UNIVERSITÄT MANNHEIM

Data Mining II
Ensembles

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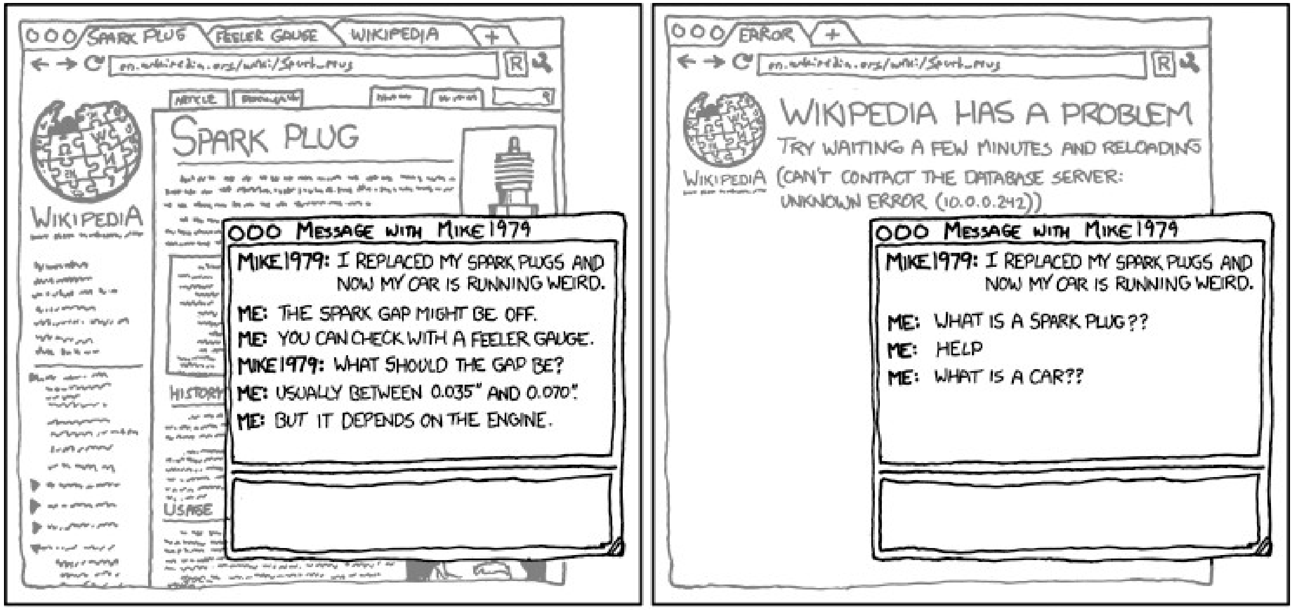
Introduction

- “Wisdom of the crowds”
  - a single individual cannot know everything
  - but together, a group of individuals knows a lot
- Examples
  - Wikipedia
  - Crowdsourcing
  - Prediction

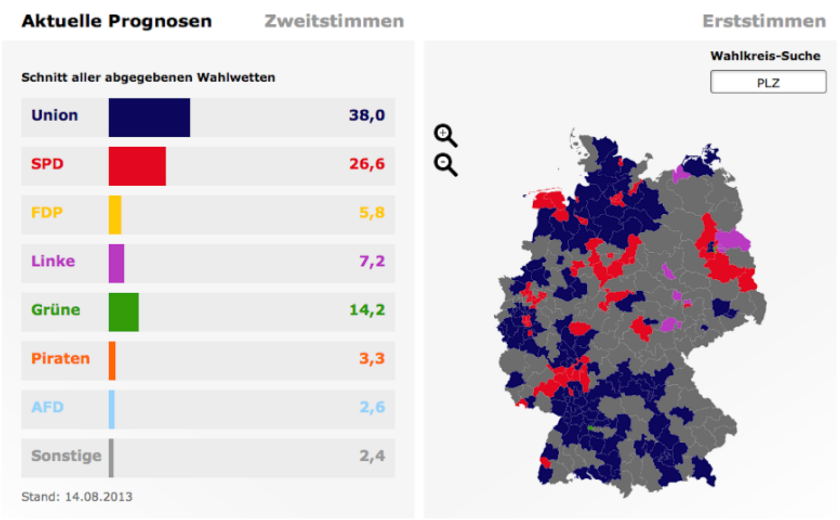


WHEN WIKIPEDIA HAS A SERVER OUTAGE, MY APPARENT IQ DROPS BY ABOUT 30 POINTS.

http://xkcd.com/903/

Introduction

- “SPIEGEL Wahlwette” (election bet) 2013
  - readers of *SPIEGEL Online* were asked to guess the federal election results
  - average across all participants:
    - only a few percentage points error for final result
    - conservative-liberal coalition cannot continue



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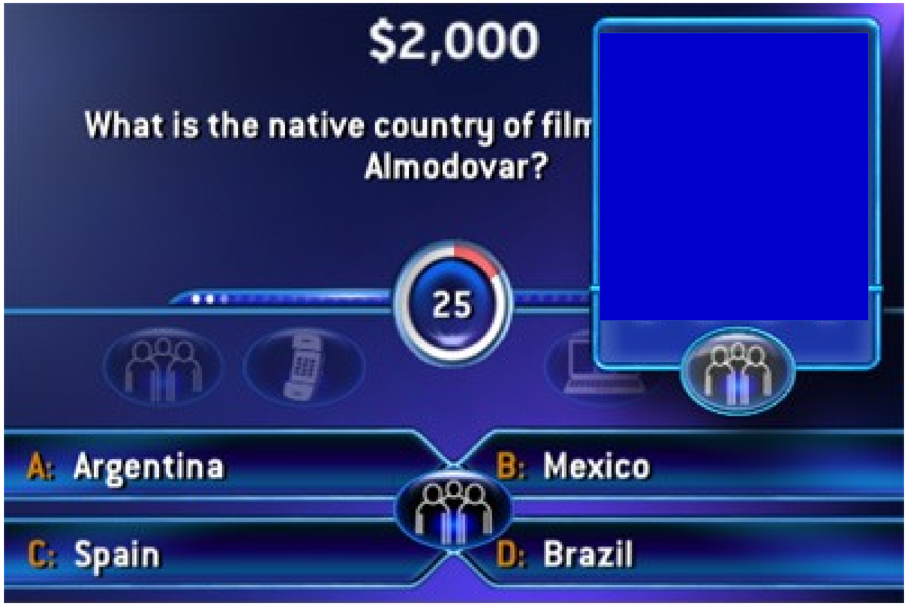
Introduction

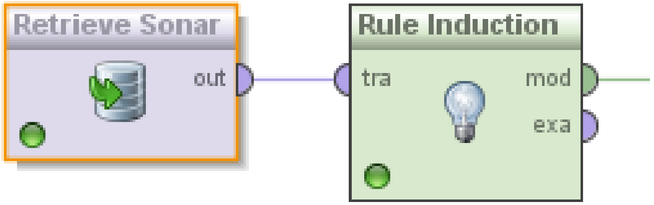
- "Who wants to be a Millionaire?"
- Analysis by Franzen and Pointner (2009):
  - "ask the audience" gives a correct majority result in 89% of all cases
  - "telephone expert": only 54%



http://hugapanda.com/wp-content/uploads/2010/05/who-wants-to-be-a-millionaire-2010.jpg

Ensembles

- So far, we have addressed a learning problem like this:



- Ensembles:
  - wisdom of the crowds for learning operators
  - instead of asking a single learner,
    combine the predictions of different learners

Ensembles

- Prerequisites for ensembles: accuracy and diversity
  - different learning operators can address a problem (accuracy)
  - different learning operators make different mistakes (diversity)

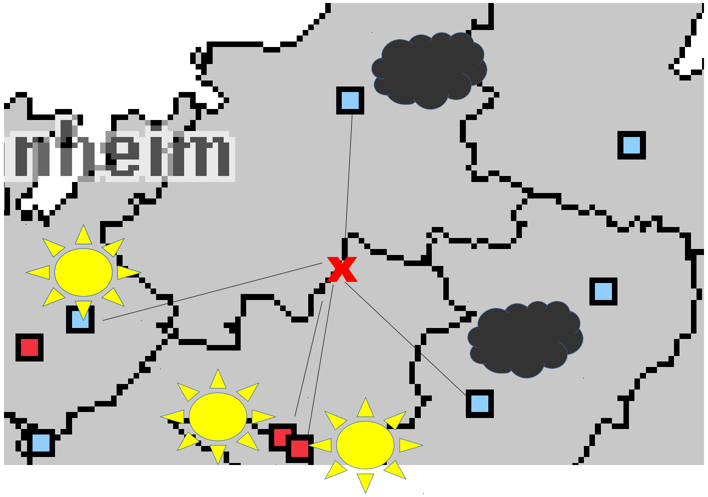
- That means:
  - predictions on a new example may differ
  - if one learner is wrong, others may be right

- Ensemble learning:
  - use various *base learners*
  - combine their results in a single prediction

Voting

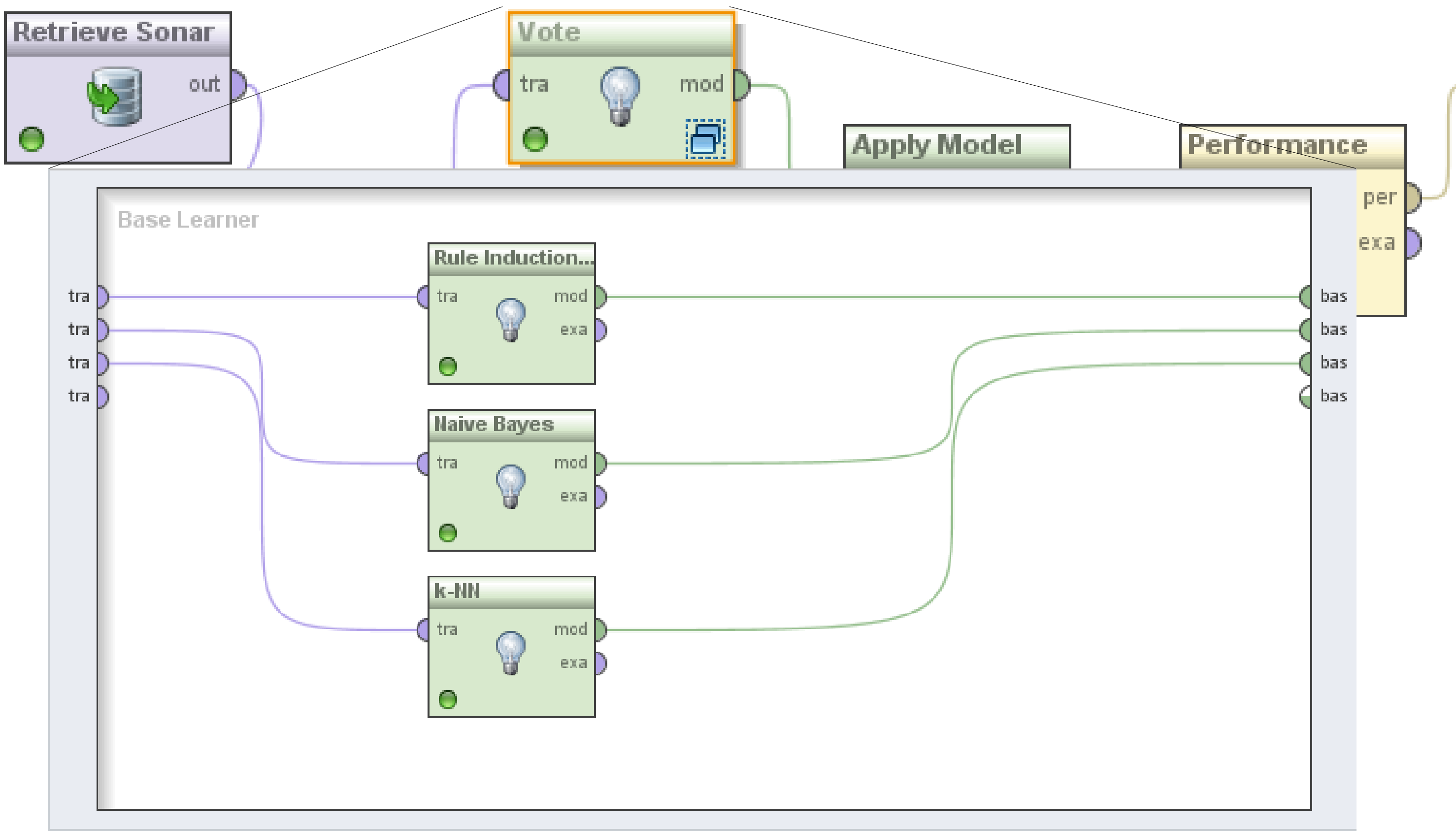
- The most straight forward approach
  - classification: use most-predicted label
  - regression: use average of predictions

- We have already seen this
  - k-nearest neighbors
  - each neighbor can be regarded as an individual classifier



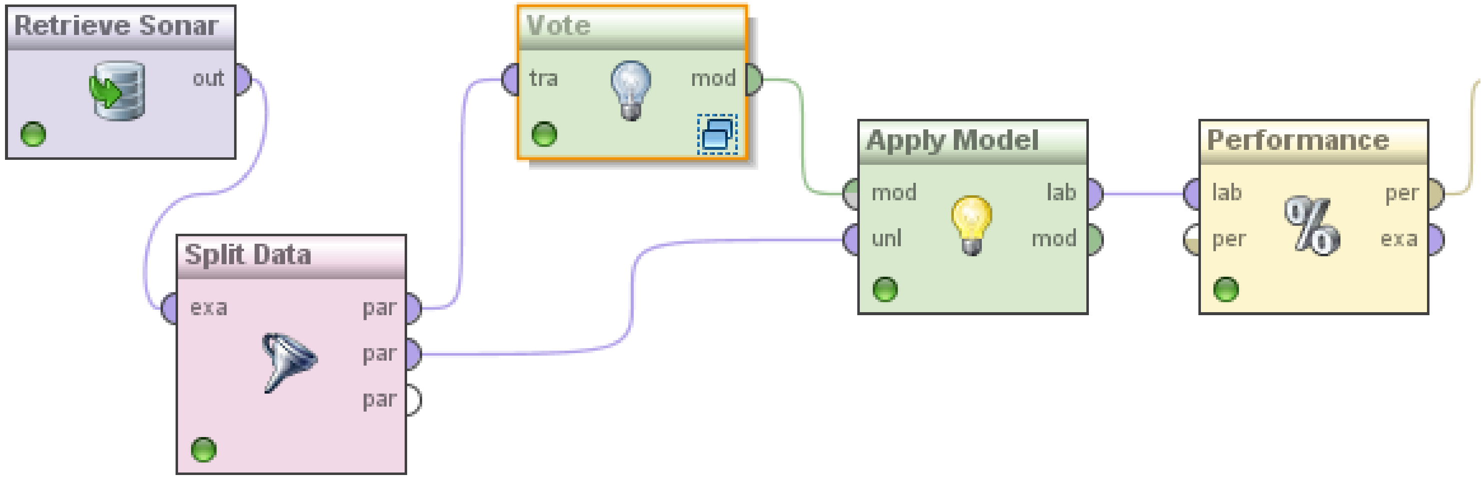
Voting in RapidMiner

- Vote operator uses different base learners



Voting in RapidMiner

- Accuracy in this example:
  - Naive Bayes: 0.71
  - Ripper: 0.71
  - k-NN: 0.81
- Voting: 0.91



Why does Voting Work?

