Logistic Regression

- Probabilistic linear classifier
- Logistic (sigmoid) function $f(x)=1/(1+e^{-x})$
  - Where $x = w_0 + \sum_i w_i x_i$
  - $f(x) = P(C=1 \mid X)$

- $w_0 + \sum_i w_i x_i = 0$ defines a hyperplane where $P(C=1 \mid X) = 0.5$ and $P(C=0 \mid X) = 0.5$

  and $w_0 + \sum_i w_i x_i$ is proportional to the distance from the hyperplane

- Learning
  - no closed form solution - optimization, e.g., with gradient descent
  - definition of a cost function (several options); $-y \log (y') - (1-y) \log (1-y')$; y in {0,1}
  - updating of weights (according to optimization results); $w_j = w_j - \alpha \sum_i (y'_i - y_i) x_{ij}$
    for all instances, multiple times

SVM

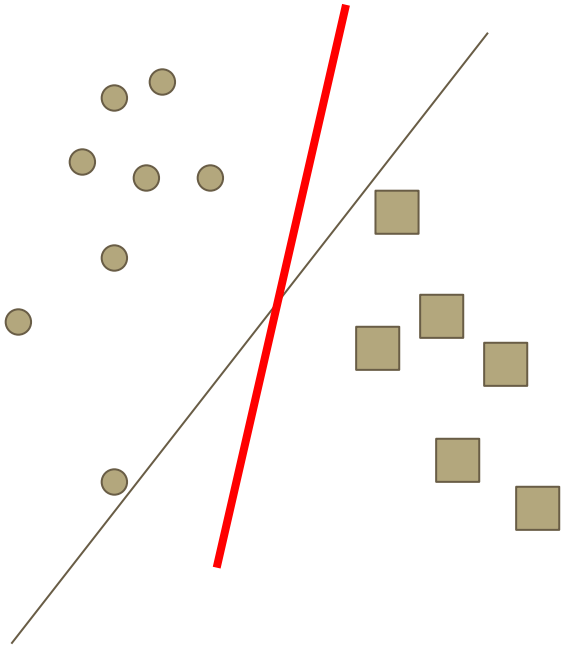
- Linear binary classifier (not probabilistic)
- Extension of linear classifiers to model non-linear decision boundaries
  - Transformation of the feature space using synthetic features of higher order

$$y' = w_0 + w_1x_1 + w_2x_2 + w_3x_1^2 + w_4x_2^2 + w_5x_1x_2$$

- But this brings problems
  - Computational complexity (a lot more parameters to learn, transformation operations)
  - Overfitting
- SVM algorithm deals with these (max. margin & SV, kernel trick & SV)

SVM - max. margin

- Model (linear, *hyperplane*) for separation of data by using the *maximal margin* principle (MAX: robustness, SV: stability)



$$\overline{W} \cdot \overline{X} + b = 0$$

$$\overline{W} \cdot \overline{X_i} + b \geq 0 \quad \forall i : y_i = +1$$

$$\overline{W} \cdot \overline{X_i} + b \leq 0 \quad \forall i : y_i = -1$$

- Learning: maximal margin (optimal hyperplane) optimization problem
- Soft margin to allow misclassifications
  - Distance on the wrong side: ξ_i
  - Parameter *C* (misclassification cost) - set with experimentation!
  - Penalty: $C \cdot \xi^r_i$

SVM - kernel trick

- Use of higher dimensions for linearly non-separable data
  - https://www.youtube.com/watch?v=3liCbRZPrZA

- Learning (optimization) involves dot products in the term to maximize:

$$L_D = \sum_{i=1}^{n} \lambda_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i \lambda_j y_i y_j \overline{X_i} \cdot \overline{X_j}$$

Dot product is needed,
(not feature values)

~similarity

classification too:

We can avoid
representing W

$$F(\overline{Z}) = \text{sign}\{\overline{W} \cdot \overline{Z} + b\} = \text{sign}\{(\sum_{i=1}^{n} \lambda_i y_i \overline{X_i} \cdot \overline{Z}) + b\}$$

SVM - kernel trick, here it is

- We do not need the feature values, just dot products
- Transformation would mean:

