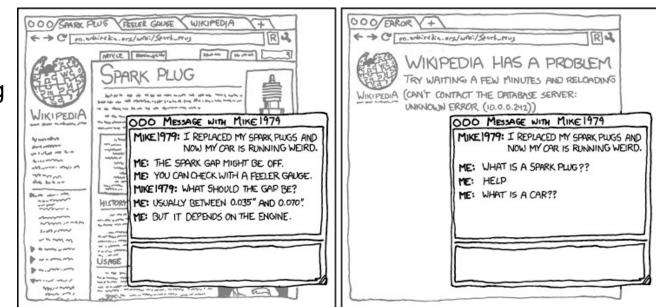
## UNIVERSITÄT MANNHEIM



**Heiko Paulheim** 

## Introduction

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

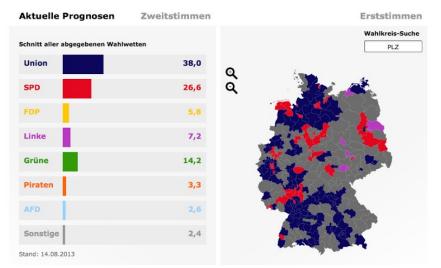


WHEN WIKIPEDIA HAS A SERVER OUTAGE, MY APPARENT IQ DROPS BY ABOUT 30 POINTS.

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

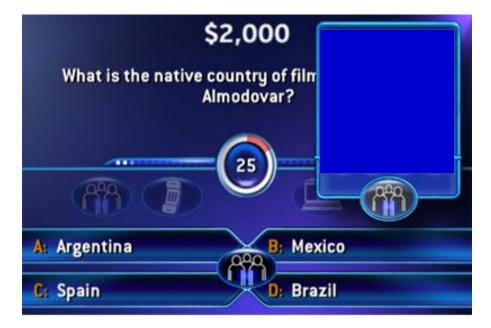


https://lh6.googleusercontent.com/-U9DXTTcT-PM/UgsdSzdV3JI/AAAAAAAAFKs/GsRydeldasg/w800-h800/ Bildschirmfoto+2013-08-14+um+07.56.01.png

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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

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#### **Ensembles**

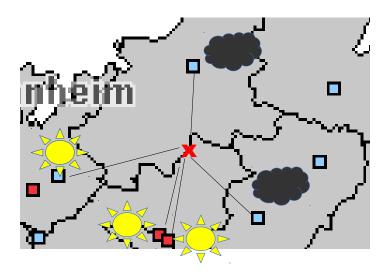
- So far, we have addressed a learning problem like this: classifier = DecisionTreeClassifier(max\_depth=5) ...and hoped for the best
- Ensembles:
  - wisdom of the crowds for learning operators
  - instead of asking a single learner, combine the predictions of different learners

#### **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

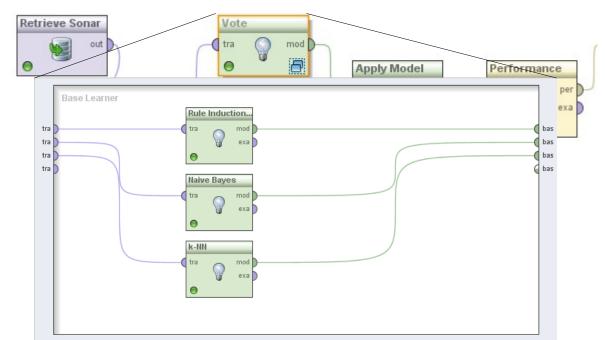
- The most straight forward approach
  - classification: use most-predicted label
  - regression: use average of predictions
- We have already seen this
  - k-nearest neighbors
  - each neighbor can be regarded as an individual classifier



## Voting in RapidMiner & SciKit Learn

- RapidMiner: Vote operator uses different base learners
- **Python:** VotingClassifier(
  - ("dt",DecisionTreeClassifier(),
    - "nb",GaussianNB(),

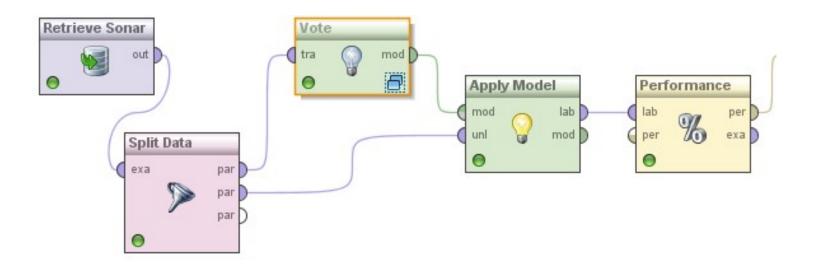
``knn",KNeighborsClassifier())



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### **Performance of Voting**

