COMP30027 Machine Learning Classifier Combination

Semester 1, 2019
Jeremy Nicholson & Tim Baldwin & Karin Verspoor



© 2019 The University of Melbourne

Lecture Outline

- 1 Introduction
- 2 Stacking
- Bagging
- 4 Random Forests
- 6 Boosting
- **6** Summary

To Date ... I

- Thus far, we have discussed individual classification algorithms and considered each of them in isolation/competition
- We have discussed ways of comparing the performance of individual classifiers over a given dataset/task, which allows us to choose the "dataset optimal" classifier
- If we were to carry out error analysis of multiple classifiers over a given dataset, would we find that the errors made by better-performing classifiers were over a proper subset of instances that worse-performing classifiers similarly misclassified? Almost certainly NO!

To Date ... II

 When evaluating, we only get one shot at classifying a given test instance and are stuck with the bias inherent in a given algorithm

Classifier Combination

- Classifier combination (aka. ensemble learning)
 constructs a set of base classifiers from a given set of
 training data and aggregates the outputs into a single
 meta-classifier
- Motivation 1: the combination of lots of weak classifiers can be at least as good as one strong classifier
- Motivation 2: the combination of a selection of strong classifiers is (usually) at least as good as the best of the base classifiers

Source(s): Tan et al. [2006, p277-80]

Why does Combination Work? I

• Suppose we have a set of 25 binary base classifiers, each with an error rate of $\epsilon=0.35$. Assuming the base classifiers are independent and we perform classifier combination by voting, the error rate of the combined classifier is:

$$\sum_{i=13}^{25} {25 \choose i} \epsilon^i (1-\epsilon)^{25-i} \approx 0.06$$

...And if the classifiers aren't independent?

Classification with Combined Classifiers

- The simplest means of classification over multiple base classifiers is simple voting:
 - for a nominal class set, run multiple base classifiers over the test data and select the class predicted by the most base classifiers (cf. k-NN)
 - for a continuous class set, average over the numeric predictions of our base classifiers

Approaches to Classifier Combination

Instance manipulation: generate multiple training datasets through sampling, and train a base classifier over each

Feature manipulation: generate multiple training datasets through different feature subsets, and train a base classifier over each

Class label manipulation: generate multiple training datasets by manipulating the class labels in a reversible manner

Algorithm manipulation: semi-randomly "tweak" internal parameters within a given algorithm to generate multiple base classifiers over a given dataset

Source(s): Tan et al. [2006, p277-80]

Lecture Outline

- 1 Introduction
- 2 Stacking
- Bagging
- 4 Random Forests
- 6 Boosting
- **6** Summary

Stacking

- Basic intuition: "smooth" errors over a range of algorithms with different biases
- Method 1: simple voting presupposes the classifiers have equal performance
- Method 2: train a classifier over the outputs of the base classifiers (meta-classification)

train using nested cross validation to reduce bias

Stacking example

- Given training dataset (X, y):
 - Train SVM
 - Train Naive Bayes
 - Train Decision Tree
- Discard (or keep) X, add new attributes for each instance:
 - predictions (labels) of the classifiers above
 - other data as available (NB scores, SVM wx + b, etc.)
- Train meta-classifier (usually Logistic Regression)

Stacking: Reflections

- Mathematically simple but computationally expensive method
- Able to combine heterogeneous classifiers with varying performance
- Generally, stacking results in as good or better results than the best of the base classifiers
- Widely seen in applied research; less interest within theoretical circles (esp. statistical learning)

Lecture Outline

- 1 Introduction
- 2 Stacking
- 3 Bagging
- 4 Random Forests
- 6 Boosting
- **6** Summary

Bagging I

- Basic intuition: the more data, the better the performance (lower the variance), so how can we get ever more data out of a fixed training dataset?
- Method: construct "novel" datasets through a combination of random sampling and replacement
 - Randomly sample the original dataset N times, with replacement
 - Thus, we get a new dataset of the same size, where any individual instance is absent with probability $(1 \frac{1}{N})^N$
 - construct k random datasets for k base classifiers, and arrive at prediction via voting

Bagging: Sampling Example

• Original training dataset:

Bootstrap samples:

:

Bagging: Classification Algorithm

- The same (weak) classification algorithm is used throughout
- As bagging is aimed towards minimising variance through sampling, the algorithm should be unstable (= high-variance) ... e.g.?