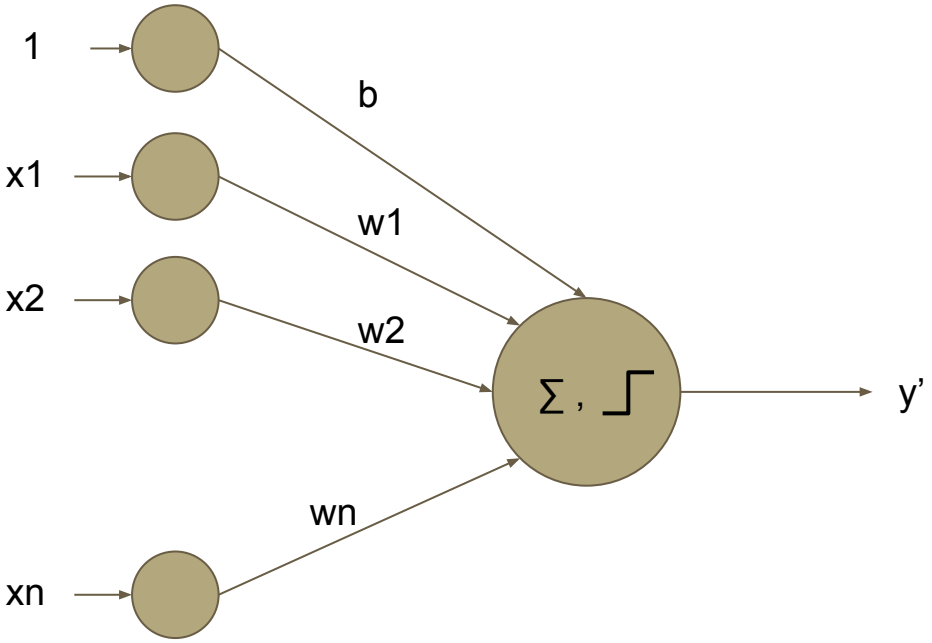
  $\Phi(x_i) \cdot \Phi(x_i)$

  calculation of transformations, then the lengthy dot products...

- Instead, we can use a function such that: $K(x_i, x_j) = \Phi(x_i) \cdot \Phi(x_i)$
  - And $K(x_i, x_j)$ is in original space!
    - EXAMPLE !
  - We can only calculate kernels (polynomial, Gaussian RBF, ...)
  - Simetric, positive semi-definite; similarity ; even for strings, graphs
  - The mapping Φ can now be only implicitly used

Neural networks - perceptron

- Inspired by (simulation of) the human nervous system



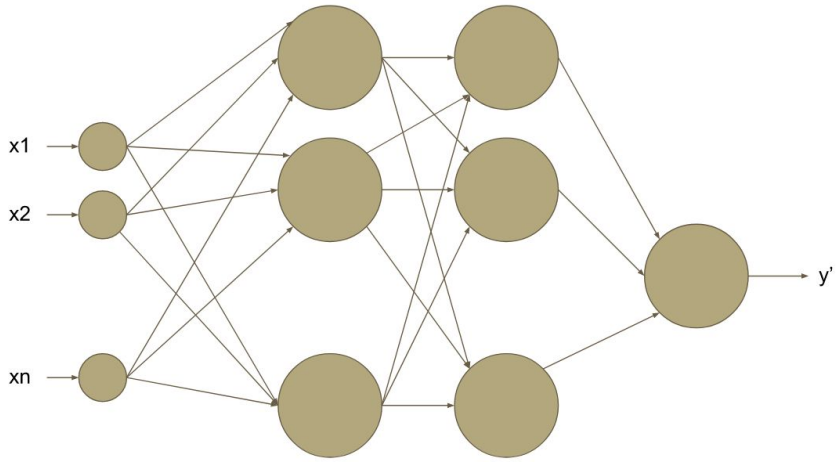
$$y' = sign(\sum_i w_i x_i + b)$$

Learning (iterative process):

- Initialize weights
- For each training item (**x**,**y**)
  - y' = f(w,x)
  - update all weights
    $w_i' = w_i + \eta(y_i - y'_i)x_i$
- Until convergence