- 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

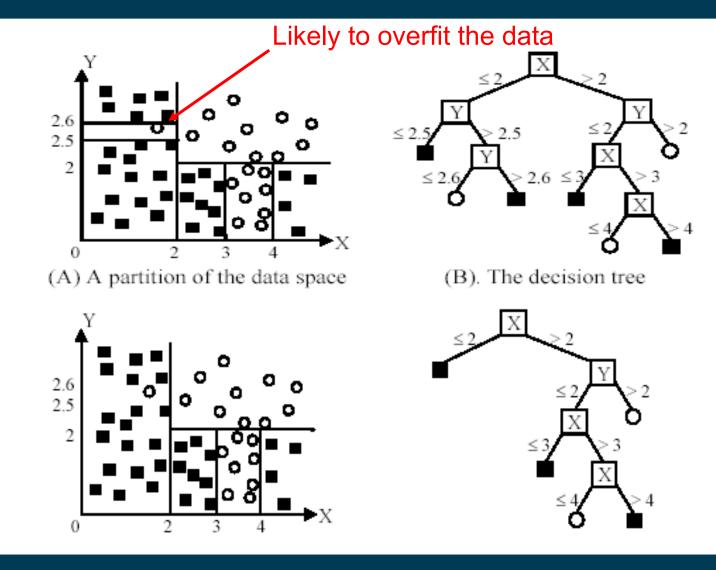
$$\sum_{i=13}^{25} \binom{25}{i} \varepsilon^i (1-\varepsilon)^{25-i} \approx 0.06 \ll \varepsilon$$

## Why does Voting Work?

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

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

#### **Recap: Overfitting and Noise**



12

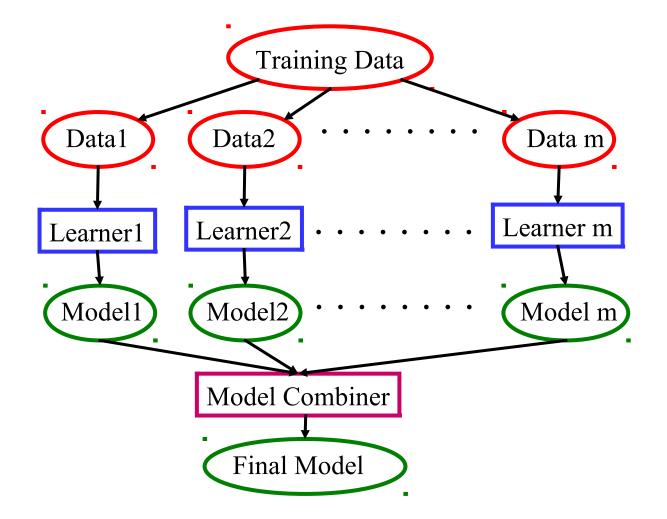
# Bagging

- 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  $\Pr(x \in D) = 1 - (1 - \frac{1}{2})^n \rightarrow 0.6322$

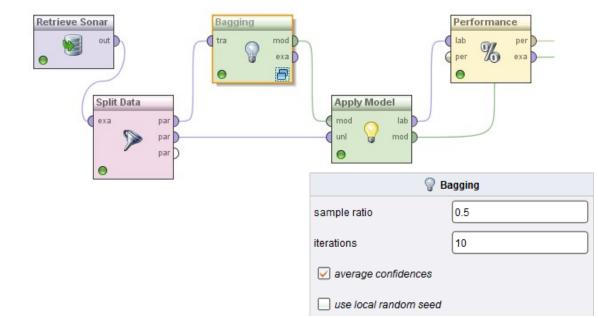
$$\Pr(x \in D_i) = 1 - (1 - \frac{1}{n}) \to 0.6322$$

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

## **Bagging in RapidMiner and Python**

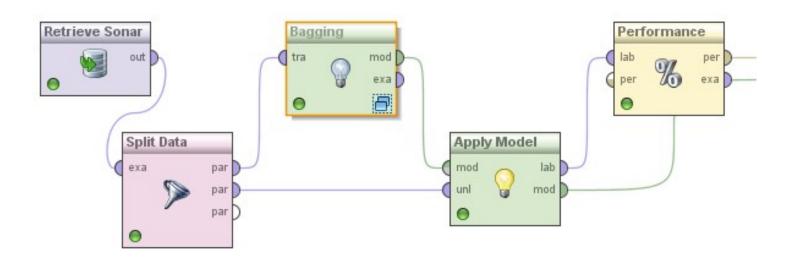
- Bagging operator uses a base learner
- Number and ratio of samples can be specified

```
- bagging = BaggingClassifier(
 DecisionTreeClassifier(),
 10,
 0.5)
```



