, where the former contains only one change and the latter suggests two different actions. However, based on the partial complexities of actions, *Mitigation 5* is less complex and strongly preferable to *Mitigation 4*.

The preferences can be extended if they are expressed against the state of the world s_{t+1} at time $t+1$, along with the utility gained (NOT_RISKY). For example supposed that it is more preferable that the dose is not changed (assuming that this represents an attribute from the state of the world that describes the dose of the active ingredient present on a field). Then, the alternative ranking step will express the preference of a particular alternative $a \in A$ as follows:

$$pref(t+1) = u'(f(a, s_{t'}), s_{t+1}). \tag{9.2}$$

Therefore, the ordered relation will be:

$$Mit.\ 4 \succ Mit.\ 7 \succ Mit.\ 8 \succ Mit.\ 3 \succ Mit.\ 5 \succ Mit.\ 6 \tag{9.3}$$

To summarize, the risk management module produces an ordered set of mitigation measures, from which the individual is supposed to select the most appropriate one. The system is limited to proposing a set and not a particular mitigation measure due to other factors that can influence the final decision, which are not included in the decision analysis. Such factors can be economical status or feasibility, which can be represented on a time scale or with the availability of specific cultivation mechanisms.

9.3 Summary

This chapter covers the presentation of results obtained during the development and implementation of quasi ex-post risk analysis in the domain of water protection.

The performance of the partial models compared to state-of-the-art models shows improvement, in particular if the timing of peak flows and their amplitude are considered. In addition, the complexity of parametrization of state-of-the-art models is overcome with the built predictive and diagnostic models.

Overall, the system has been evaluated on real case scenarios. The team of experts at ARVALIS provided information from previous diagnoses done on a small set of fields in France, used to parametrize the system with required input information. The results have been compared to the recommendations that the experts proposed to the farmers as a part of the diagnosis processes used for the evaluation. The system provided more precise sets of mitigation measures compared to the diagnosis reports filled out by the experts as their recommendation. Recommendations were improved because the system considers predicted values for the uncertain attributes that describe the state of the field. Additionally, improvement comes from the possibility to evaluate the recommendations in terms of individuals' preferences with regard to the state of a field that would eventually take place upon application of the corresponding alternative.

However, the case-study implementation of the quasi ex-post risk analysis is limited in applicability to the particular region of Western France, since the data were collected from one experimental site. This issue can be overcome if data are available for each representative experimental site registered by the FOCUS group, which will lead to building predictive models that can cover a wider spatial region.

The case-study implementation shows the applicability and performance improvement of quasi ex-post risk analysis (the methodological framework). However, the usability of the methodological framework can be limited by the availability of data regarding the decision problem under consideration, which would lead to an implementation that will be based on expert knowledge only.

Chapter 10

Conclusions

The thesis addresses the problem of imperfect knowledge that influences multi-criteria decision making and causes risk and uncertainty about the state of the world and possible outcomes. Uncertainty and risk can be related to the state of the world at time t (time of decision making), at time t' (before a chosen alternative is realized or applied) and at time $t+1$ (after a chosen alternative is applied). The thesis addresses decision maker preferences and how they are expressed.

Existing MCDA methods for dealing with uncertainty and risk consider only the state of the world at time t and express preference in terms of the outcome. This is the case because all of them use the ex-ante approach to risk assessment that tries to use simulation or forecasting techniques to estimate the probability distribution of states of the world.

A combination of risk analysis and decision analysis with existing risk assessment approaches *ex-ante* and *ex-post* suffers from limitations that influence the complete decision analysis. The former has limitations regarding the availability of information at the beginning of the period under consideration, while the latter is limited (for most real-world problems) due to the requirement that decision making needs to be performed at the beginning of the period in question. Consequently, the goal of the thesis was to present a methodological framework that overcomes the limitations of existing risk assessment approaches.

Furthermore, existing risk assessment approaches appear as partial steps in a complete risk analysis that have to be done separately. This limits the autonomy of decision analysis and requires additional efforts to be delivered as decision support to decision makers. Thus, the second goal of the thesis was to upgrade the methodological framework towards a framework for decision analysis that can be easily incorporated into a decision support system which allows assessed risk to be managed autonomously, in a way defined by the decision maker. Finally, the developed methodological framework has been implemented and applied on a case-study in the domain of water protection from pesticides used in agriculture, which was the third goal of the thesis.

10.1 Contributions of the Thesis

The main novelty of the study in the thesis consists in the following contributions and corresponding results:

Contribution 1

We have proposed quasi ex-post risk analysis as a complementary approach to ex-post risk analysis that considers the classical ex-post approach over a predicted or diagnosed state of the world. The former is achieved by introducing a predictive layer

within the risk assessment module, while the latter is accomplished by introducing a diagnostic layer. Both layers are embedded into the risk assessment module of the proposed methodological framework.

Contribution 2
We further extended the methodological framework to allow defining the output format in accordance with the three decision making tasks, by introducing a risk management module. The risk management module has also been designed to allow consideration of the state of the world at time $t+1$ along with the gained utility.

Contribution 3
The risk assessment and the risk management modules have been formalized in a methodological framework of quasi ex-post risk analysis.

Contribution 4
We have applied the methodological framework on a case-study where the decision problem is in the domain of agriculture, in particular to the decision problem regarding water protection from pesticides used in agriculture.

The aforementioned contributions have been verified by confirming the hypothesis stated at the beginning of the thesis:

Hypothesis 1
The introduction of quasi ex-post risk assessment enriches the process of decision analysis with additional information with quantified certainty, filling the gap in imperfect knowledge. The predictive and diagnostic layers of quasi ex-post risk assessment inherit properties of the ex-post approach, and additionally try to discover uncertain attributes in the process, and quantify the risk. The introduction of the predictive and the diagnostic layer and their implementation in the case-study confirms the hypothesis that the uncertain state of the world can be better estimated in terms of providing additional information during risk assessment.