- Can learn (converge) in linearly separable situations
- Finds (some!) linear separation

Neural networks with hidden layers



- Very powerful in capturing arbitrary functions
  - having non-linear activation functions; careful selection to facilitate learning
- Automatic generation of (higher-level) features!
  - last level is similar to logreg on generated (relevant) high-level features, not all quadratic, cubic, ... which easily go into hundreds of thousands.
- Drawbacks
  - computationally demanding learning (recently alleviated)
  - more layers - more power - more prone to overfitting
  - black-box models

Neural network - use (forward propagation)

Use of a neural network

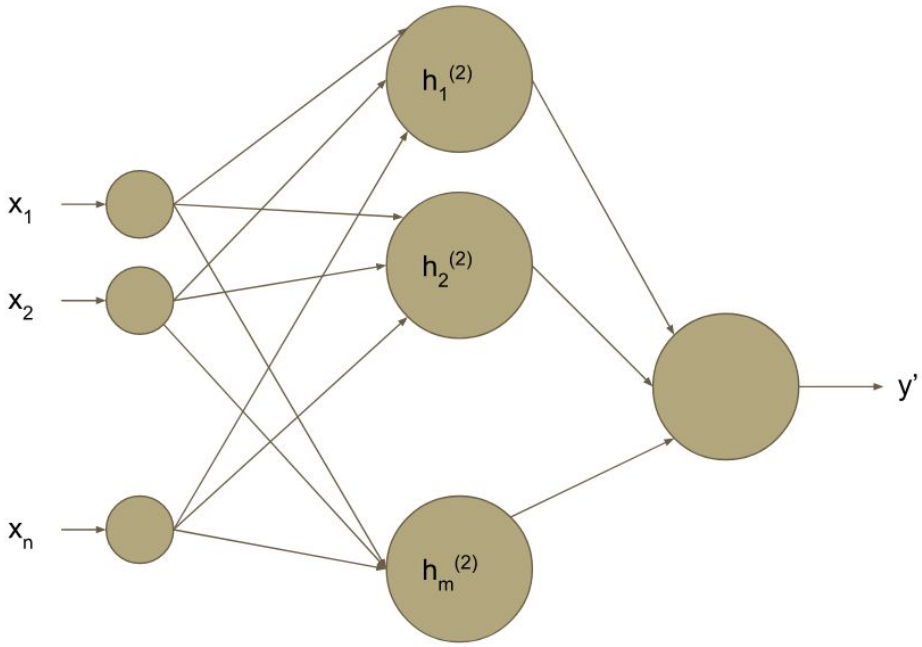
$$h_1^{(2)} = f(w_{11}^{(1)}x_1 + w_{12}^{(1)}x_2 + \ldots + w_{1n}^{(1)}x_n)$$

$$h_2^{(2)} = f(w_{21}^{(1)}x_1 + w_{22}^{(1)}x_2 + \ldots + w_{2n}^{(1)}x_n)$$

...

$$h_m^{(2)} = f(w_{m1}^{(1)}x_1 + w_{m2}^{(1)}x_2 + \ldots + w_{mn}^{(1)}x_n)$$

$$y' = f(w_{11}^{(2)}h_1^{(2)} + w_{12}^{(2)}h_2^{(2)} + \ldots + w_{1m}^{(2)}h_m)$$



Neural networks - learning

- Two things to learn:
  - Structure: expert knowledge and experimentation
  - Parameters/weights : backpropagation (and other optimization approaches)
    - Gradient descent (consequence: step → sigmoid; error 0/1 → $(y-y')^2$)
      - Optimum can be local !
    - Can be done in a batch or online mode
    - Overfitting problem - stop on check with holdout, ...
    - Computationally demanding
    - Nice explanation of the procedure in the Weka book CHECK!
      - Activation function selection was not random ;)

Ensemble methods

- Combine results of multiple classifiers
  - Different learners
  - Different training data subsets
  - Combined predictions
    - averaging
    - weighted voting
    - model of combination
- Helps tackling error components
  - Bias
    - Model assumptions (e.g., linear separation)
    - Consistently incorrect for some instances
  - Variance
    - Data variations leading to very different models (~ overfitting)
    - Inconsistently classified data
  - Noise
    - Intrinsic error in target class
    - Some algorithms are more affected, some less