Bagging: Reflections

- Simple method based on sampling and voting
- Possibility to parallelise computation of individual base classifiers
- Highly effective over noisy datasets (outliers may vanish)
- Performance is generally significantly better than the base classifiers and only occasionally substantially worse

Lecture Outline

- 1 Introduction
- Stacking
- Bagging
- 4 Random Forests
- 6 Boosting
- **6** Summary

Random Tree

A "Random Tree" is a Decision Tree where:

- At each node, only some of the possible attributes are considered
- For example, a fixed proportion τ of all of the attributes, except the ones used earlier in the tree
- Attempts to control for unhelpful attributes in the feature set
- Much faster to build than a "deterministic" Decision Tree, but increases model variance

Random Forests

A "Random Forest" is:

- An ensemble of Random Trees (many trees = forest)
- Each tree is built using a different Bagged training dataset
- As with Bagging the combined classification is via voting
- The idea behind them is to minimise overall model variance, without introducing (combined) model bias

Random Forests (cont.)

- Hyperparameters:
 - number of trees B (can be tuned, e.g. based on "out-of-bag" error rate)
 - feature sub-sample size (e.g. $|\log_2|F| + 1|$)
- Interpretation:
 - logic behind predictions on individual instances can be tediously followed through the various trees
 - logic behind overall model: ???

Practical Properties of Random Forests

- Generally a very strong performer
- Embarrassingly parallelisable
- Surprisingly efficient
- Robust to overfitting
- Interpretability sacrificed

Lecture Outline

- 1 Introduction
- Stacking
- Bagging
- 4 Random Forests
- 5 Boosting
- **6** Summary

Boosting

- Basic intuition: tune base classifiers to focus on the "hard to classify" instances
- Method: iteratively change the distribution and weights of training instances to reflect the performance of the classifier on the previous iteration
 - start with each training instance having a $\frac{1}{N}$ probability of being included in the sample
 - over T iterations, train a classifier and update the weight of each instance according to whether it is correctly classified
 - combine the base classifiers via weighted voting

Boosting: Sampling Example

• Original training dataset:

Boosting samples:

Boosting Example: AdaBoost I

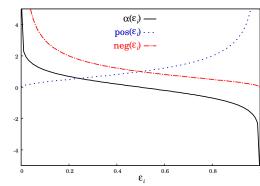
- Base classifiers: $C_1, C_2, ..., C_T$
- Training instances $\{(x_j, y_j)| j = 1, 2, ..., N\}$
- Initial instance weights $\{w_i^{(0)} = \frac{1}{N} | j = 1, 2, ..., N\}$
- Error rate for C_i:

$$\epsilon_i = \frac{1}{N} \sum_{i=1}^{N} w_j^{(i)} \delta(C_i(x_j) \neq y_j)$$

Boosting Example: AdaBoost II

• "Importance" of C_i (i.e. the weight associated with the classifiers' votes):

$$\alpha_i = \frac{1}{2} \log_e \frac{1 - \epsilon_i}{\epsilon_i}$$



Boosting Example: AdaBoost III

• Instance weights for i > 0:

$$w_j^{(i+1)} = \frac{w_j^{(i)}}{Z_i} \times \left\{ \begin{array}{l} e^{-\alpha_i} & \text{if } C_i(x_j) = y_j \\ e^{\alpha_i} & \text{if } C_i(x_j) \neq y_j \end{array} \right.$$

Boosting Example: AdaBoost IV

- Continue iterating for i = 1, 2, ..., T, but reinitialise the instance weights whenever $\epsilon_i > 0.5$
- Classification:

$$C^*(x) = \underset{y}{\operatorname{arg max}} \sum_{j=1}^{T} \alpha_j \ \delta(C_j(x) = y)$$

 Base classification algorithm: decision stumps (OneR) or decision trees

Boosting: Reflections

- Mathematically complicated but computationally cheap method based on iterative sampling and weighted voting
- More computationally expensive than bagging
- The method has guaranteed performance in the form of error bounds over the training data
- Interesting effect with convergence of the error rate over the training vs. test data
- In practical applications, boosting has the tendency to overfit

Bagging/RF vs. Boosting

Bagging/RF	Boosting
Parallel sampling	Iterative sampling
Simple voting	Weighted voting
Single classification algorithm	Single classification algorithm
Minimise variance	Minimise (instance) bias
Not prone to overfitting	Prone to overfitting

Lecture Outline

- 1 Introduction
- 2 Stacking
- Bagging
- 4 Random Forests
- 6 Boosting
- **6** Summary

Summary

- What is classifier combination?
- What is bagging and what is the basic thinking behind it?
- What is boosting and what is the basic thinking behind it?
- What is stacking and what is the basic thinking behind it?
- How do bagging and boosting compare?

References I

Leo Breiman. Random forests. Machine Learning, 45(1):5-32, 2001.

Pang-Ning Tan, Michael Steinbach, and Vipin Kumar. *Introduction to Data Mining*. Addison Wesley, 2006.

Ian H. Witten and Eibe Frank. Data Mining: Practical Machine Learning Tools and Techniques with Java Implementations. Morgan Kaufmann, San Francisco, USA, second edition, 2005.