- Suppose there are 25 base classifiers
  - Each classifier has an accuracy of 0.65, i.e., error rate $\varepsilon = 0.35$
  - Assume classifiers are independent
    - i.e., probability that a classifier makes a mistake does not depend on whether other classifiers made a mistake
    - **Note:** in practice they are not independent!
- Probability that the ensemble classifier makes a wrong prediction
  - The ensemble makes a wrong prediction if the majority of the classifiers makes a wrong prediction
  - The probability that 13 or more classifiers are wrong is

$$\sum_{i=13}^{25} \binom{25}{i} \varepsilon^i (1-\varepsilon)^{25-i} \approx 0.06 \ll \varepsilon$$

Why does Voting Work?

- In theory, we can lower the error infinitely
  - just by adding more base learners

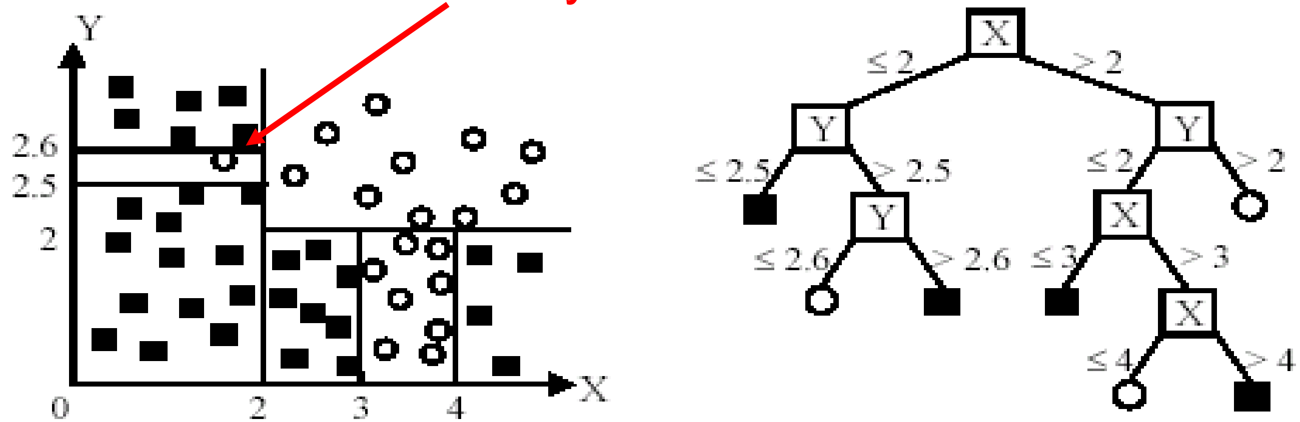
$$\sum_{i=13}^{25} \binom{25}{i} \varepsilon^{i} (1-\varepsilon)^{25-i} \approx 0.06 \ll \varepsilon$$

- But that is hard in practice
  - Why?

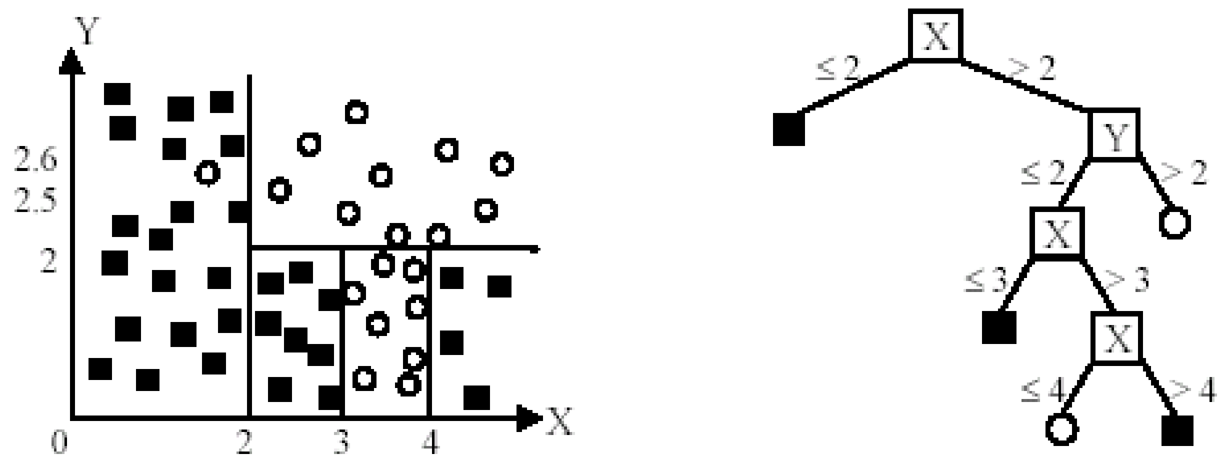
- The formula only holds for *independent* base learners
  - It is hard to find many truly independent base learners
  - ...at a decent level of accuracy
- Recap: we need both *accuracy* and *diversity*

Recap: Overfitting and Noise

Likely to overfit the data



(A) A partition of the data space (B). The decision tree



Bagging

- Biases in data samples may mislead classifiers
  - overfitting problem
  - model is overfit to single noise points

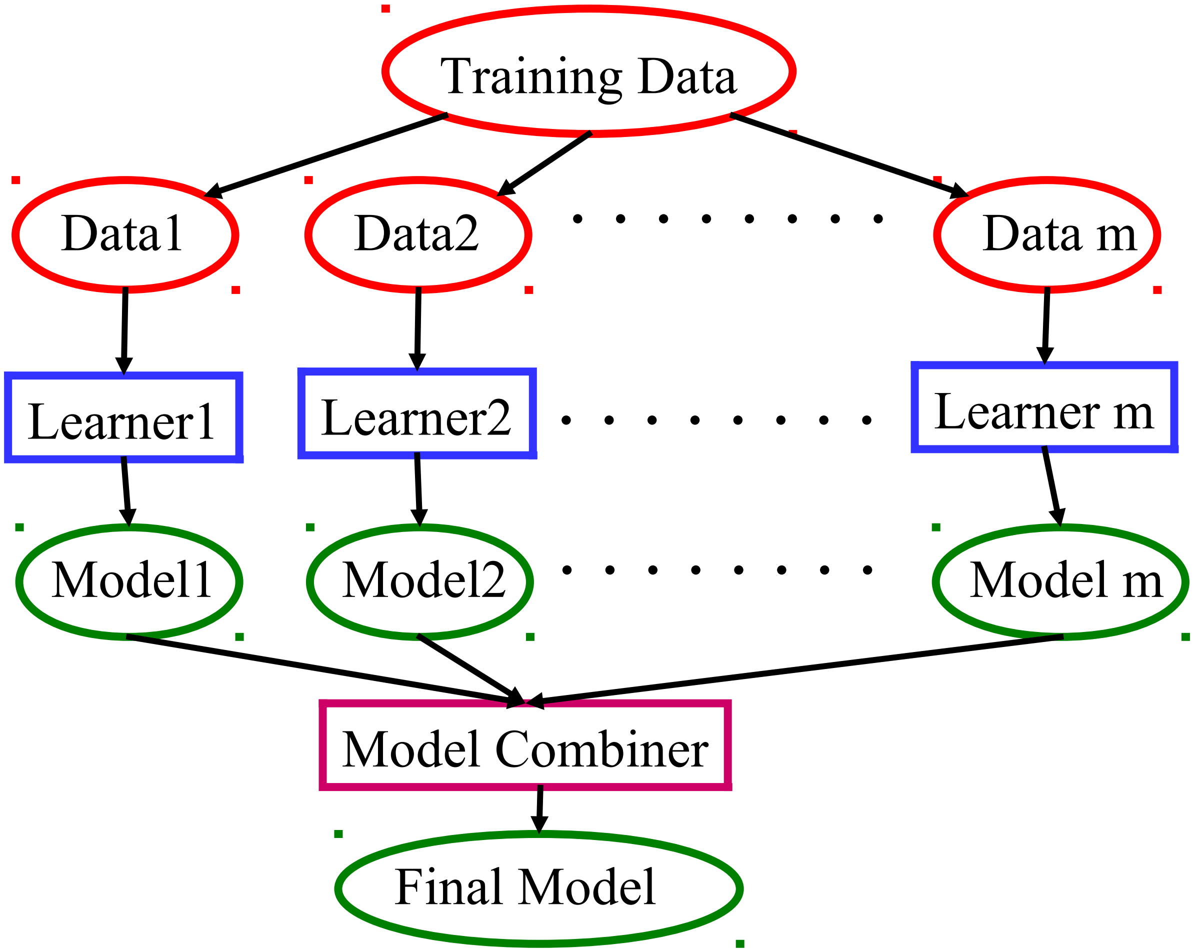
- If we *had* different samples
  - e.g., data sets collected at different times, in different places, …
  - ...and trained a single model on each of those data sets...
  - only one model would overfit to each noise point
  - voting could help address these issues

- But usually, we only have one dataset!

Bagging

- Models may differ when learned on different data samples
- Idea of bagging:
  - create samples by picking examples *with replacement*
  - learn a model on each sample
  - combine models
- Usually, the same base learner is used
- Samples
  - differ in the subset of examples
  - replacement randomly re-weights instances (see later)

Bagging: illustration



Bagging: Generating Samples

- Generate new training sets using sampling with replacement (bootstrap samples)

Original Data	1	2	3	4	5	6	7	8	9	10
Bagging (Round 1)	7	8	10	8	2	5	10	10	5	9
Bagging (Round 2)	1	4	9	1	2	3	2	7	3	2
Bagging (Round 3)	1	8	5	10	5	5	9	6	3	7

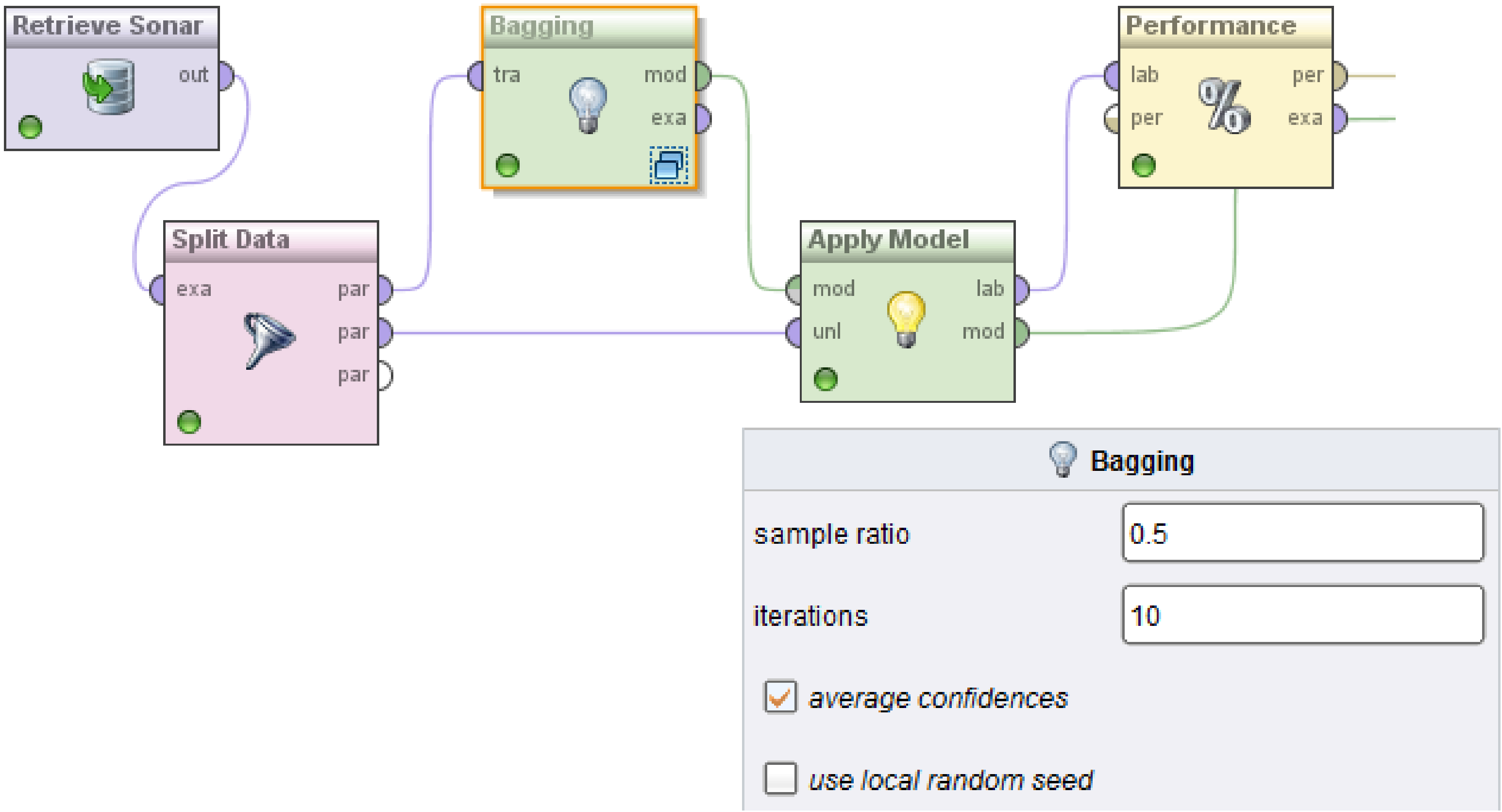
  - some examples may appear in more than one set
  - some examples will appear more than once in a set
  - for each set of size n, the probability that a given example appears in it is

$$Pr(x \in D_i) = 1 - (1 - \frac{1}{n})^n \rightarrow 0.6322$$

    - i.e., on average, less than 2/3 of the examples appear in any single bootstrap sample