Bagging

- Single learning algorithm
- *k* data samples with replacement
- *k* learned (same kind) classifiers
- Majority vote
- Reduces variance (makes sense for low bias learners, e.g. deep trees)
- Models are independent, can be built in parallel

Boosting

- Single learning algorithm
- Weighted training instances
  - Adapted learning
  - Weighted data sampling
- Iterative reweighting according to classifier performance
- Focus on misclassified instances in next iteration (increased weights)
  - Various increase approaches and termination criteria
- Aggregation of weighted (according to performance) predictions
- Reduces overall bias (to be used with simple, high bias, models)
- Reduction of variance depends on intensity of reweighting scheme
  - No reweighting in iterations == bagging
- Sensitive to noise (training can focus on bad data!)
- Models depend on previous ones, sequential process

Stacking

- Combination of predictions with another machine learned model
- Two level classification, two data subsets
- *k* classifiers (bagged, boosted or from different learners) learned on the first subset
- Their outputs on second subset are *k* new features
- Second level classifier is trained on
  - new feature space (of size *k*), or
  - combined feature space (old+new)

Random forest

- Similar as bagging with decision trees, but promotes more diverse trees
  - Decision trees in bagging tend to be similar
- Randomness at splits:
  - A random subset of attributes
  - Often advised: $\log_2(\#all\_atribs)+1$
- Usually no or minimal pruning
- Also bootstrapped data samples (as in bagging)
- Majority vote
- Efficient (less attributes considered at splits)
- Resistant to noise, outliers and overfitting

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Gradient boosted trees

- Construct a (regression) tree and let the residuals (y-F(x)) become a new target for another model in the iteration
- Next model learns the residuals of the first one
  - Using original features and the new target
- Taking the two models together we get a better prediction
- Repeat *m* times, until stopping criterion...
- In fact: a gradient of a differentiable loss function is usually modelled instead of actual residuals (added parameter: step size)
- Sensitive to noise
- Sequential (cannot run in parallel)

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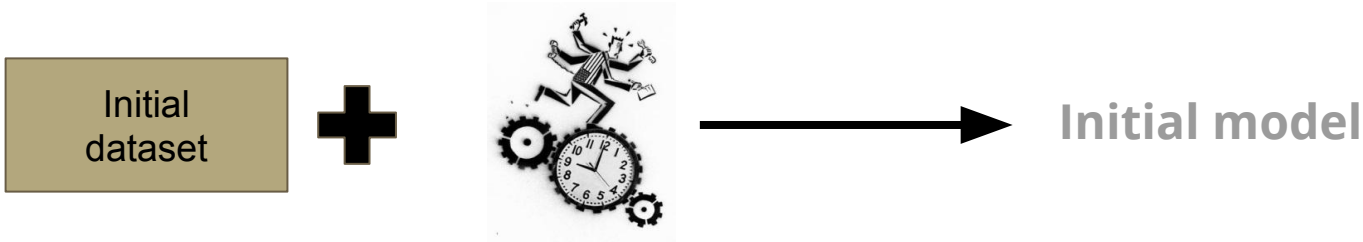
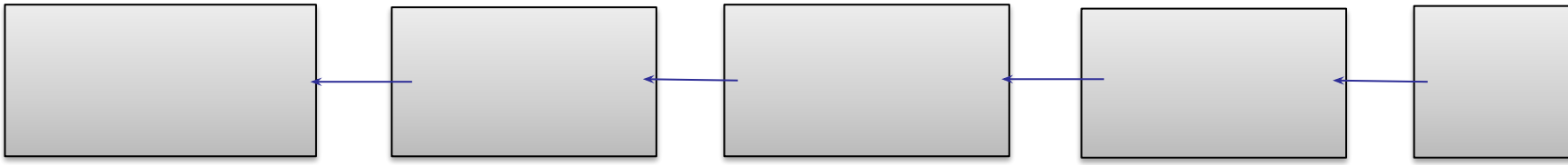
→ **ESA challenge example**

Active learning

- Labels are sometimes hard or expensive to get
  - Time restrictions in dynamic settings
- AL aims at getting the most of information with the least amount of labels
- Components
  - Querying system : selects the instances to be labelled
  - Oracle : provides labels
- Querying strategies
  - Highest uncertainty regions (danger: querying in low data quality areas)
  - Expected error of variance reduction
  - Representativeness
    - Equal representativeness of regions (weighted by density)
  - And many others and their mixtures...

