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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



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



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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



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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

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

- 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



Intermezzo: Learning with Weighted Instances

- Handling imbalanced classification problems
- So far:
 - undersampling
 - removes examples \rightarrow loss of information
 - oversampling
 - adds examples \rightarrow larger data (performance!)
 - also: synthetic data points (SMOTE)
- 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 α_m

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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


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



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, parallel to the axes
- 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 Ir₁
 - By minimizing the sum of squared errors
- The second iteration aims at learning a LR Ir₂ 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



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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|x₂) = 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

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- x₂ is relabeled to "stall"

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

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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 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					

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
	low	1	0	1	2	4
	medium	2	1	0	1	2
actual	high	4	2	1	0	1
act	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?