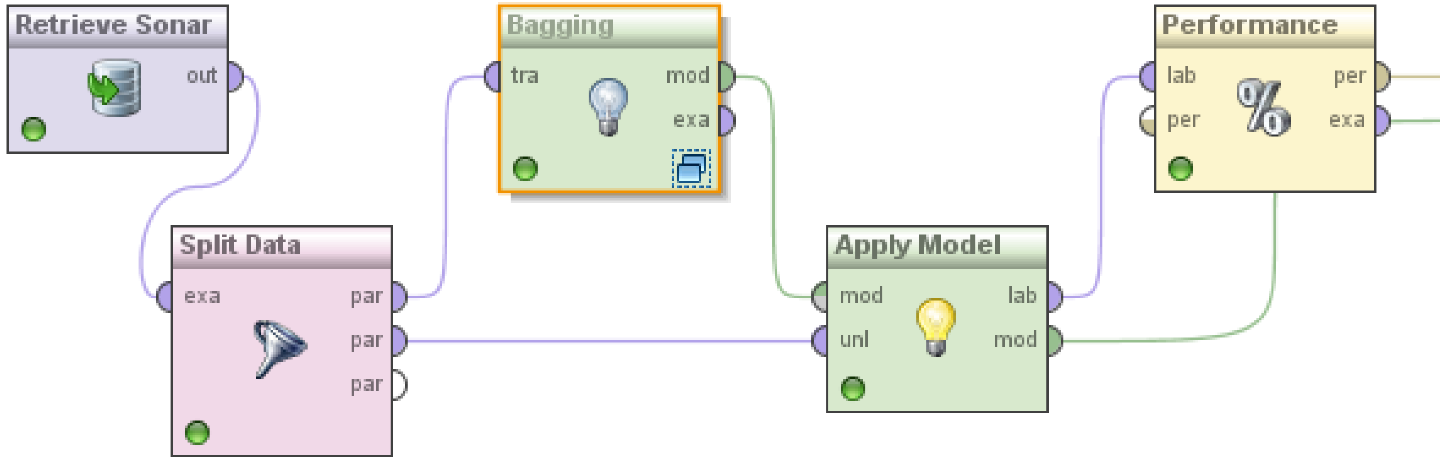
Bagging in RapidMiner

- Bagging operator uses a base learner
- Number and ratio of samples can be specified



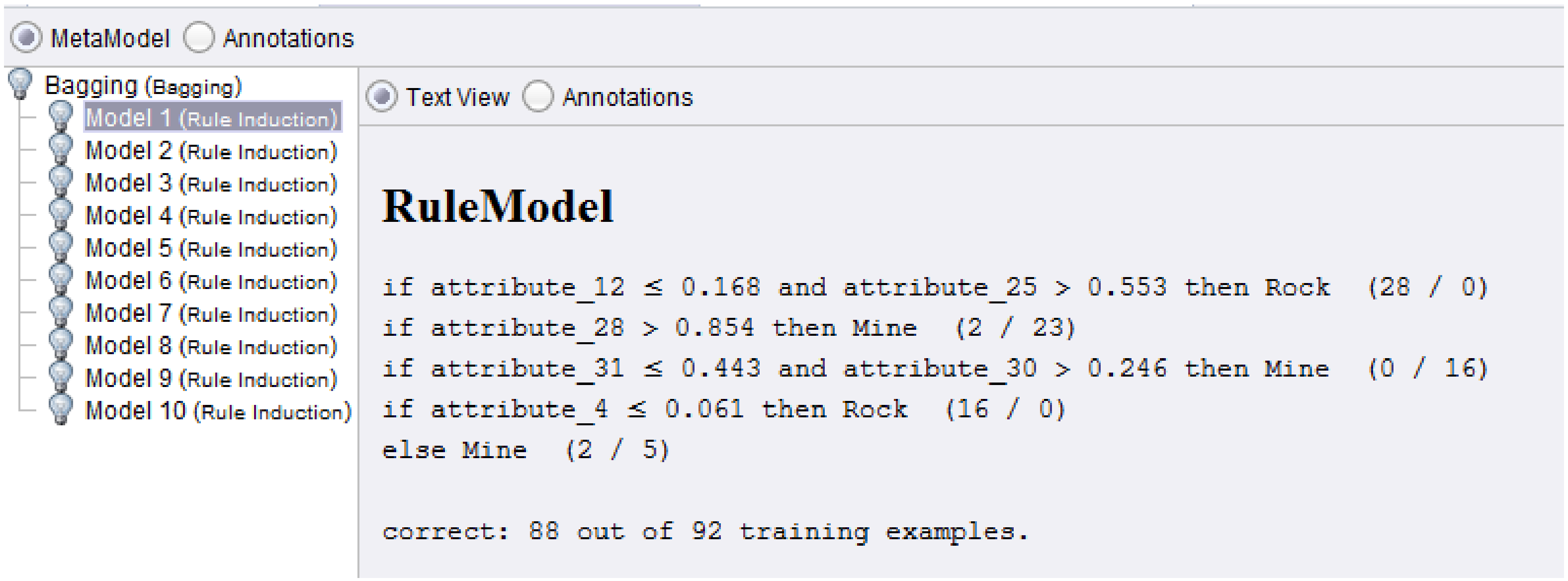
Bagging in RapidMiner

- Accuracy in this example:
  - Ripper alone: 0.71
  - Ripper with bagging (10x0.5): 0.86



Bagging in RapidMiner

- 10 different rule models are learned:

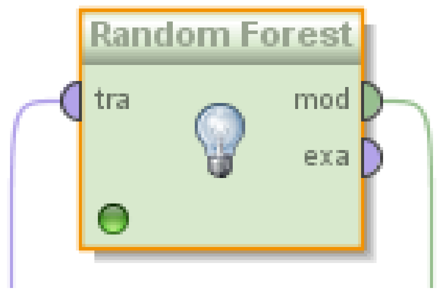


Variant of Bagging: Randomization

- Randomize the learning algorithm instead of the input data
- Some algorithms already have a random component
  - e.g. initial weights in neural net
- Most algorithms can be randomized, e.g., greedy algorithms:
  - Pick from the *N* best options at random instead of always picking the best options
  - e.g.: test selection in decision trees or rule learning
- Can be combined with bagging

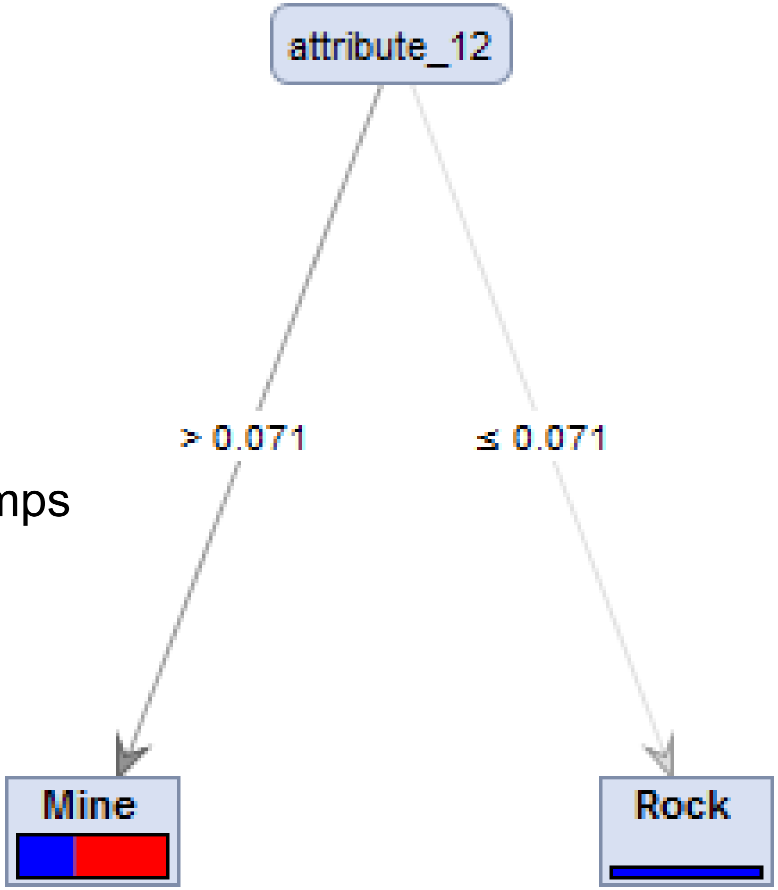
Random Forests

- A variation of bagging with decision trees
- Train a number of individual decision trees
  - each on a random subset of examples
  - only analyze a random subset of attributes for each split
    *(Recap: classic DT learners analyze **all** attributes at each split)*
  - usually, the individual trees are left unpruned



Paradigm Shift: Many Simple Learners

- So far, we have looked at learners that are as good as possible
- Bagging allows a different approach
  - several simple models instead of a single complex one
  - Analogy: the SPIEGEL poll (mostly no political scientists, nevertheless: accurate results)
  - extreme case: using only decision stumps
- Decision stumps:
  - decision trees with only one node

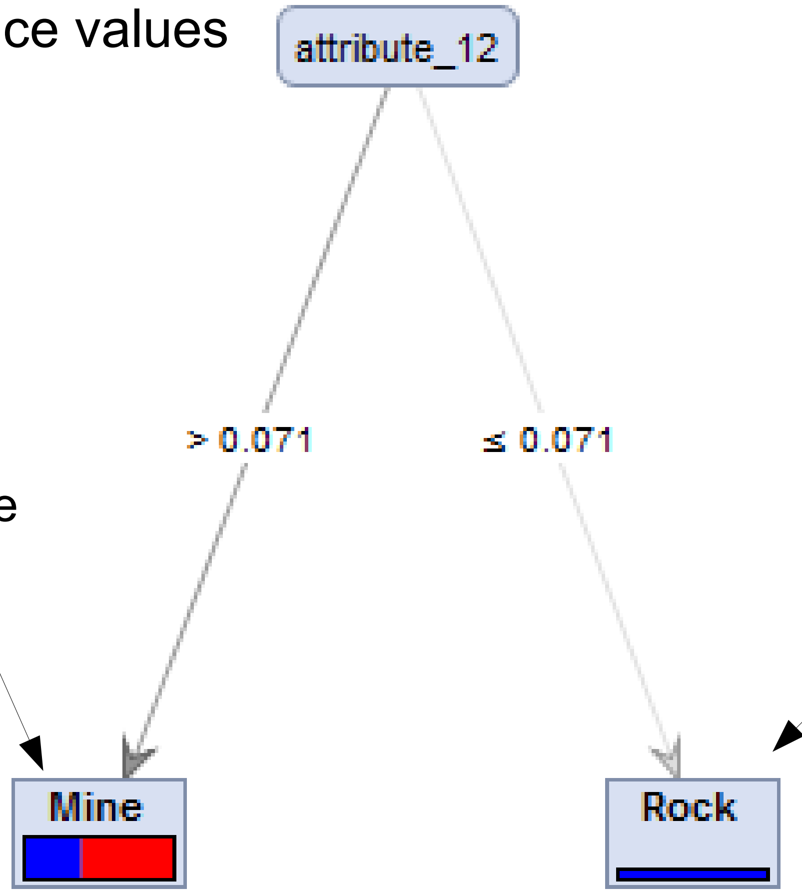


Bagging with Weighted Voting

- Some learners provide confidence values
  - e.g., decision tree learners
  - e.g., Naive Bayes
- Weighted voting
  - use those confidence values for weighting the votes
  - some models may be rather sure about an example, while others may be indifferent

Weighted Voting with Decision Stumps

- Weights: confidence values in each leaf



lower confidence
that it is mine
(weight = 0.6)

high confidence
that it is rock
(weight = 1.0)

Intermediate Recap

- What we've seen so far
  - ensembles often perform better than single base learners
  - simple approach: voting, bagging
- More complex approaches coming up
  - Boosting
  - Stacking
- Boosting requires learning with *weighted instances*
  - we'll have a closer look at that problem first

Intermezzo: Learning with Weighted Instances

- So far, we have looked at learning problems where each example is equally important
- Weighted instances
  - assign each instance a weight (*think:* importance)
  - getting a high-weighted instance wrong is more expensive
  - accuracy etc. can be adapted
- Example:
  - data collected from different sources (e.g., sensors)
  - sources are not equally reliable
    - we want to assign more weight to the data from reliable sources

Intermezzo: Learning with Weighted Instances

- Two possible strategies of dealing with weighted instances

- Changing the learning algorithm
  - e.g., decision trees, rule learners: adapt splitting/rule growing heuristics, example on following slides

- Duplicating instances
  - an instance with weight n is copied n times
  - simple method that can be used on all learning algorithms

Recap: Accuracy

- Most frequently used metrics:

$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN}$$

$$\text{Error Rate} = 1 - Accuracy$$

	PREDICTED CLASS		
ACTUAL CLASS		Class=Yes	Class=No
	Class=Yes	TP	FN
	Class=No	FP	TN

Accuracy with Weights

- Definition of accuracy

$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN}$$

- Without weights, TP, FP etc. are *counts* of instances
- With weights, they are *sums of their weights*
  - classic TP, FP etc. are the special case where all weights are 1