Active learning

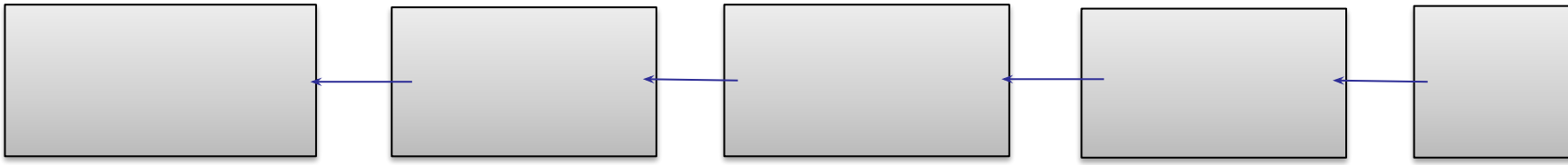


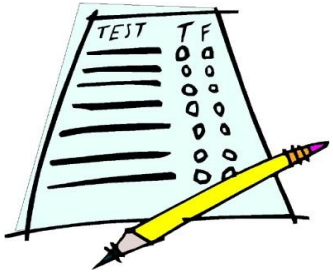


Active learning

Initial dataset

Initial model





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Active learning

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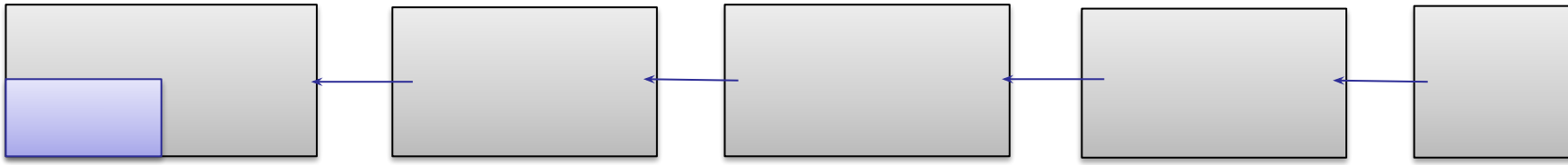

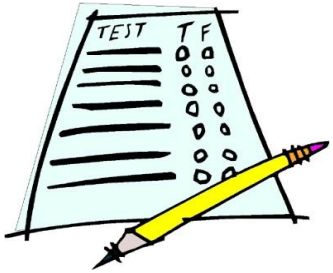

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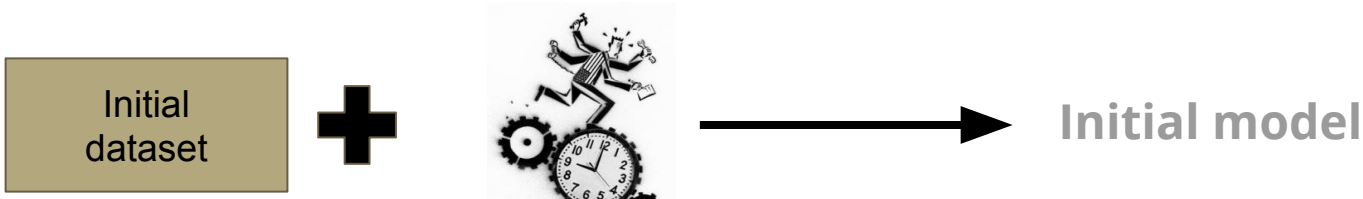
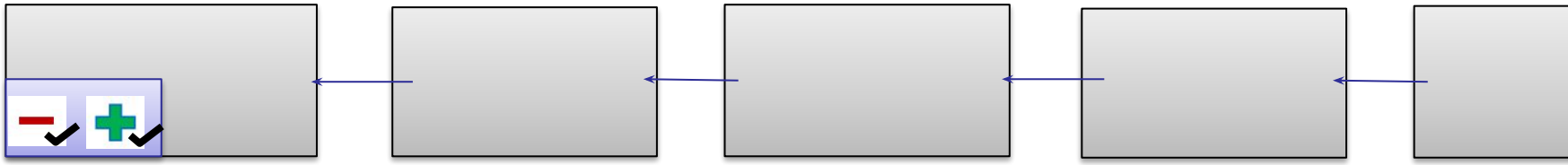
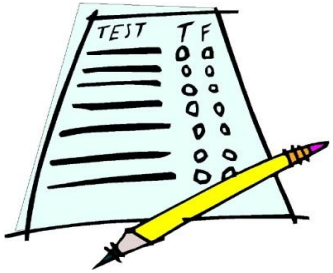
Active learning