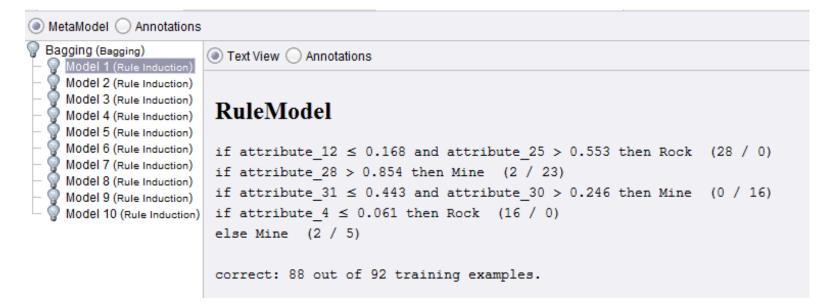
## **Performance of Bagging**

- 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

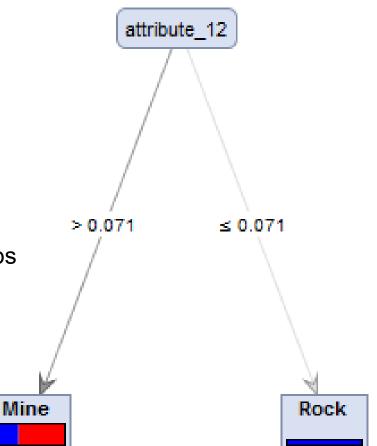
#### **Random Forests**

- 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
  - rf = RandomForestClassifier(n\_estimators=10)



## **Paradigm Shift: Many Simple Learners**

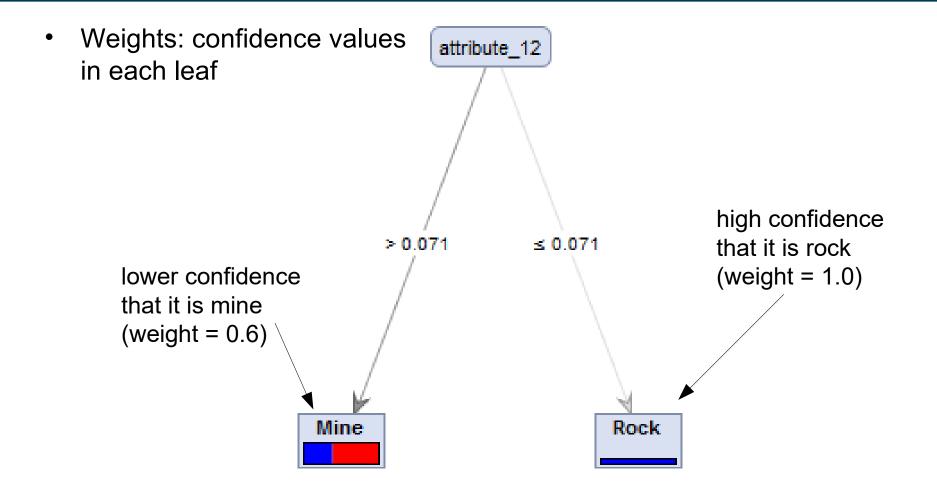
- So far, we have looked at learners that are as good as possible
- Bagging allows a different approach
  - several simple models instead of a single complex one
  - Analogy: the SPIEGEL poll (mostly no political scientists, nevertheless: accurate results)
  - extreme case: using only decision stumps
- 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
  - Python: parameter voting=soft
    - sums up all confidences for each class and predicts argmax
    - caution: requires *comparable* confidence scores!

## **Weighted Voting with Decision Stumps**



#### **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:

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

Error Rate = 1 - Accuracy

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

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### **Accuracy with Weights**

• Definition of accuracy

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

- 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**

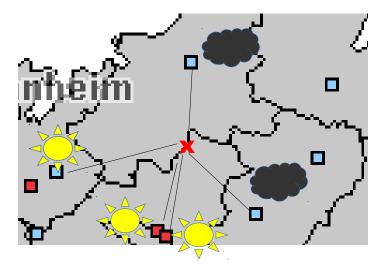
• Recap: Gini index as splitting criterion