Adapting Algorithms: Decision Trees

- Recap: Gini index as splitting criterion

$$GINI(t) = 1 - \sum_j [p(j \mid t)]^2$$

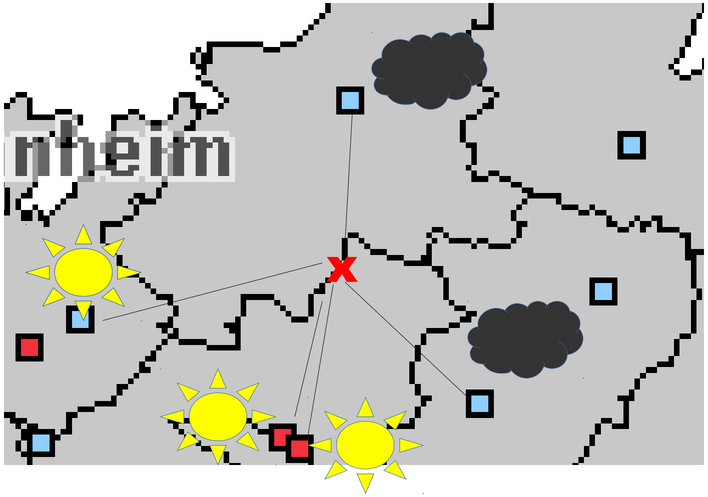
- The probabilities are obtained by counting examples
  - Again, we can sum up weights instead

- The same works for rule-based classifiers and their heuristics

Adapting Algorithms: k-NN

- Standard approach
  - use average of neighbor predictions

- With weighted instances
  - weighted average



Back to Ensembles: Boosting

- Idea of boosting
  - train a set of classifiers, one after another
  - later classifiers focus on examples that were misclassified by earlier classifiers
  - weight the predictions of the classifiers with their error
- Realization
  - perform multiple iterations
    - each time using different example weights
  - weight update between iterations
    - *increase* the weight of *incorrectly* classified examples
    - so they become more important in the next iterations (misclassification errors for these examples count more heavily)
  - combine results of all iterations
    - weighted by their respective error measures

Boosting – Algorithm AdaBoost.M1

1. initialize example weights $w_i = 1/N \quad (i = 1..N)$
2. for $m = 1$ to t // t ... number of iterations
   a) learn a classifier C_m using the current example weights
   b) compute a weighted error estimate $$err_m = \frac{\sum w_i \textit{ of all incorrectly classified } e_i}{\sum_{i=1}^{N} w_i}$$
      $= 1$ because weights are normalized
   c) if $err_m > 0.5 \rightarrow$ exit loop
   d) compute a classifier weight $\alpha_m = \frac{1}{2} \ln\left(\frac{1 - err_m}{err_m}\right)$
   e) for all correctly classified examples e_i: $w_i \leftarrow w_i e^{-\alpha_m}$
   f) for all incorrectly classified examples e_i: $w_i \leftarrow w_i e^{\alpha_m}$
   g) normalize the weights w_i so that they sum to 1

   update weights so that sum of correctly classified examples equals sum of incorrectly classified examples
3. for each test example
   a) try all classifiers C_m
   b) predict the class that receives the highest sum of weights α_m

Illustration of the Weights

- Classifier Weights α_m
  - differences near 0 or 1 are emphasized
- Good classifier
  - $\rightarrow$ highly positive weight
- Bad classifier
  - $\rightarrow$ highly negative weight
- Classifier with error 0.5
  - $\rightarrow$ weight 0
  - $\rightarrow$ this is equal to guessing!

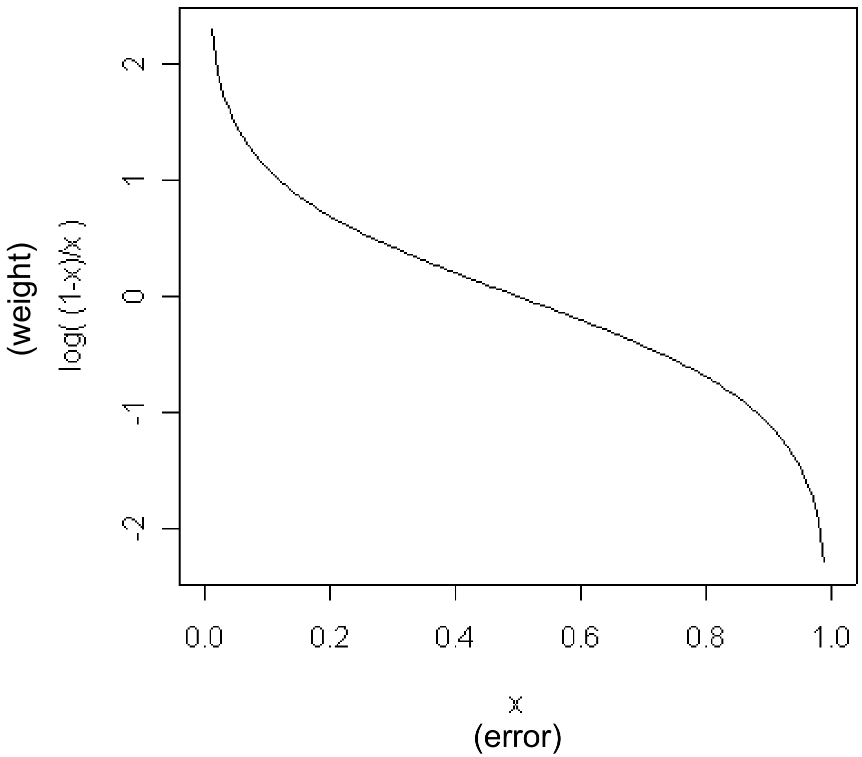
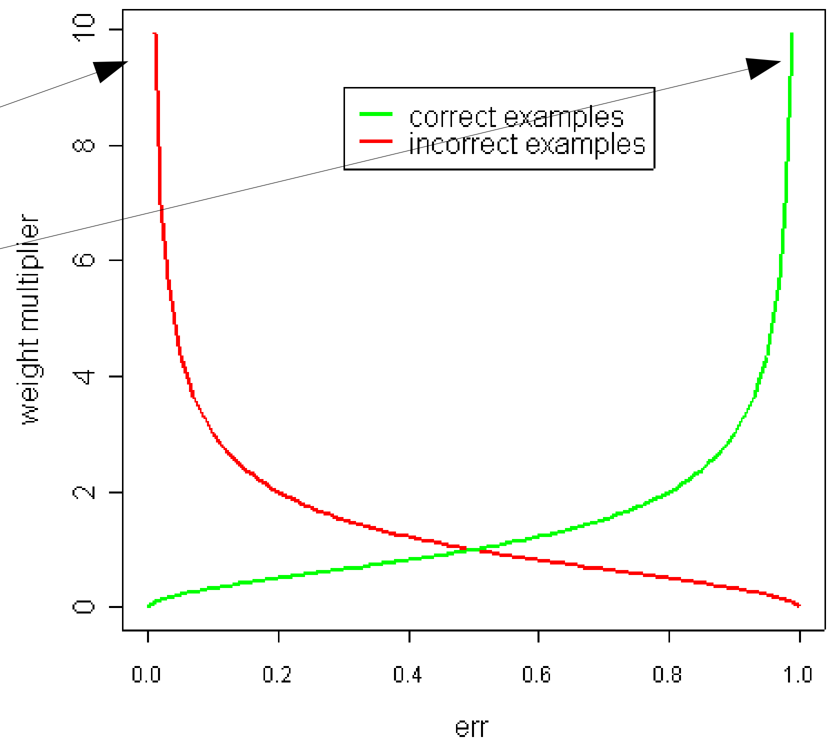


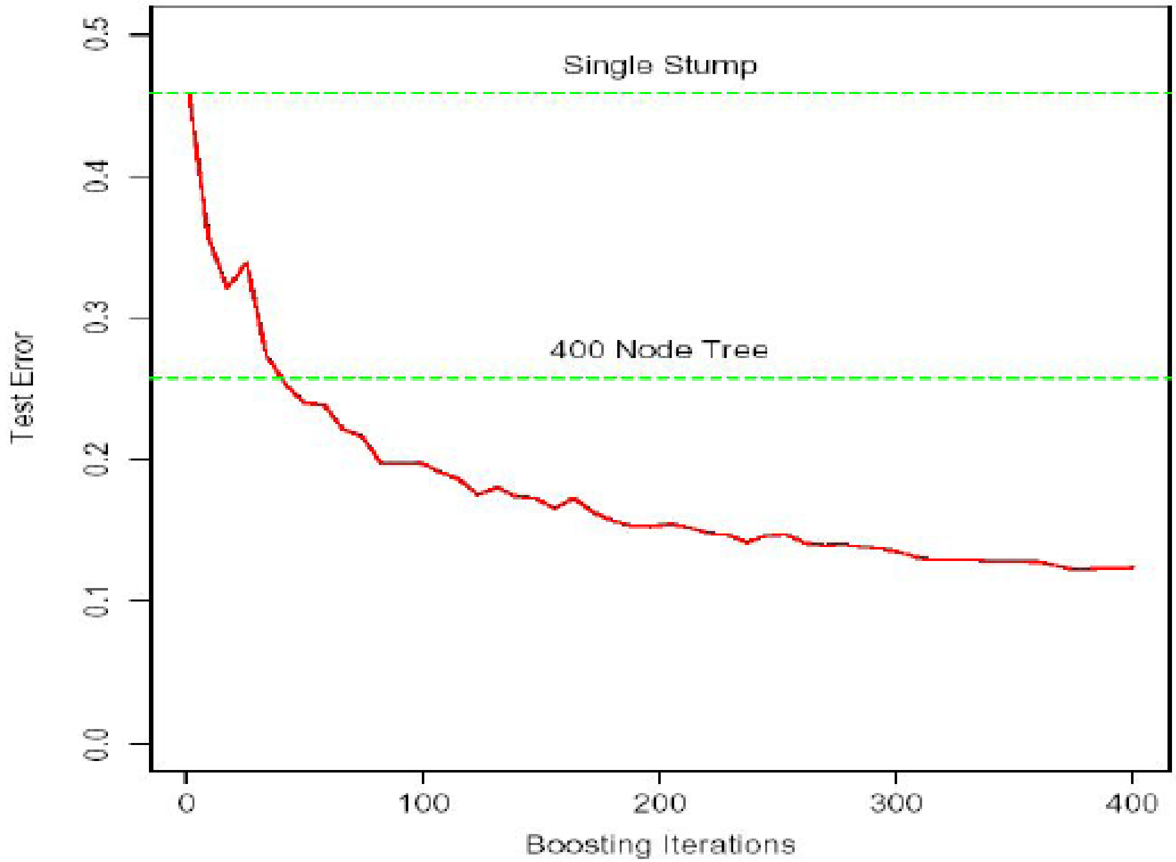
Illustration of the Weights

- Example Weights
  - multiplier for correct and incorrect examples
  - depending on error
- Later iterations need to focus on examples that are
  - Incorrectly classified by a good classifier
  - Correctly classified by a bad classifier



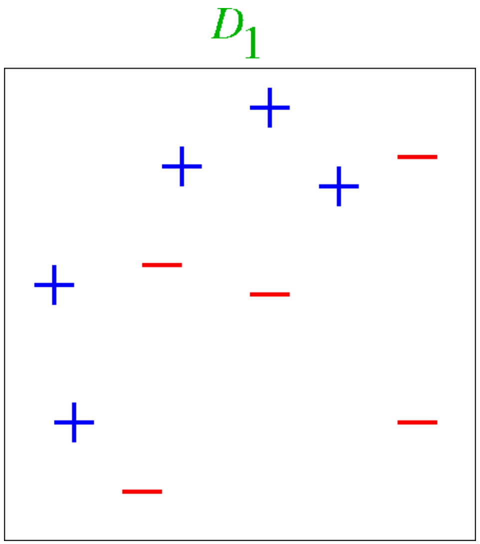
Boosting – Error Rate Example

- boosting of decision stumps on simulated data



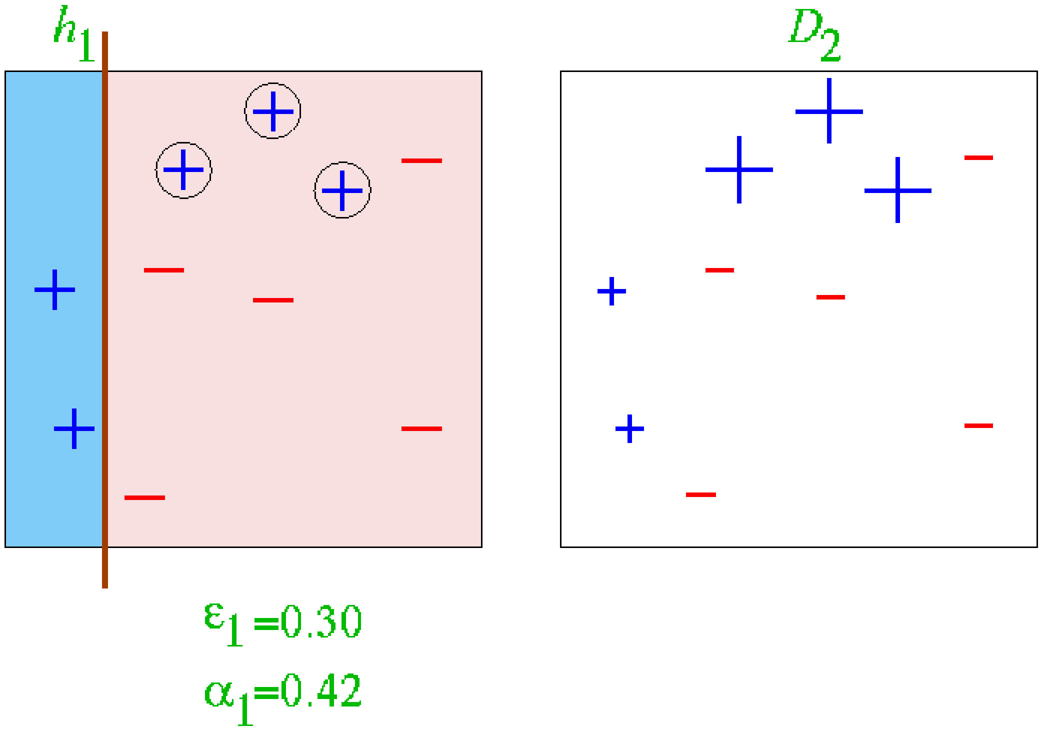
from Hastie, Tibshirani, Friedman: The Elements of Statistical Learning, Springer Verlag 2001