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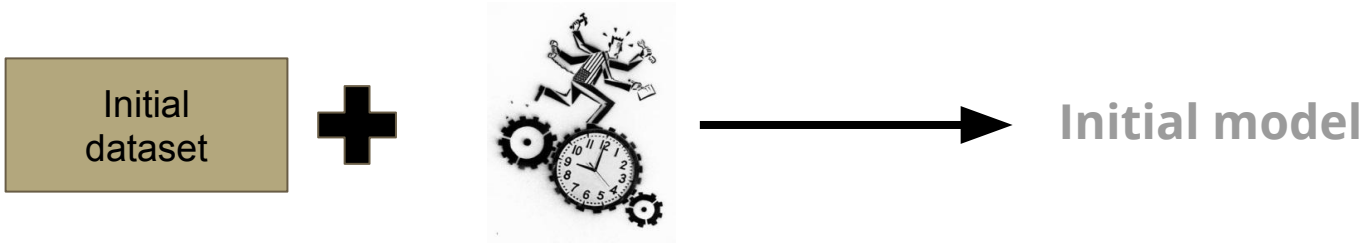

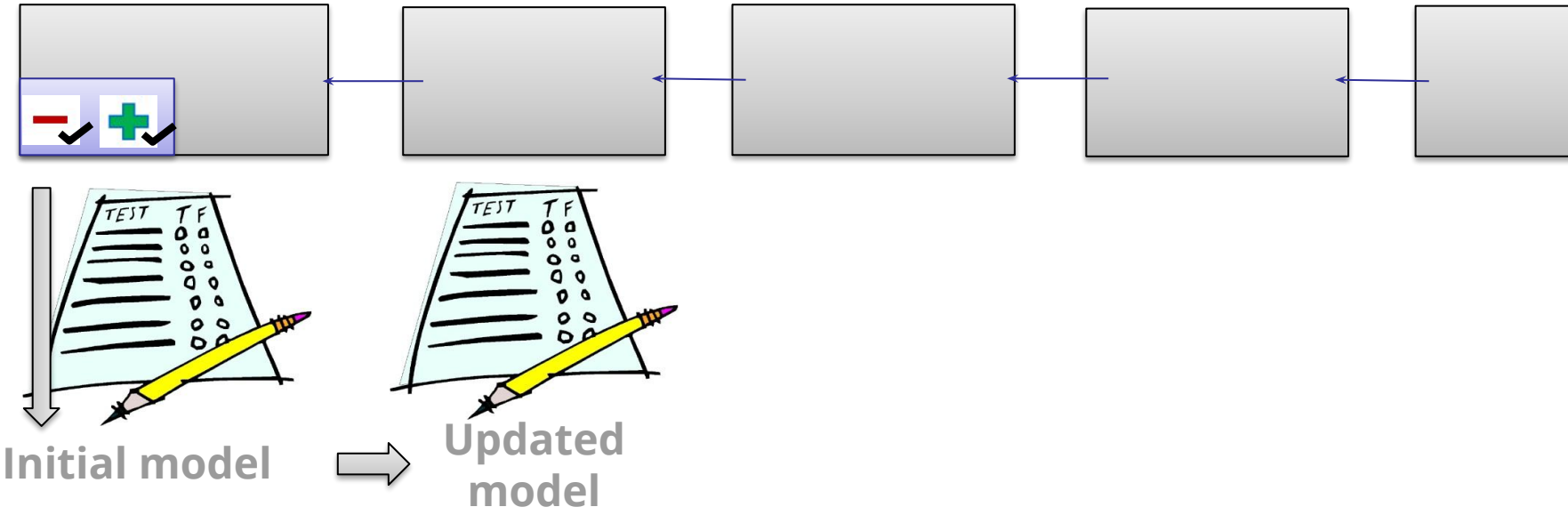

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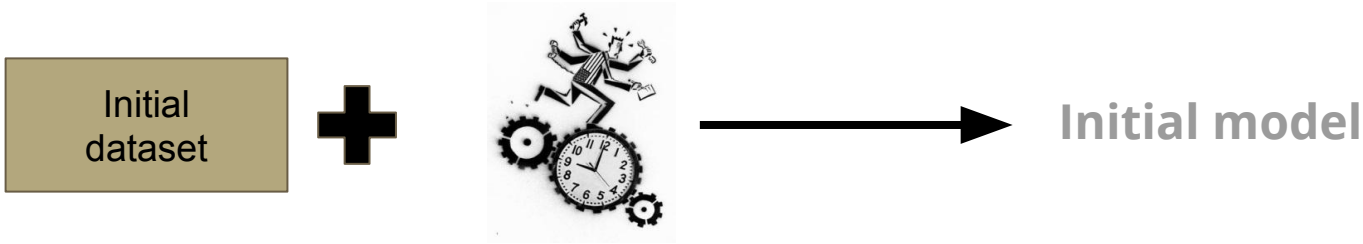