$$GINI(t) = 1 - \sum_{j} [p(j | t)]^{2}$$

- 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



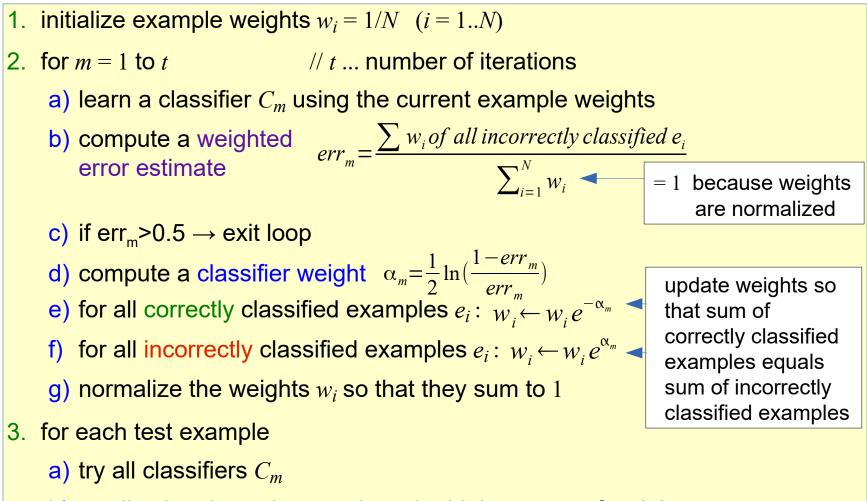
## Intermezzo: Learning with Weighted Instances

- Handling imbalanced classification problems
- So far:
  - undersampling
    - removes examples  $\rightarrow$  loss of information
  - oversampling
    - adds examples → larger data (performance!)
- Alternative:
  - lowering instance weights for larger class
  - simplest approach: weight 1/|C| for each instance in class C

#### **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**

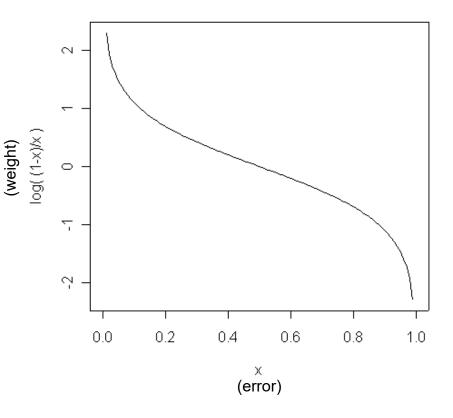


b) predict the class that receives the highest sum of weights  $\alpha_m$ 

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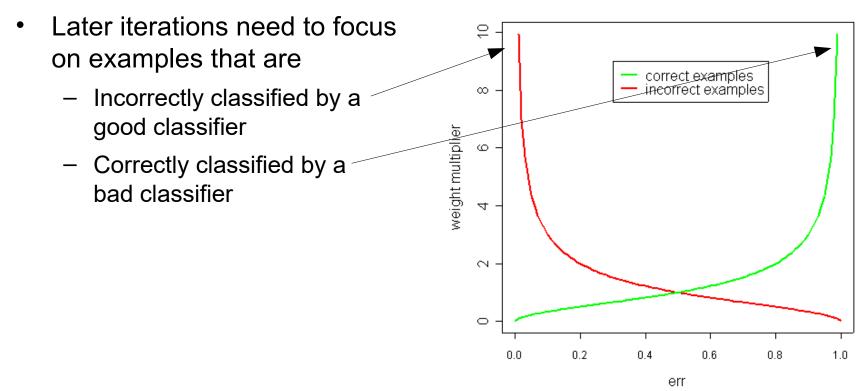
## **Illustration of the Weights**

- Classifier Weights  $\alpha_m$ 
  - 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!



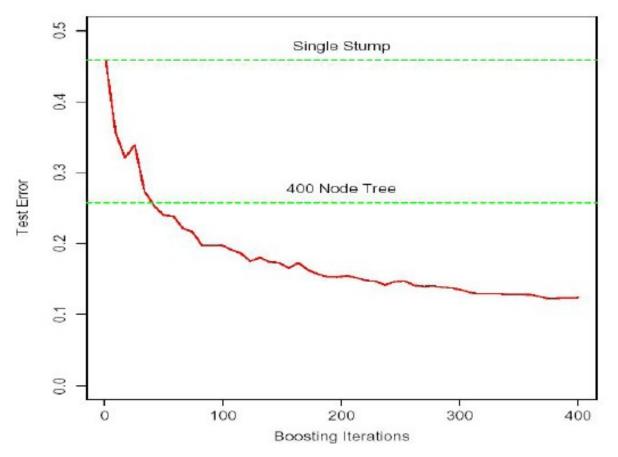
## **Illustration of the Weights**

- Example Weights
  - multiplier for correct and incorrect examples
  - depending on error



#### **Boosting – Error Rate Example**

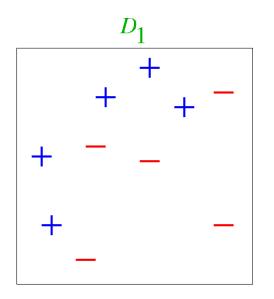
boosting of decision stumps on simulated data