Toy Example

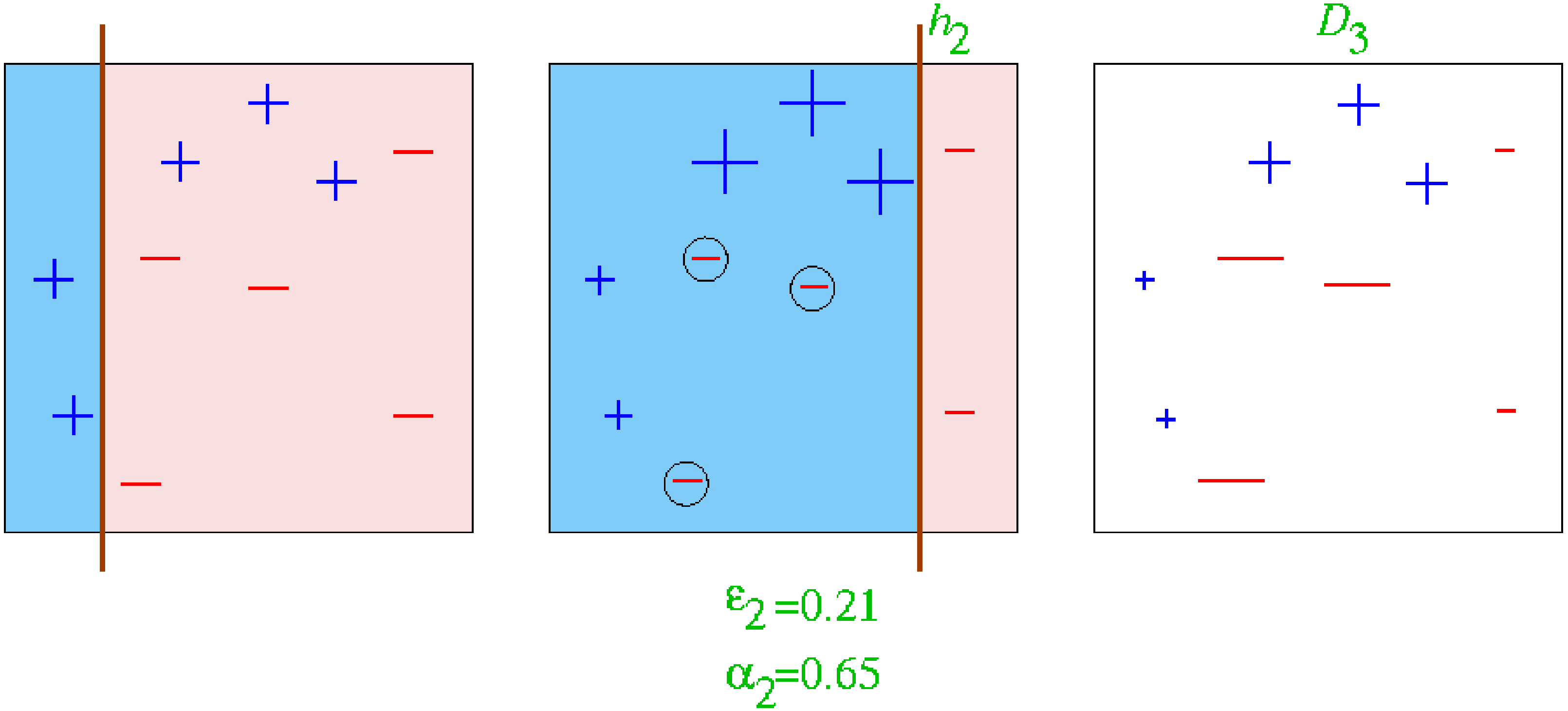


(taken from Verma & Thrun, Slides to CALD Course CMU 15-781,
Machine Learning, Fall 2000)

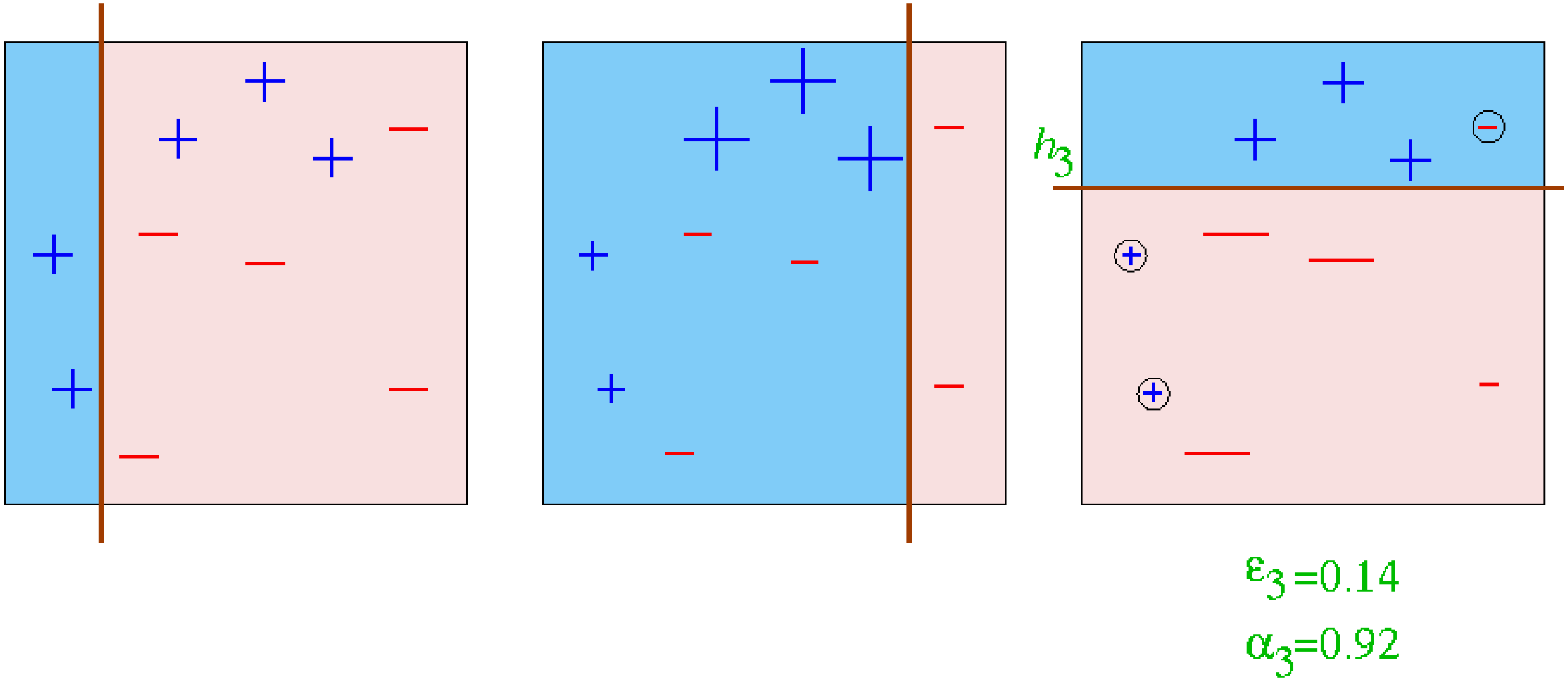
Round 1



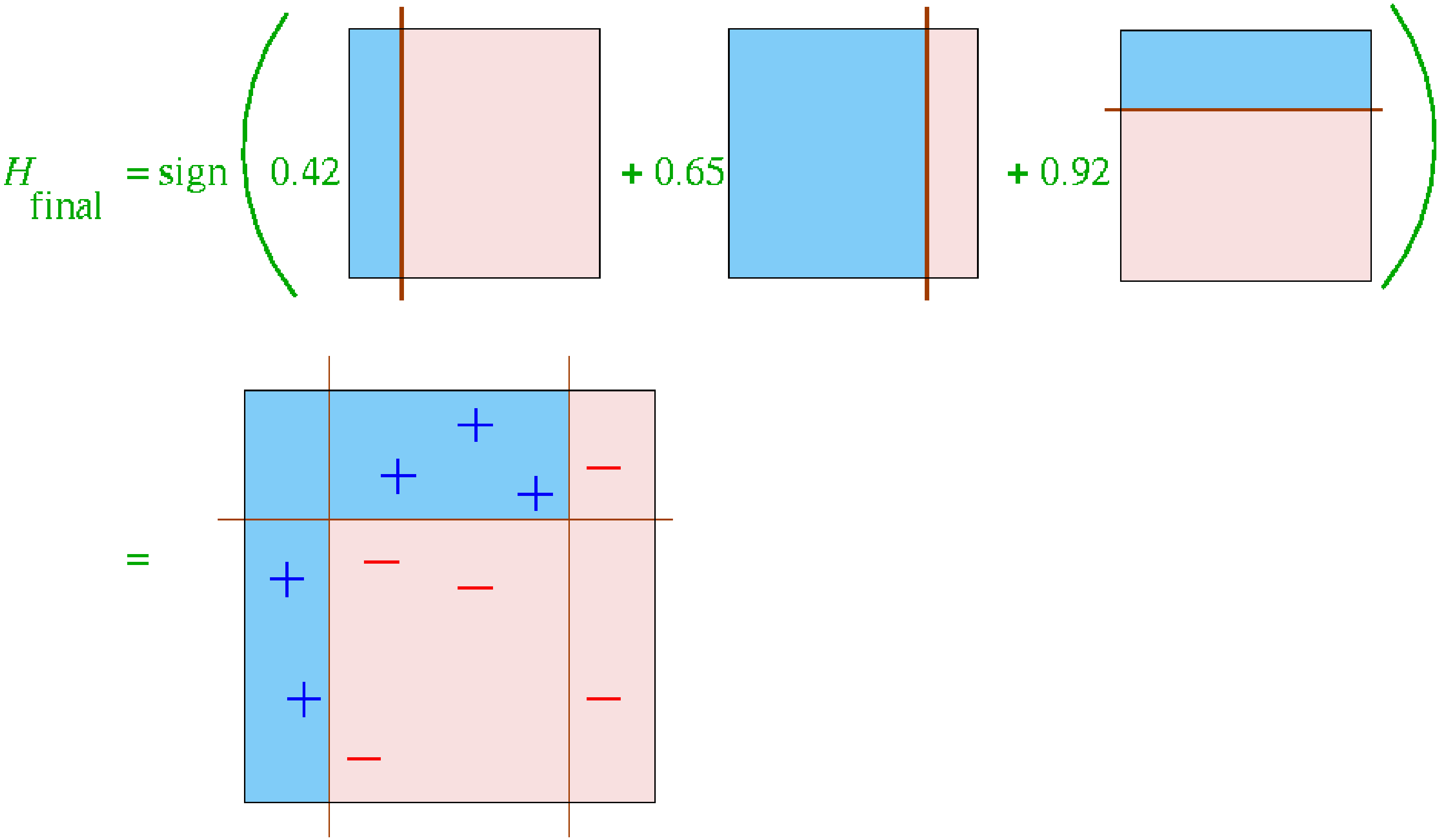
Round 2



Round 3



Final Hypothesis

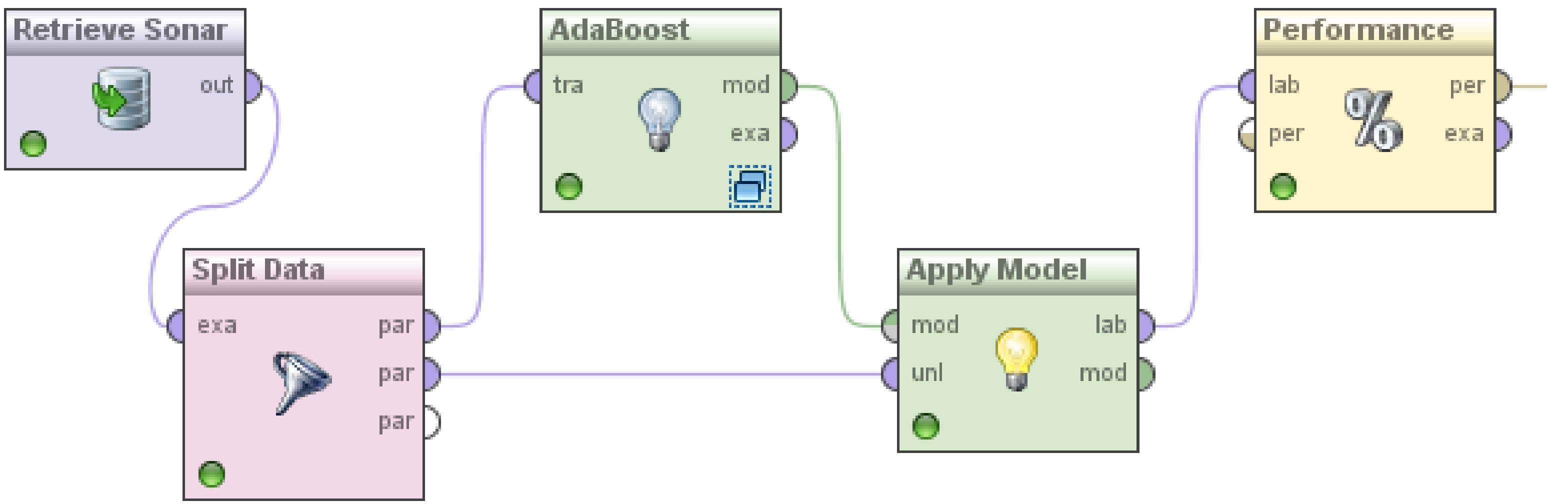


Hypothesis Space of Ensembles

- Each learner has a *hypothesis space*
  - e.g., decision stumps: a linear separation of the dataset
- The hypothesis space of an ensemble
  - can be larger than that of its base learners
- Example: bagging with decision stumps
  - different stumps → different linear separations
  - resulting hypothesis space also allows polygon separations