Hypothesis 2
The risk management module further extends the proposed methodological framework in order to find a solution for the assessed risk. This module supports the autonomy of the process and delivers support to the decision maker. Moreover, the support delivered can cover additional steps in order to satisfy the decision maker's criteria or requirements of how the support should be designed. Namely, the risk management module contains resources to process the decision support along the lines of decision making tasks defined by Roy (2005): choosing, sorting and ranking tasks. In addition, the risk management module has the ability to express preferences in accordance with the gained utility and the state of the world that would take place at time $t+1$. The formalization of the risk management module and its implementation in the case-study confirms the corresponding hypothesis.

Hypothesis 3
The applicability and evaluation of the proposed methodological framework is tested on a case-study in the domain of agriculture and environmental protection for the problem of surface and ground water pollution with pesticides used in agriculture. The implementation of the methodological framework confirms this hypothesis of applicability of the proposed framework to complex decision problems. Furthermore, it evaluates the performance of the predictive and diagnostic layers by comparison with measured data collected from the experimental site. The case-study results in

a decision support system that covers the post-market risk evaluation of pesticides used in agriculture. Such a system allows farmers to evaluate the risk already when planning a plant protection programme. This results in suggestions or recommendations of mitigation measures to be considered in case the programme is assessed to be risky.

The developed decision support system over the implementation of the proposed methodological framework directly contributes in filling the gap between EU Directives (Regulations) (European Parliament & Council, 2009a, 2000) for water protection, which are characterized as very general but still complex and restrictive, and the agriculture that may suffer collateral damage from the implementation of those regulations. Finally, the developed decision support system is web-based and has a graphical user interface, which makes it widely accessible to farmers and the their advisers.

The formalized methodological framework of quasi ex-post risk analysis can be implemented on a wide variety of cases from different domains. However, there are limitations that can be presented as requirements for an implementation of the framework. Namely, the methodological framework will not be of added value if (**1**) the decision problem does not require evaluation of the alternative set in accordance with states of the world at times t' or $t+1$; (**2**) data and expert knowledge are not available in order to build a predictive or a diagnostic layer that will fill the gap of imperfect knowledge.

10.2 Further Work

The work presented in the thesis and the implementation of the proposed methodological framework raise new challenges in different segments of the framework. In the risk assessment module of quasi ex-post risk analysis, the following are seen as possible improvements:

1. Implementation of different machine learning methods and decision models for learning and diagnostic layers;

2. Improvement in the scope of uncertainty quantification when multiple models are integrated within a predictive layer and investigating of the sensitivity of the risk management module when uncertainty quantification varies.

Research directions for further work also arise in the risk management module. The current methodological framework requires well defined models for each task within a module, which could be improved by introducing behavioral learning or personalization:

1. The task of alternative evaluation could be improved in time with different optimization techniques, instead of exhaustive search;

2. The task of choice-set selection could be replaced with deductive choice-set determination, which would attempt to learn a model for choosing a set of alternatives on the basis of a decision maker's behavior;

3. The task of ranking could be replaced with a deductive ranking model, learned from previous decision maker's selections and orderings.

Overall, the research directions for further work could be focused on automation of the implementation by developing a workflow system. This system could offer a graphical user interface as a tool for automatic implementation. Finally, implementation of the proposed methodological framework over wider domains of decision problems will extend its design, power and usefulness.

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Bibliography

Publications Related to the Thesis

Journal Articles

Kuzmanovski, V., Trajanov, A., Leprince, F., Džeroski, S., & Debeljak, M. (2015). Modeling water outflow from tile-drained agricultural fields. *Science of The Total Environment*, *505*(1), 390–401. doi:http://dx.doi.org/10.1016/j.scitotenv.2014.10.009

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Conference Abstracts

Kuzmanovski, V., Leprince, F., Džeroski, S., & Debeljak, M. (2013). Modeling the water outflow in an arable ecosystem. In *Book of abstracts : isem 2013, ecological modelling for ecosystem sustainability*.

Trajanov, A., Kuzmanovski, V., Leprince, F., Réal, B., Dutertre, A., Maillet-Mezeray, J., ... Debeljak, M. (2014). Studying the drainage periods for agricultural fields with data mining : la jaillière case study. In *Book of abstracts - discovery science 2014*.

Other Publications

Journal Articles

Ceci, M., Pio, G., Kuzmanovski, V., & Džeroski, S. (2015). Semi-supervised multi-view learning for gene network reconstruction. *PloS one*, *10*(12).

Biography

Vladimir Kuzmanovski was born on 9 February 1987 in Kumanovo, Republic of Macedonia. He has completed secondary school in his birthplace. In 2005 he started his studies at the Institute of Informatics, Faculty of Mathematics and Natural Sciences, University Ss Cyril and Methodius in Skopje, Republic of Macedonia.

He was enrolled in BSc program in the area of Computer and Software Engineering. He defended his BSc thesis titled "FastBit optimization of bitmap indices" under the supervision of Professor Goran Velinov.

Later, in 2012 he has completed master studies at the Jožef Stefan International Postgraduate School, Ljubljana, Slovenia. He defended his MSc thesis titled "Integration of expert knowledge and predictive learning: Modelling water flows in agriculture" under the supervision of Prof. Dr. Marko Debeljak.

In 2012 he started his doctoral studies at the Jožef Stefan International Postgraduate School, Ljubljana, Slovenia. His research is in the field of data mining and decision support systems and includes the study, developments and application of different data mining algorithms. The results of his research work were published in several journals and presented at several conferences.