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

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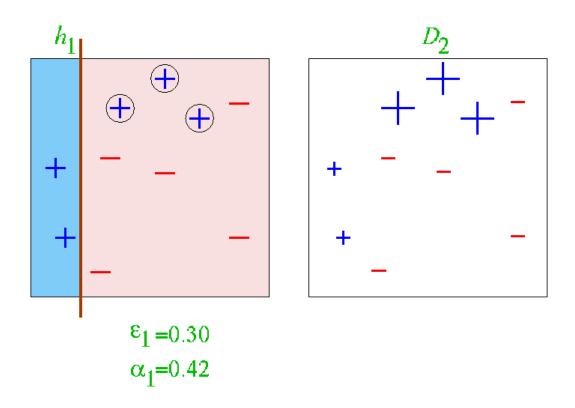
#### **Toy Example**



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

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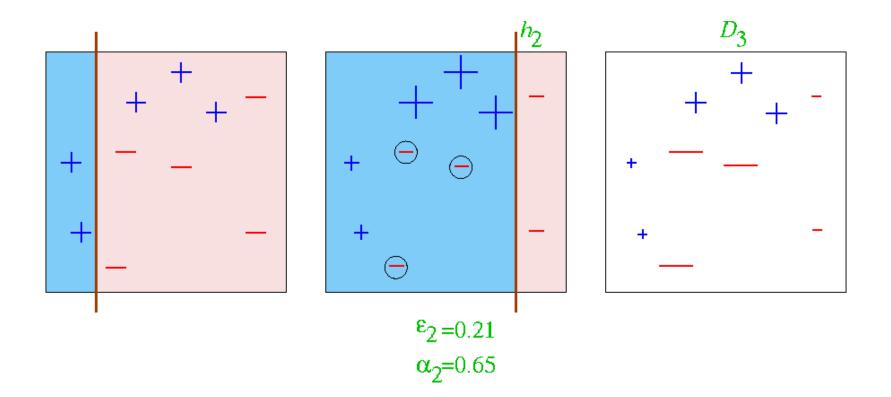
Round 1



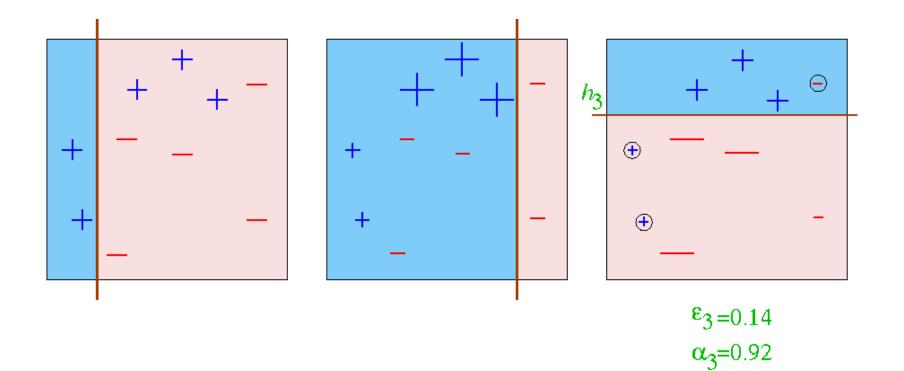
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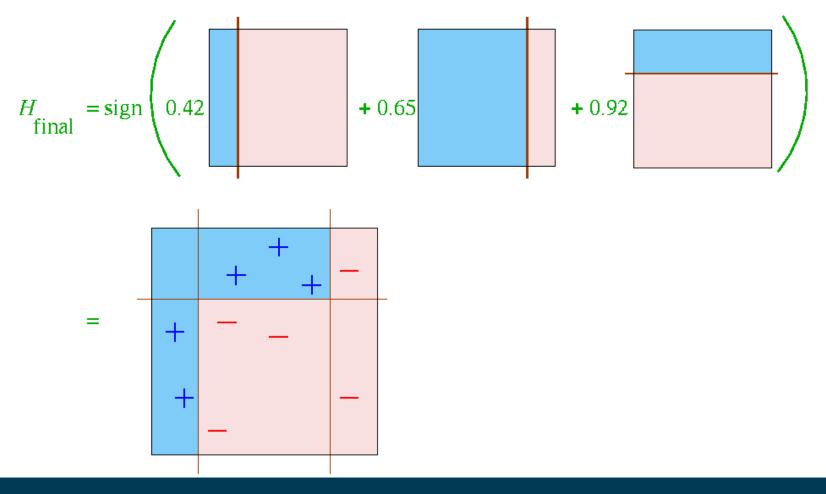
Round 2