Boosting in RapidMiner

- Just like voting and bagging



Experimental Results on Ensembles

- Ensembles have been used to improve generalization accuracy on a wide variety of problems
- On average, Boosting provides a larger increase in accuracy than Bagging
  - Boosting on rare occasions can degrade accuracy
  - Bagging more consistently provides a modest improvement
- Boosting is particularly subject to over-fitting when there is significant noise in the training data
  - subsequent learners over-focus on noise points

(Freund & Schapire, 1996; Quinlan, 1996)

Back to Combining Predictions

- Voting
  - each ensemble member votes for one of the classes
  - predict the class with the highest number of vote (e.g., bagging)
- Weighted Voting
  - make a *weighted* sum of the votes of the ensemble members
  - weights typically depend
    - on the classifier's confidence in its prediction (e.g., the estimated probability of the predicted class)
    - on error estimates of the classifier (e.g., boosting)

Mannheim RapidMiner Toolbox

- Stacking
  - Why not use a classifier for making the final decision?
  - training material are the class labels of the training data and the (cross-validated) predictions of the ensemble members

Stacking

- Basic Idea:
  - learn a function that combines the predictions of the individual classifiers
- Algorithm:
  - train n different classifiers $C_1 \ldots C_n$ (the *base classifiers*)
  - obtain predictions of the classifiers for the training examples
  - form a new data set (the *meta data*)
    - **classes**
      - the same as the original dataset
    - **attributes**
      - one attribute for each base classifier
      - value is the prediction of this classifier on the example
  - train a separate classifier M (the *meta classifier*)

Stacking (2)

- Example:

Attributes			Class
x_{11}	...	x_{1n_a}	t
x_{21}	...	x_{2n_a}	f
...	...	...	...
x_{n_e1}	...	$x_{n_en_a}$	t

training set

C_1	C_2	...	C_{n_c}
t	t	...	f
f	t	...	t
...	...	...	...
f	f	...	t

predictions of the classfiers

C_1	C_2	...	C_{n_c}	Class
t	t	...	f	t
f	t	...	t	f
...	...	...	...	...
f	f	...	t	t

training set for stacking

- Using a stacked classifier:
  - try each of the classifiers $C_1 ... C_n$
  - form a feature vector consisting of their predictions
  - submit these feature vectors to the meta classifier M

Stacking and Overfitting

- Consider a dumb base learner D, which works as follows:
  - during training: store each training example
  - during classification: if example is stored, return its class

    otherwise: return a random prediction

do you know that classifier?

- If D is used along with a number of classifiers in stacking, what will the meta classifier look like?
  - D is perfect on the training set
  - so the meta classifier will say: always use D's result

Implementation in RapidMiner :-(

Stacking and Overfitting

- Solution 1: split dataset (e.g., 50/50)
  - use one portion for training the base classifiers
  - use other portion to train meta model

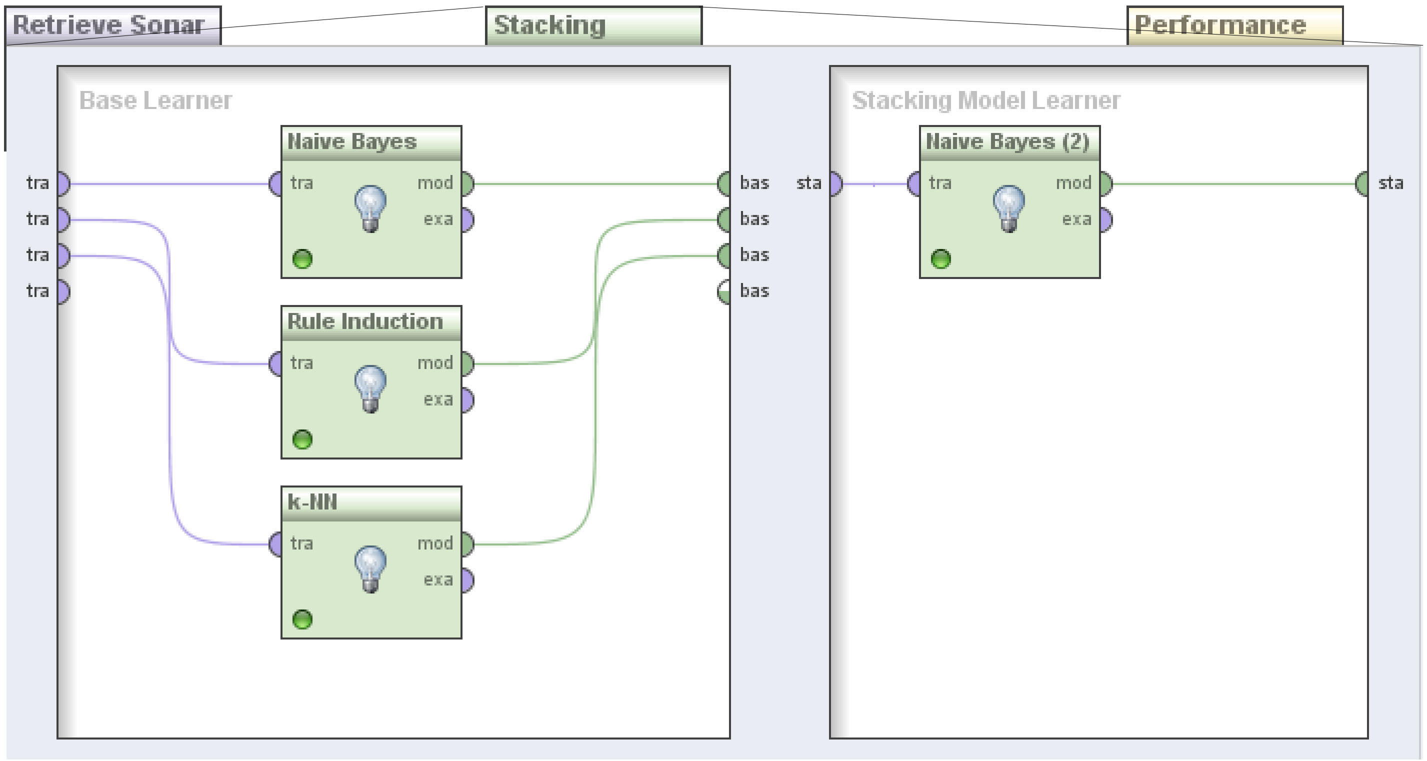
- Solution 2: cross-validate base classifiers
  - train classifier on 90% of training data
  - create features for the remaining 10% on that classifier
  - repeat 10 times

X-Stacking in Mannheim RapidMiner Toolbox :-)

- The second solution is better in most cases
  - uses whole dataset for meta learner
  - uses 90% of the dataset for base learners

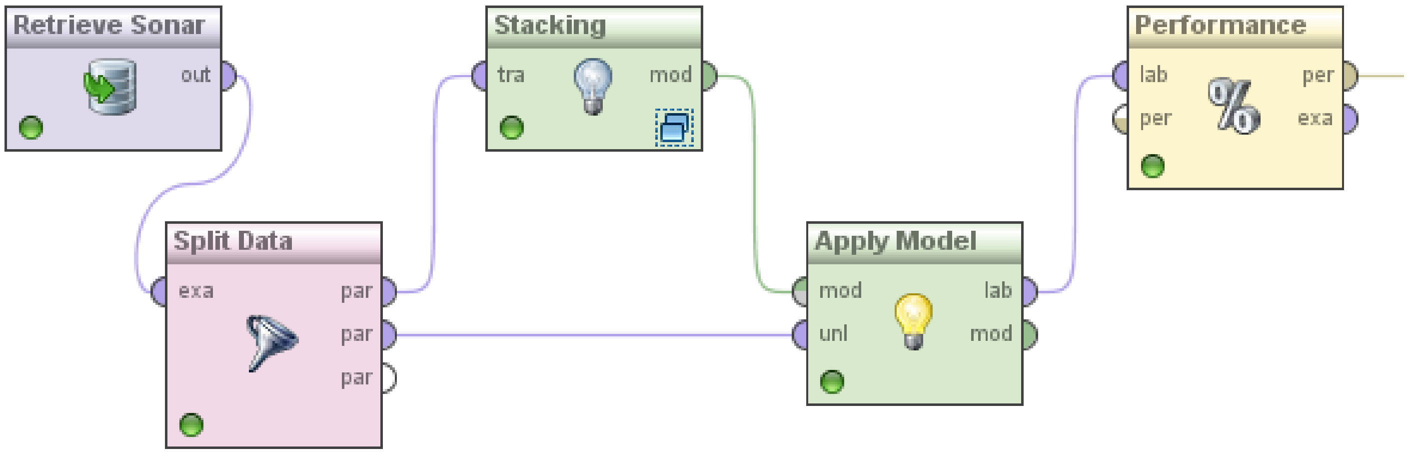
Stacking in RapidMiner

- Looks familiar again
  - we need a set of base learners (like for voting)
  - and a learner for the stacking model



Stacking in RapidMiner

- Accuracy in this experiment:
  - Naive Bayes: 0.71
  - k-NN: 0.81
  - Ripper: 0.71
- Stacked model: 0.86



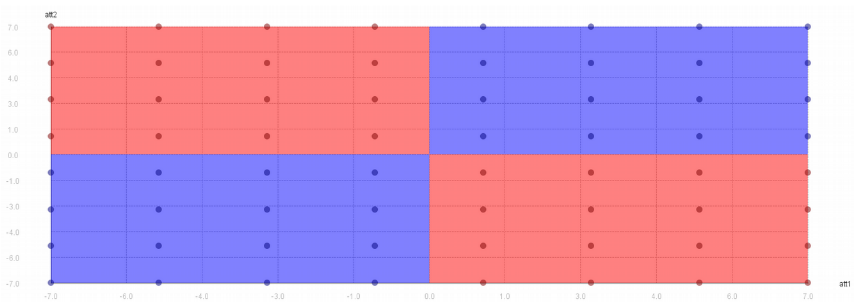
Stacking

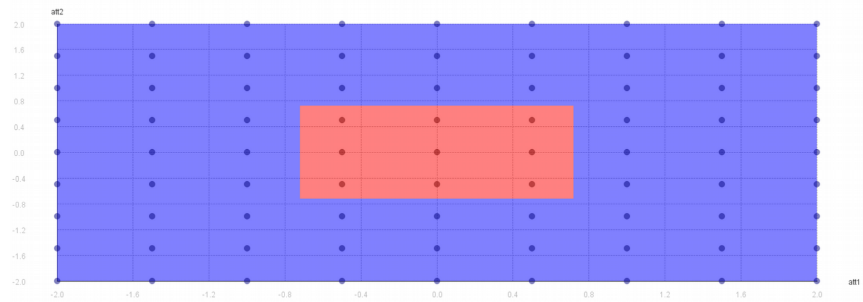
- Variant: also keep the original attributes
- Predictions of base learners are additional attributes for the stacking predictor
  - allows the identification of “blind spots” of individual base learners

- Variant: stacking with confidence values
  - if learners output confidence values, those can be used by the stacking learner
  - often further improves the results

The Classifier Selection Problem

- Question: decision trees or rule learner – which one is better?
- Two corner cases – recap from Data Mining 1





Accuracy:

- Baseline: 0.45
- Decision Tree: 0.45
- Rule Learner: 0.7

- Voting: 0.65
- Weighted Voting: 0.7
- Stacking: 0.83

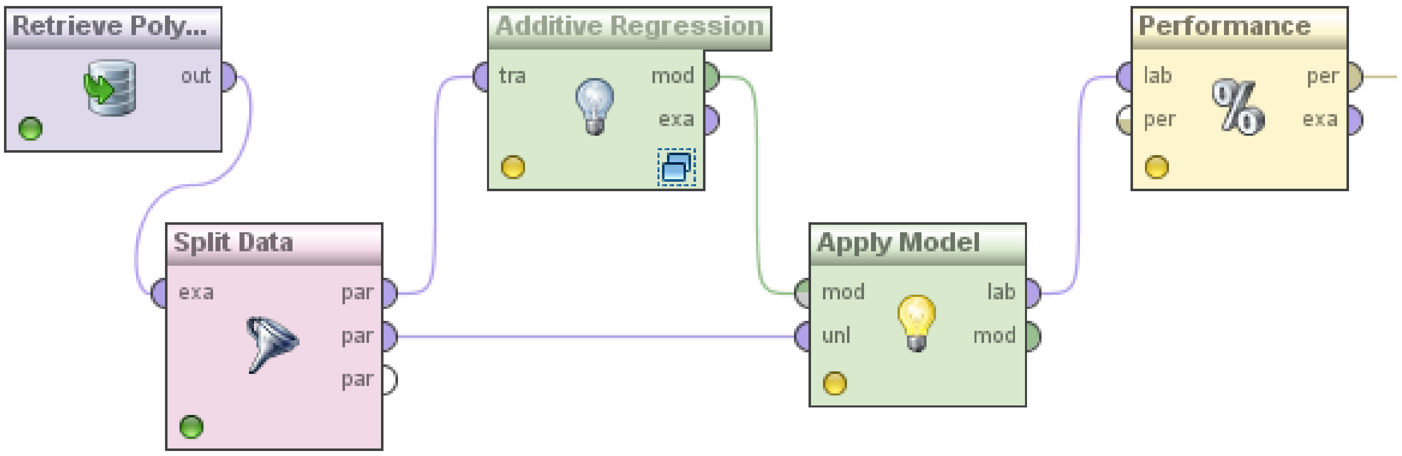
Accuracy:

- Baseline: 0.89
- Decision Tree: 1.0
- Rule Learner: 0.89

- Voting: 0.89
- Weighted Voting: 1.0
- Stacking: 1.0

Regression Ensembles

- Most ensemble methods also work for regression
  - voting: use average
  - bagging: use average or weighted average
  - stacking: learn *regression* model as stacking model!
  - boosting: the regression variant is called *additive regression*



Additive Regression

- Boosting can be seen as a greedy algorithm for fitting additive models
- Same kind of algorithm for numeric prediction:
  - Build standard regression model
  - Gather residuals, learn model predicting residuals, and repeat
    - Given a prediction p(x), residual = $(x-p(x))^2$
- To predict, simply sum up weighted individual predictions from all models

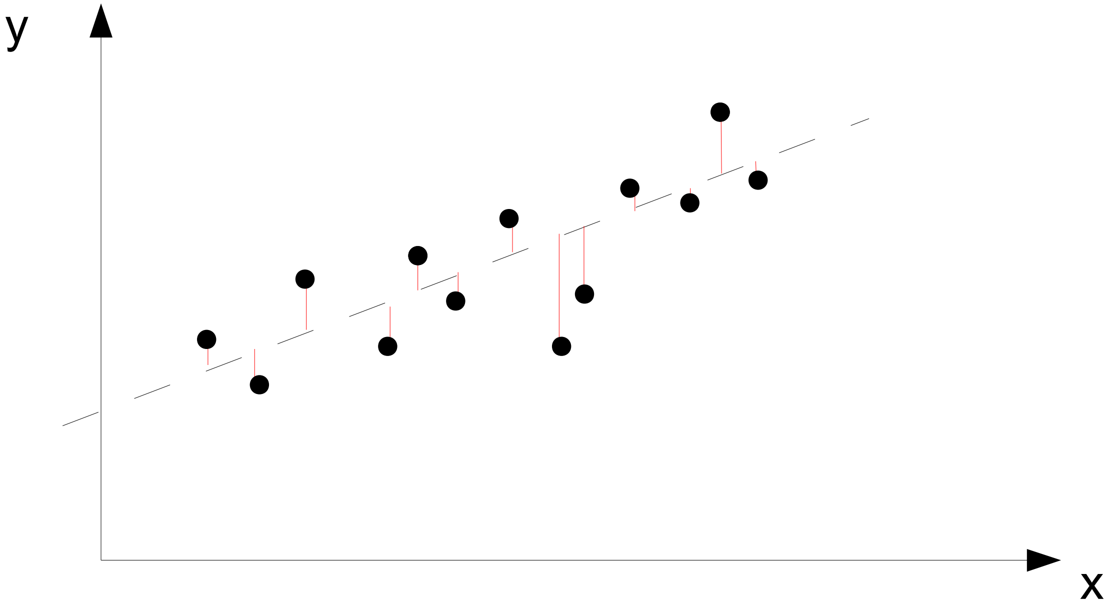
Additive Regression w/ Linear Regression

- What happens if we use Linear Regression inside of Additive Regression?