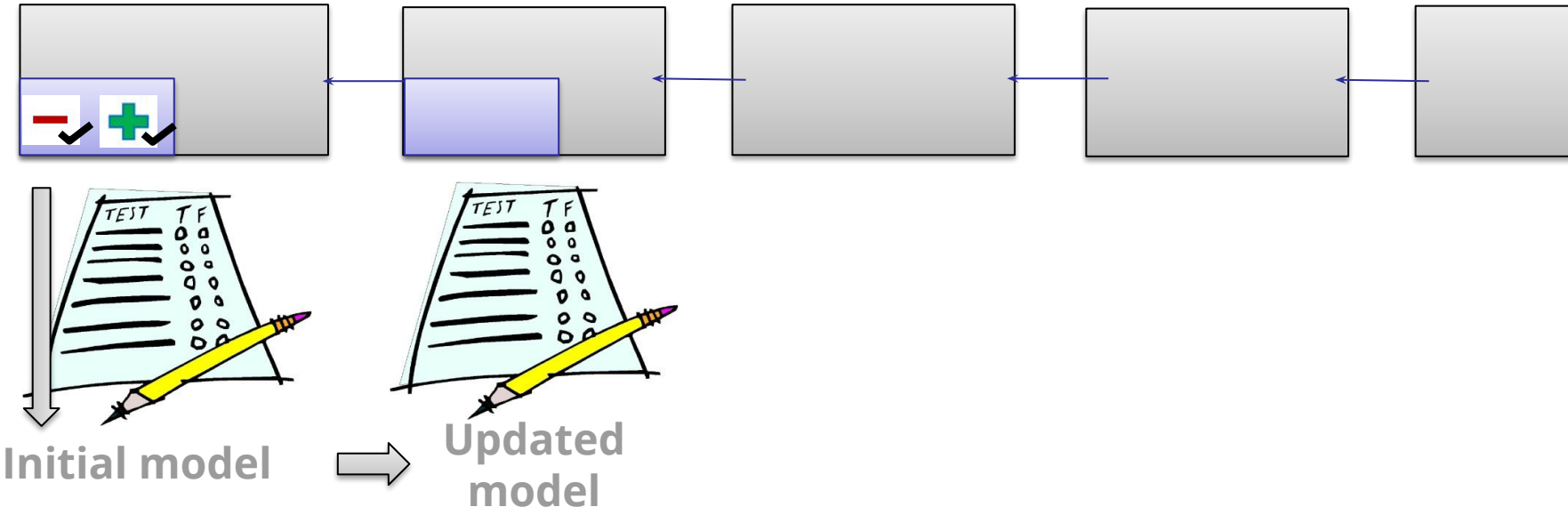

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