Round 3



#### **Final Hypothesis**



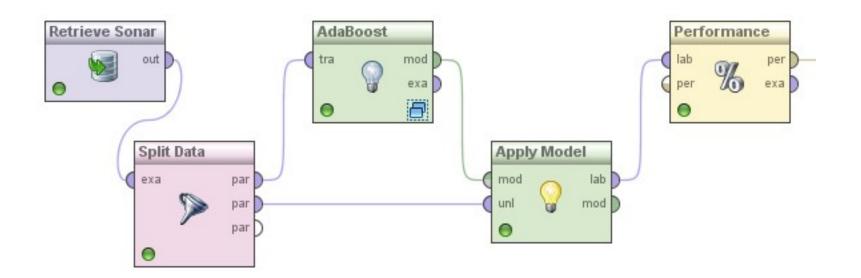
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#### **Hypothesis Space of Ensembles**

- 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  $\rightarrow$  different linear separations
  - resulting hypothesis space also allows polygon separations

### **Boosting in RapidMiner and Python**

- Just like voting and bagging
  - bdt = AdaBoostClassifier(
     DecisionTreeClassifier),
     n\_estimators=200)



# **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)
- 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

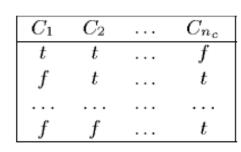
- Basic Idea:
  - learn a function that combines the predictions of the individual classifiers
- Algorithm:
  - train *n* different classifiers  $C_{1}...C_{n}$  (the base classifiers)
  - obtain predictions of the classifiers for the training examples
  - form a new data set (the meta data)
    - classes
      - 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:

A	Class	
$x_{11}$	 $x_{1n_a}$	t
$x_{21}$	 $x_{2n_a}$	f
$x_{n_e1}$	 $x_{n_e n_a}$	t

training set



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

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## **Stacking and Overfitting**

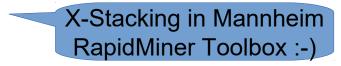
- Consider a dumb base learner D, which works as follows:
  - during training: store each training example
  - during classification: if example is stored, return its class otherwise: return a random prediction
- If D is used along with a number of classifiers in stacking, what will the meta classifier look like?
  - D is perfect on the training set
  - so the meta classifier will say: always use D's result

Implementation in RapidMiner :-(

do you know that classifier?

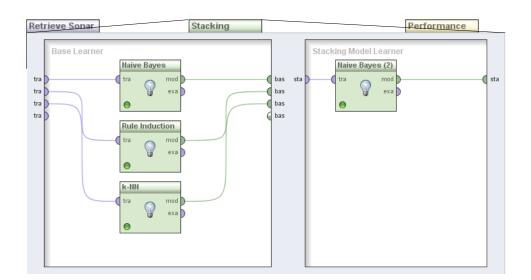
## **Stacking and Overfitting**

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



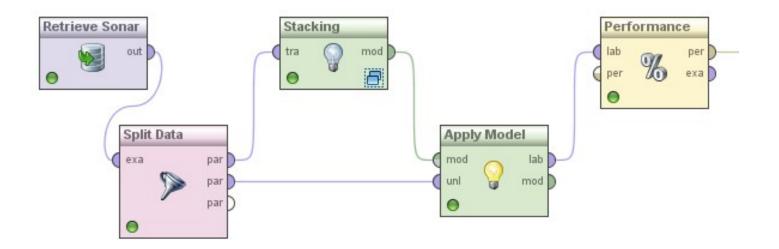
### Stacking in RapidMiner and Python

- Looks familiar again
  - we need a set of base learners (like for voting)
  - and a learner for the stacking model
- Python: not in scikit-learn, use, e.g., package mlxtend
  - requires setting base classifiers and meta learner as well



#### **Performance of Stacking**

- 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

9					•			
•		•	•	•	•	•	•	•
	•	•			•			
•	•	•	•	•	•	•	•	•
•	•	•	•	•	•	•	•	•
•	•	•	•	•	•	•	•	•
-2.0	-1.6	-1.2 -0.8	-0.4		0.4		1.6	2.0

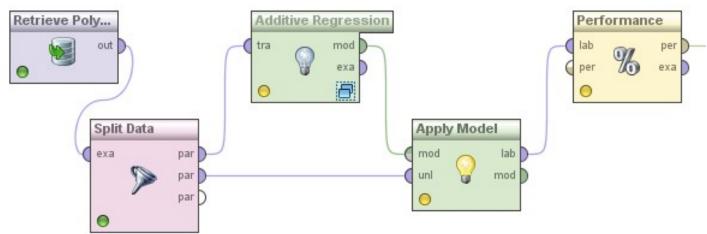
Accuracy:

- Baseline: 0.89
- Decision Tree: 1.0
- Rule Learner: 0.89
- Voting: 0.89
- Weighted Voting: 1.0
- Stacking: 1.0

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#### **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*
- In Python: usually the same class ending in *Regressor* instead of *Classifier*