- The first iteration learns a linear regression model lr_1
  - By minimizing the sum of squared errors
- The second iteration aims at learning a LR lr_2 model for
  - $x' = (x-lr_1(x))^2$
  - Since $(x-lr_1(x))^2$ is already minimal, lr_2 cannot improve upon this
    - Hence, the subsequent linear models will always be a constant 0

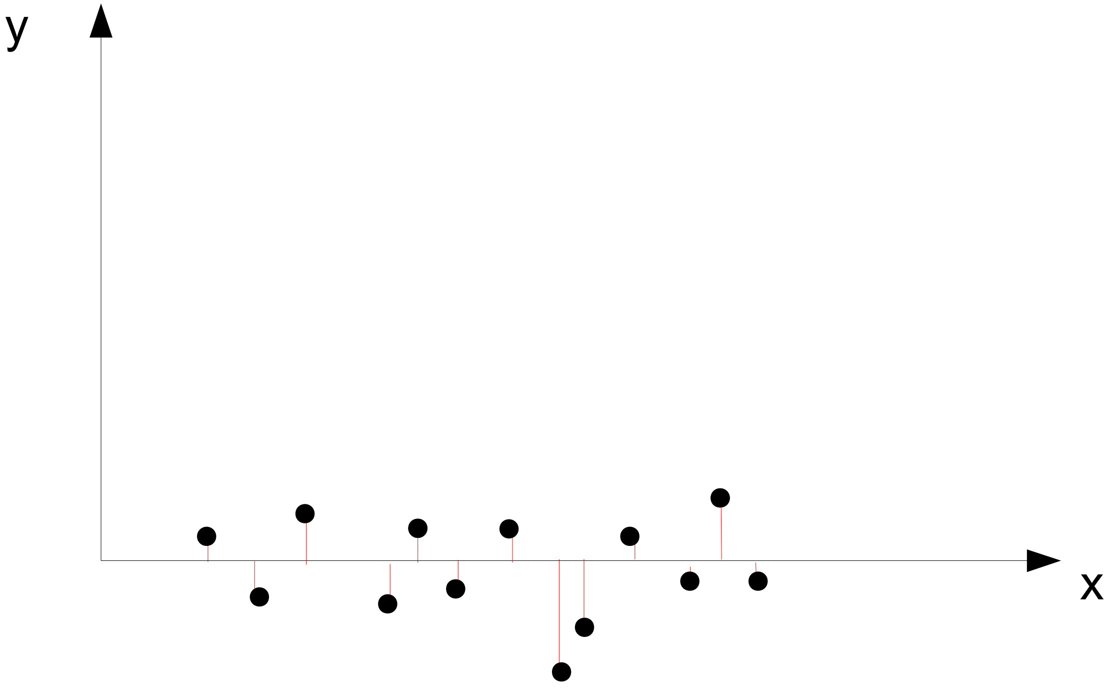
Additive Regression w/ Linear Regression

- First regression model:

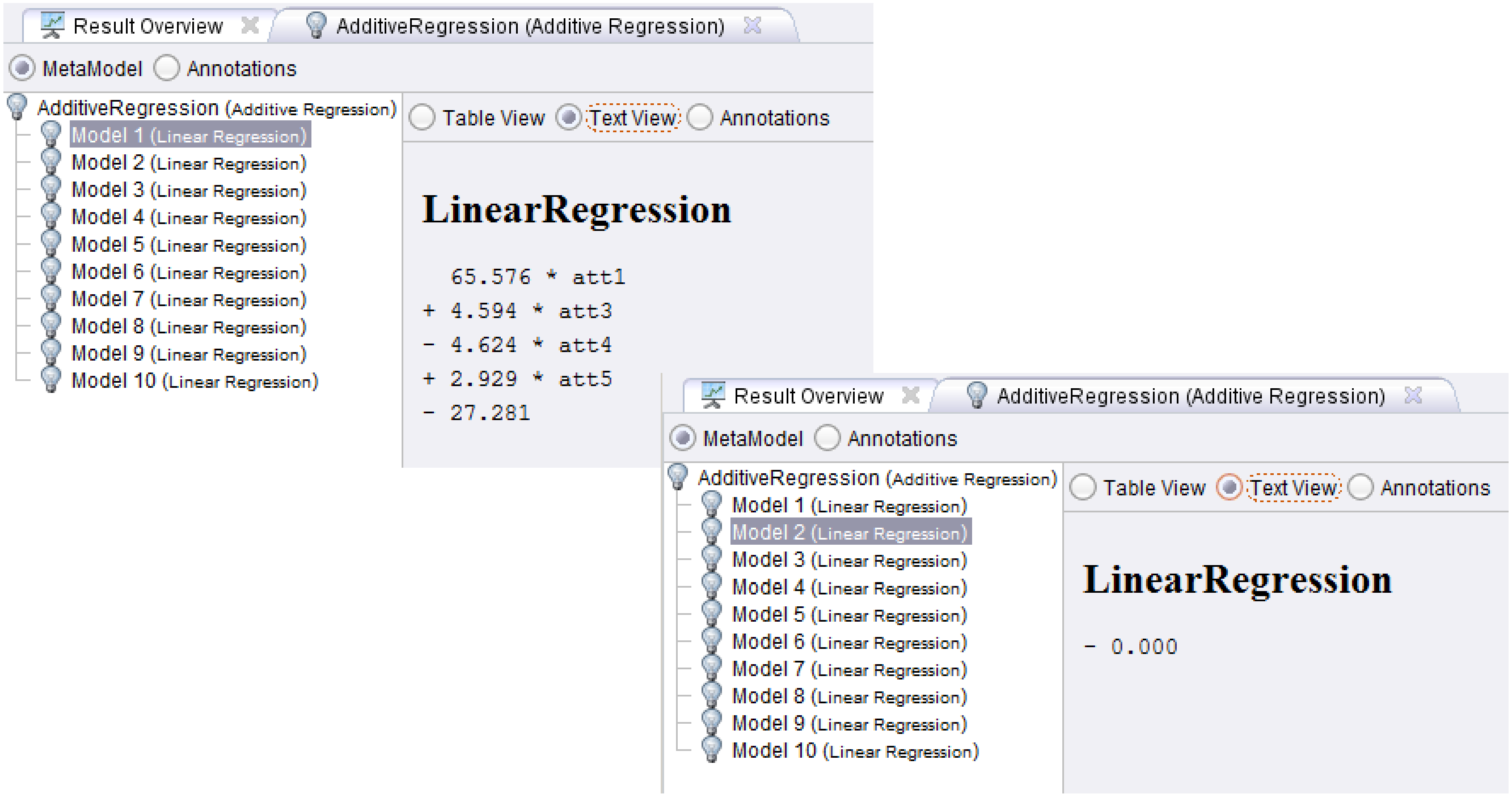


Additive Regression w/ Linear Regression

- Second (and third, fourth, ...) regression model:

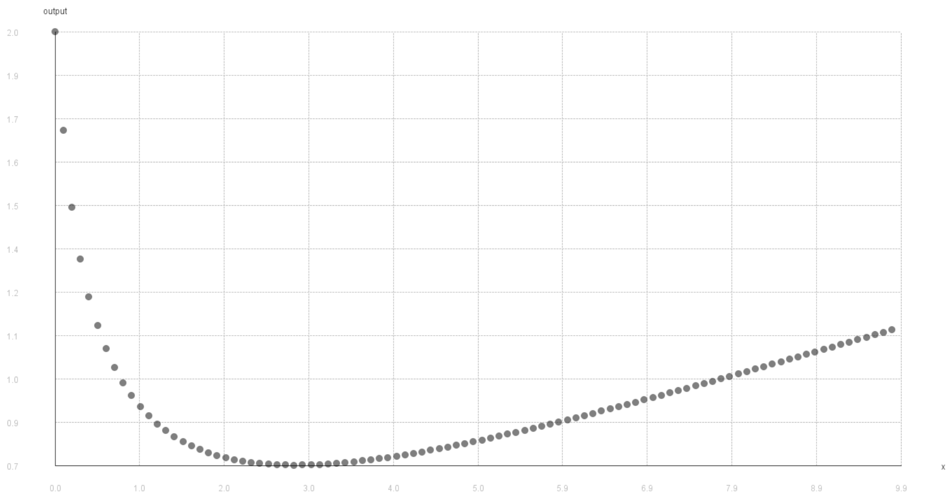


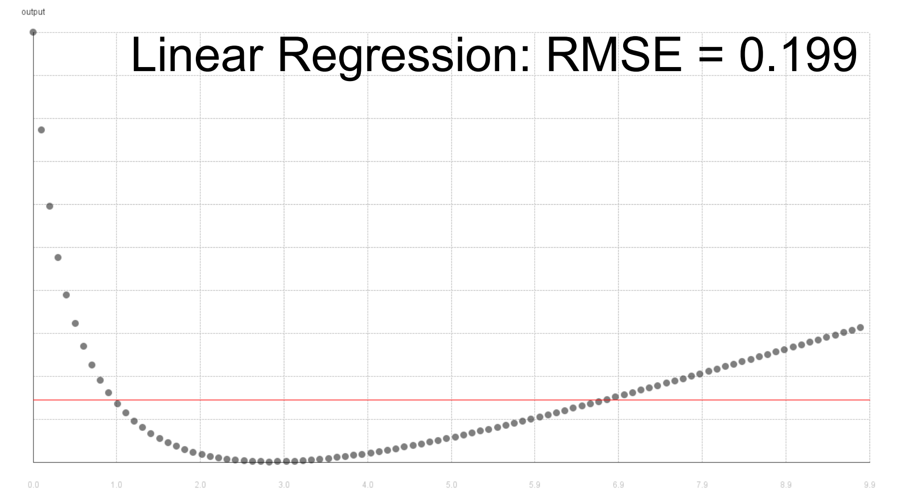
Additive Regression

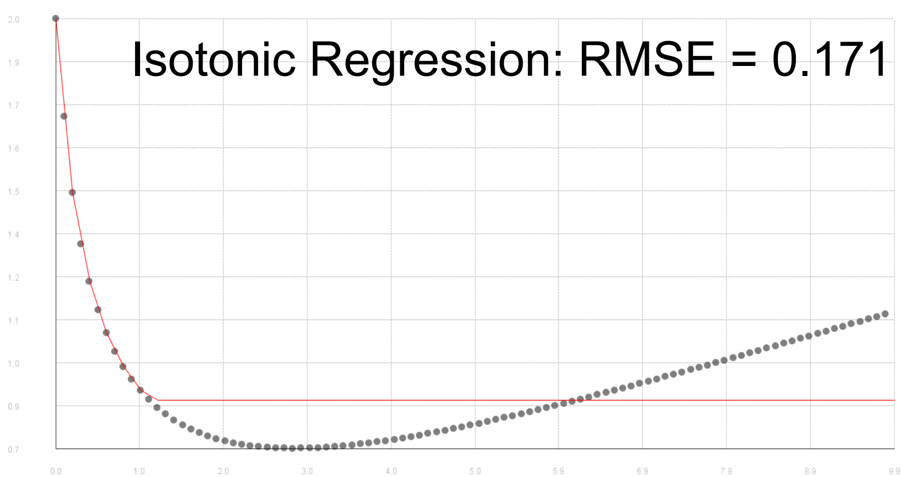


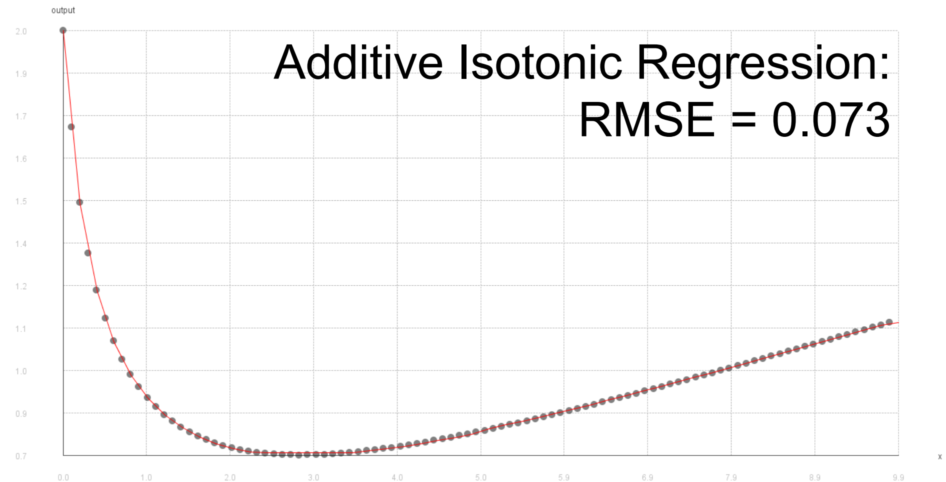
- Bottom line: additive and linear regression are not a good match