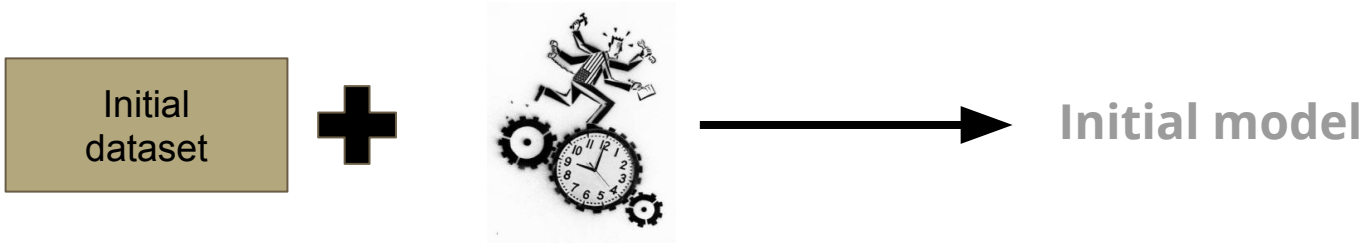

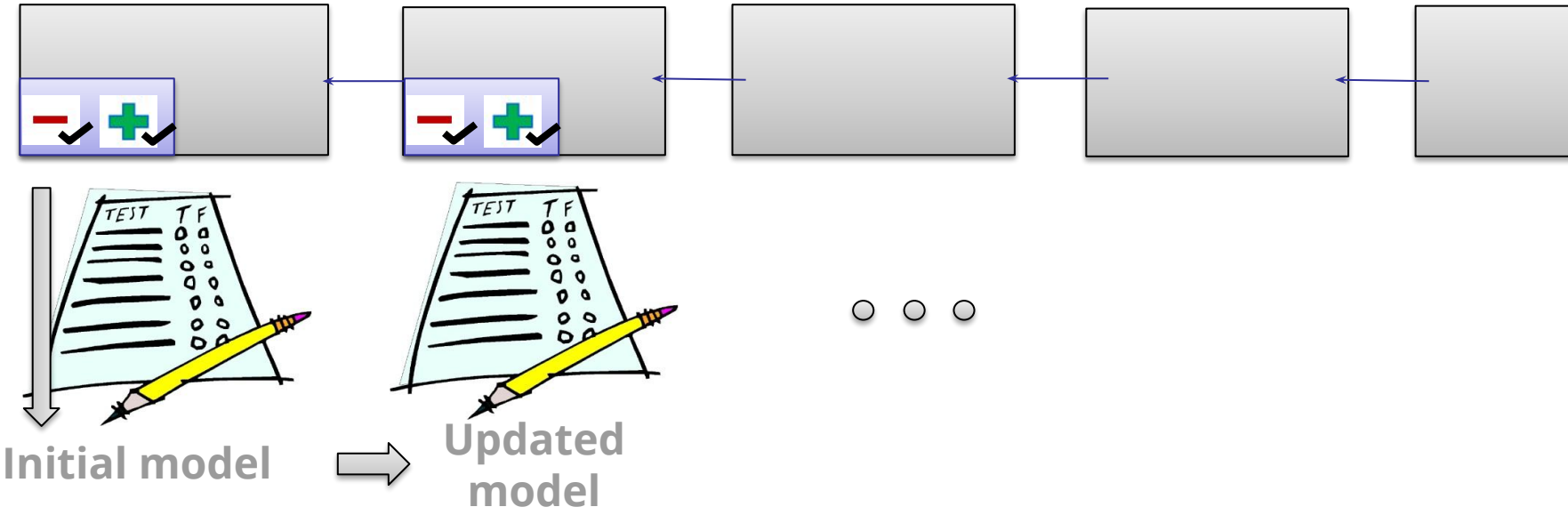

Active learning