### **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

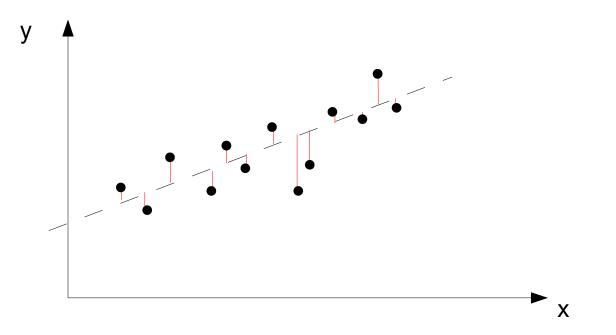
- What happens if we use Linear Regression inside of Additive Regression?
- The first iteration learns a linear regression model Ir<sub>1</sub>
  - By minimizing the sum of squared errors
- The second iteration aims at learning a LR Ir<sub>2</sub> model for

 $- x' = (x-lr_1(x))^2$ 

- Since  $(x-Ir_1(x))^2$  is already minimal,  $Ir_2$  cannot improve upon this
  - Hence, the subsequent linear models will always be a constant 0

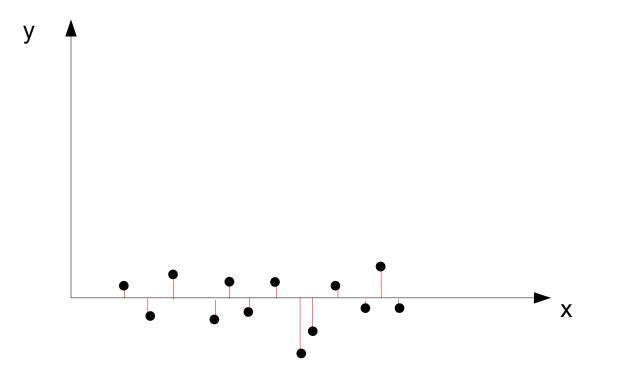
#### Additive Regression w/ Linear Regression

• First regression model:

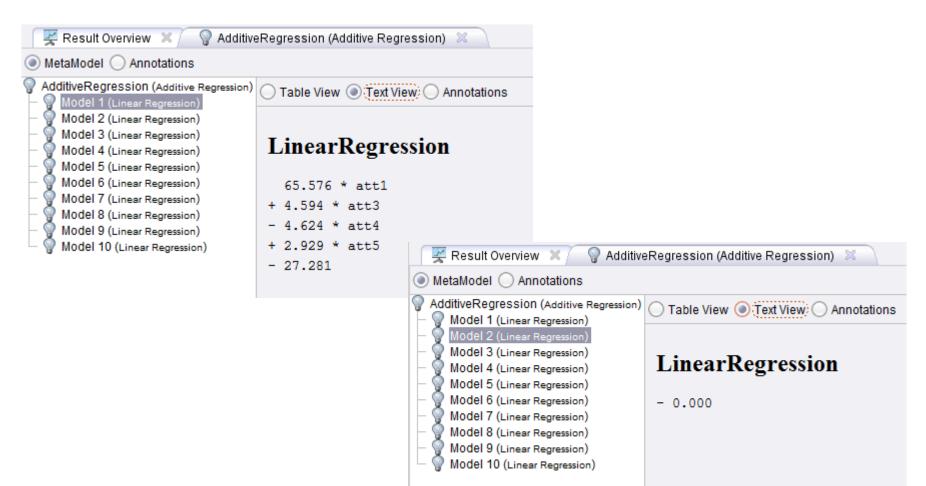


#### **Additive Regression w/ Linear Regression**

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

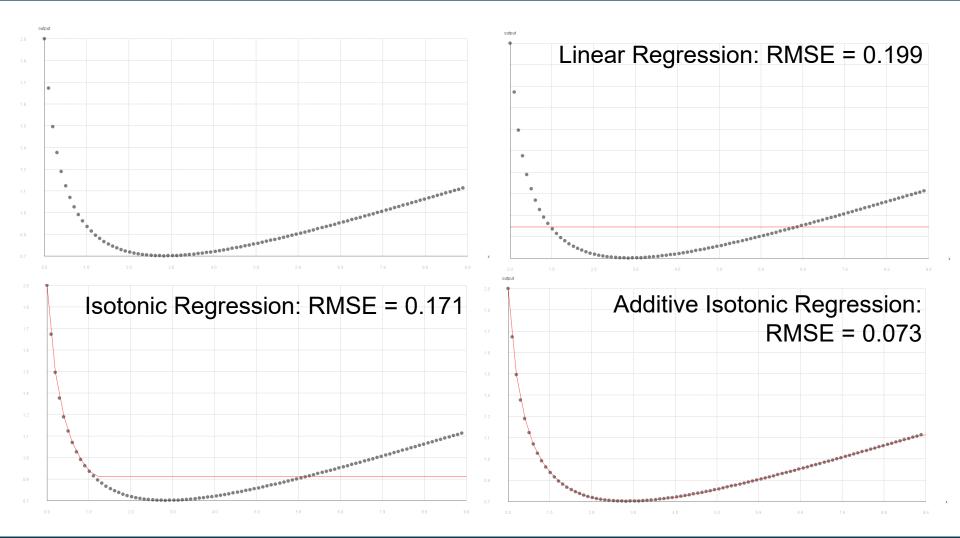


### **Additive Regression**



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

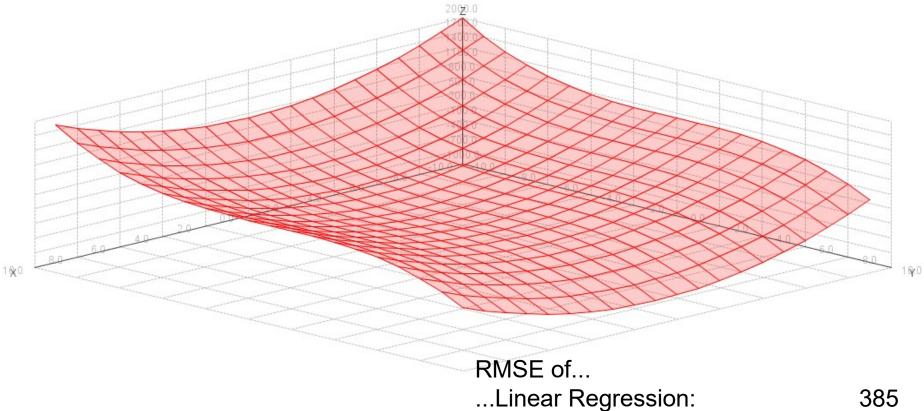
#### **Example 1: One-dimensional, Non-linear**



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#### **Example 2: Multidimensional, Non-Linear**





- ...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  $\rightarrow$  very expensive
  - actual: false, predicted true  $\rightarrow$  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<sub>2</sub>) = 0.9
- Risk values:
  - $R(stall|x_1) = P(stall|x_1)*C(stall,stall) + P(no|x_1)*C(stall,no) = 0.2*1 = 0.2$

actual

stall

no stall

8/10 classifiers

are correct

-  $R(no|x_1) = P(stall|x_1)*C(no,stall) + P(no|x_1)*C(no,no) = 0.8*10 = 8$ 

=0

- $R(stall|x_2) = P(stall|x_2)*C(stall,stall) + P(no|x_2)*C(stall,no) = 0.9*1 = 0.9$
- $R(no|x_2) = P(stall|x_2)*C(no,stall) + P(no|x_2)*C(no,no) = 0.1*10 = 1$
- Since 0.9<1
  - x<sub>2</sub> is relabeled to "stall"

http://i.telegraph.co.uk/multimedia/archive/01419/plane\_1419831c.jpg



predicted

no stall

10

0

stall

0

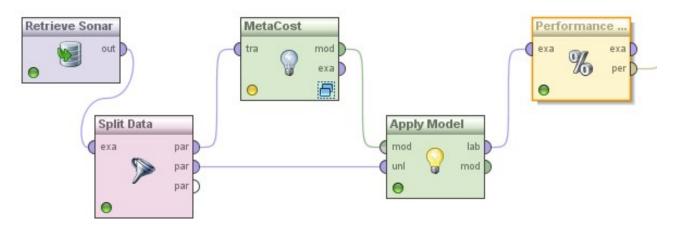
1

#### 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

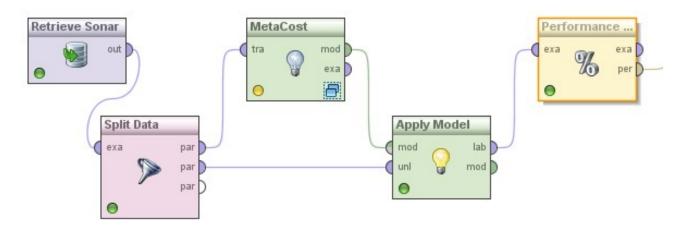
• Hint: use the performance (cost) operator for evaluation



Edit Parameter Matrix: cost matrix    X      Edit Parameter Matrix: cost matrix    Edit Parameter Matrix: cost matrix      The matrix of missclassification costs. Columns and Rows in order of internal mapping.							
Cost Matrix	True Class 1	True Class 2					
Predicted Class 1	0.0	1.0					
Predicted Class 2	2.0	0.0					
	Increase Size	crease Size 🖌 OK 🄀 Cancel					

#### 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
- Typical cost matrix:

		predicted				
		very low	low	medium	high	very high
	very low	0	1	2	4	8
actual	low	1	0	1	2	4
	medium	2	1	0	1	2
	high	4	2	1	0	1
	very high	8	4	2	1	0

## 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?**