Example 1: One-dimensional, Non-linear



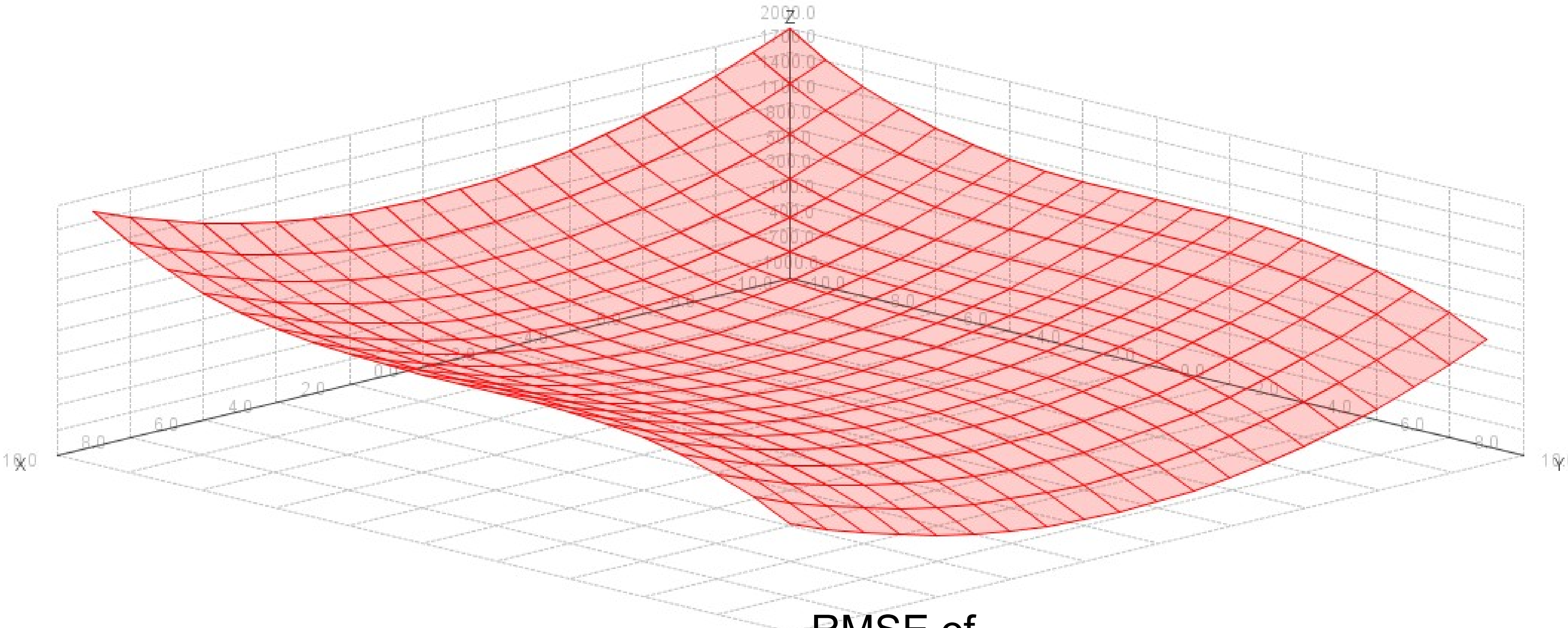






Example 2: Multidimensional, Non-Linear

- $z = 10x^2 - y^3$



RMSE of...

...Linear Regression:	385
...Isotonic Regression:	293
...Additive Isotonic Regression:	122

XGBoost

- Currently wins most Kaggle competitions etc.
- Additive Regression w/ Regression Trees
- Regularization
  - Respect size of trees
  - Larger trees: more likely to overfit!
    - Introduce penalty for tree size
  - Overcomes the problem of overfitting in boosting

Intermediate Recap

- Ensemble methods
  - outperform base learners
  - Help minimizing shortcomings of single learners/models
  - simple and complex methods for method combination

- Reasons for performance improvements
  - individual errors of single learners can be “outvoted”
  - more complex hypothesis space

Ensembles for Other Problems

- There are ensembles also for...
- ...clustering (Vega-Pons and Ruiz-Shulkloper, 2011)
  – trying to unify different clusterings
  – using a consensus function mapping different clusterings to each other
- ...outlier detection (Zimek et al., 2014)
  – unifying outlier scores of different approaches
  – requires score normalization and/or rank aggregation
- etc.

Learning with Costs

- Most classifiers aim at reducing the number of errors
  - all errors are regarded as being equally important

- In reality, misclassification costs may differ
- Consider a warning system in an airplane
  - issue a warning if stall is likely to occur
  - based on a classifier using different sensor data
  - wrong warnings may be ignored by the pilot
  - missing warnings may cause the plane to crash
- Here, we have different costs for
  - actual: true, predicted: false → very expensive
  - actual: false, predicted true → not so expensive

http://i.telegraph.co.uk/multimedia/archive/01419/plane_1419831c.jpg

The MetaCost Algorithm

- Form multiple bootstrap replicates of the training set
  - Learn a classifier on each training set
  - i.e., perform bagging
- Estimate each class’s probability for each example
  - by the fraction of votes that it receives from the ensemble
- Use conditional risk equation to relabel each training example
  - with the estimated optimal class
- Reapply the classifier to the relabeled training set

MetaCost

- Conditional risk $R(i|x)$ is the expected cost of predicting that x belongs to class i
  - $R(i|x) = \sum P(j|x)C(i, j)$
  - $C(i,j)$ are the classification costs
    (classify an example of class j as class i)
  - $P(j|x)$ are obtained by running the bagged classifiers
- The goal of MetaCost procedure is: to relabel the training examples with their “optimal” classes
  - i.e., those with lowest risk
- Then, re-run the classifier to build a final model
  - the resulting classifier will be defensive,
    i.e., make low-risk predictions
  - in the end, the costs are minimized

MetaCost

- Pilot stall alarm example
  - x_1: stall, $P(stall|x_1) = 0.8$
  - x_2: no, $P(no|x_2) = 0.9$

8/10 classifiers are correct

		predicted	
		stall	no stall
actual	stall	0	10
	no stall	1	0

- Risk values:
  - $R(stall|x_1) = P(stall|x_1)*\underbrace{C(stall,stall)}_{=0} + P(no|x_1)*C(stall,no) = 0.2*1 = 0.2$
  - $R(no|x_1) = P(stall|x_1)*C(no,stall) + P(no|x_1)*C(no,no) = 0.8*10 = 8$
  - $R(stall|x_2) = P(stall|x_2)*C(stall,stall) + P(no|x_2)*C(stall,no) = 0.9*1 = 0.9$
  - $R(no|x_2) = P(stall|x_2)*C(no,stall) + P(no|x_2)*C(no,no) = 0.1*10 = 1$
- Since 0.9<1
  - x_2 is relabeled to "stall"

http://i.telegraph.co.uk/multimedia/archive/01419/plane_1419831c.jpg

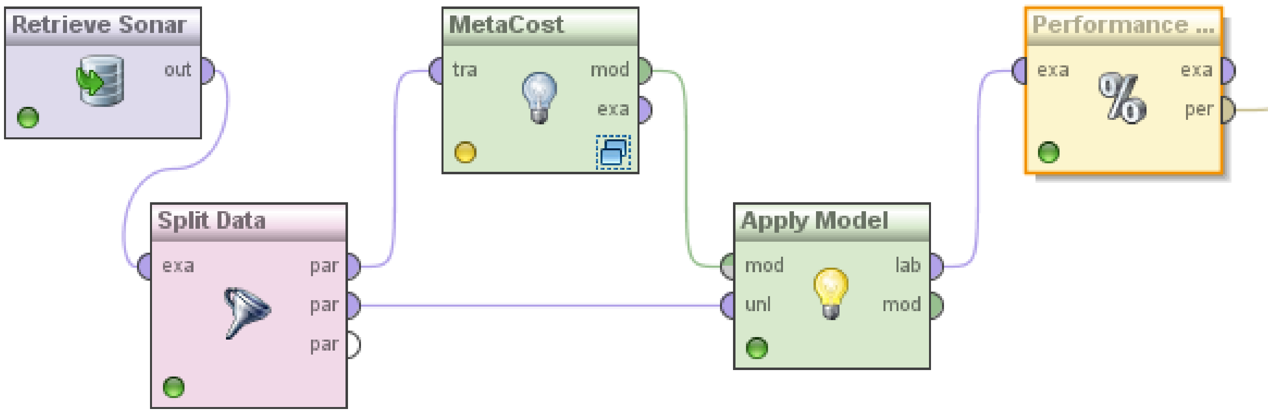
MetaCost vs. Balancing

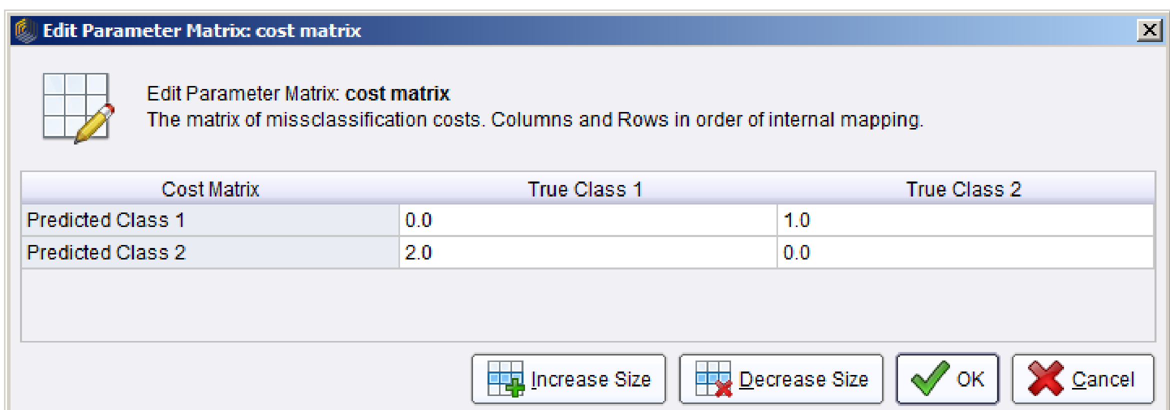
- Recap balancing:
  - in an unbalanced dataset, there is a bias towards the larger class
  - balancing the dataset helps building more meaningful models

- MetaCost:
  - incidentally unbalance the dataset,
    labeling more instances with the “cheap” class
  - make the learner have a bias towards the “cheap” class
    - i.e., expensive mis-classifications are avoided
  - in the end, the overall cost is reduced
- In the example:
  - there will be more false alarms (stall warning, but actually no stall)
  - the risk of not issuing a warning is reduced

MetaCost in RapidMiner

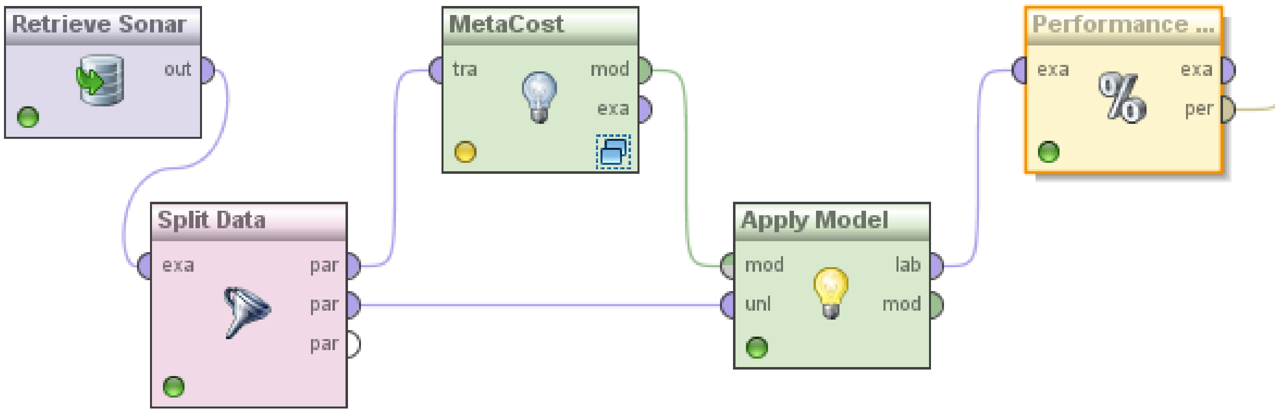
- Hint: use the performance (cost) operator for evaluation





MetaCost in RapidMiner

- Experiment: set misclassification cost
  Rock → Mine = 2; Mine → Rock = 1
- Non-cost sensitive decision tree:
  - misclassification cost = 0.33
- MetaCost with decision tree:
  - misclassification cost = 0.24



Another Example for Cost-Sensitive Prediction

- Predicting *ordinal* attributes
  - e.g., very low, low, medium, high, very high
- A standard classifier just looks at correct/incorrect classifications
  - i.e., for a *very low* instance, predicting *low* or *very high* is equally bad
- In practice, predicting *low* for a *very low* instance is much better than predicting *very high*
- Solution: assign costs C(actual,predicted) to predictions
  - C(very low, very low) = 0, C(very low, low) = 1, C(very low, medium) = 2 ...

Wrap-up

- Ensemble methods in general
  - build a strong model from several weak ones
- Ingredients
  - base learners
  - a combination method
- Variants
  - Voting
  - Bagging (based on sampling)
  - Boosting (based on reweighting instances)
  - Stacking (use learner for combination)
- Also used for cost-sensitive predictions (MetaCost)

Questions?