Lecture 16: Ensemble Learning

COMP90049

Semester 1, 2021

Lea Frermann, CIS

Acknowledgement: Jeremy Nicholson, Tim Baldwin & Karin Verspoor

Roadmap

So far...

- individual classification algorithms in isolation
- choose the ”optimal” classifier by comparing the performance of individual classifiers over a given dataset/task
- When evaluating, we only get one shot at classifying a given test instance and are stuck with the bias inherent in a given algorithm

Today

- Wrapping up classification:
  - aside on (non)-linear classification
  - aside on (non)-parametric machine learning
- Ensembles: combining multiple (weak) models into one strong model!

Aside: (Non)-linear and (non)-parametric classification

Linear classifiers

- Naive Bayes
- Logistic Regression
- Perceptron

... because their **decision boundary** is a linear function of the input x.
(There's still a non-linear activation function, so y is not a linear function of x).

Aside I: linear vs. non-linear classification

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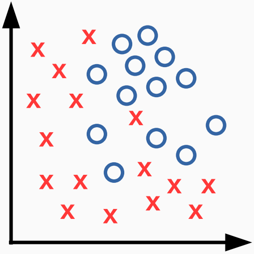
Non-linear classifiers

- Multi-layer perceptron (with non-linear activations)
- K-Nearest Neighbors
- Decision trees

... because their **decision boundary** is *not* a linear function of the input x.
They can learn more complex decision boundaries.

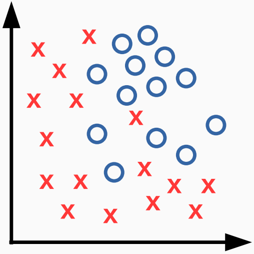
Aside I: linear vs. non-linear classification

Decision boundary of a well-trained **decision tree**



Appropriate-fitting

Decision boundary of a well-trained **Naive Bayes classifier**



Appropriate-fitting

Aside II: parametric vs. non-parametric models

Warning: these terms are ambiguous and several definitions exist. We'll adopt the following.

Parametric Models

- Naive Bayes, Logistic Regression, Multi-layer perceptron, ...

... because they have a **constant number of parameters**, irrespective of the **amount of training data**. We can write down the model $y = f(x; \theta)$ which holds true no matter what x. We fit parameters to a **given model**.

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Non-parametric models

- K-Nearest Neighbors, Decision trees, ...

... because the parameters grow with the training data and are **possibly infinite**. We **learn our model directly from the data**.

- Discuss: what's 'non-parametric' about KNN?
- Discuss: what's 'non-parametric' about Decision Trees?

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Now, on to ensembles

Ensembles I

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

Ensembles II

- When does ensemble learning work?
  - the base classifiers should not make the same mistakes
  - the base classifiers are reasonably accurate

	t_1	t_2	t_3
C_1	√	√	x
C_2	x	√	√
C_3	√	x	√
C^*	√	√	√

	t_1	t_2	t_3
C_1	√	√	x
C_2	√	√	x
C_3	√	√	x
C^*	√	√	x

	t_1	t_2	t_3
C_1	√	x	x
C_2	x	√	x
C_3	x	x	√
C^*	x	x	x

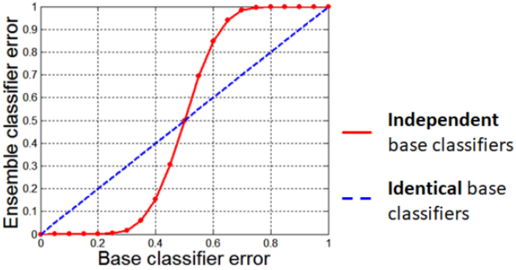
Ensembles III

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

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

Ensembles VI

- When does ensemble learning work?



- 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 (e.g. k-NN)
  - for a continuous class set, average over the numeric predictions of our base classifiers

Approaches to Ensemble Learning

- **Instance manipulation**: generate multiple training datasets through sampling, and train a base classifier over each dataset
- **Feature manipulation**: generate multiple training datasets through different feature subsets, and train a base classifier over each dataset
- **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

Stacking

Stacking I

- **Intuition**: “smooth” errors over a range of algorithms with different biases
- **Simple Voting**: generate multiple training datasets through different feature subsets, and train a base classifier over each dataset
    - presupposes the classifiers have equal performance
- **Meta Classification**: train a classifier over the outputs of the base classifiers
    - train using nested cross validation to reduce bias

Stacking II

- Given training dataset (X, y):
  - Train Neural Network
  - 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 etc.)
- Train meta-classifier (usually Logistic Regression or Neural Network)

Stacking III

- 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)

Bagging

Bagging I

- **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 (bootstrap)
    - 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 II

- Original dataset:

1	2	3	4	5	6	7	8	9	10

- Bootstrap Samples

7	2	6	7	5	4	8	8	1	10

1	3	8	10	3	5	8	10	1	9

2	9	4	2	7	9	3	10	1	10

⋮

Bagging III

- 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 VI

- 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

Bagging - Random Forest

Random Forest I

A “Random Tree” is a Decision Tree where:

- At each node, only some of the possible attributes are considered
- For example, a fixed proportion 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 Forest II

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

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Random Forest III

Hyperparameters:

- number of trees B (can be tuned, e.g. based on “out-of-bag” error rate)
- feature sub-sample size (e.g. $(\log|F| + 1)$

Interpretation:

- logic behind predictions on individual instances can be tediously followed through the various trees
- logic behind overall model: ???

Random Forest VI

Practical Properties of Random Forests:

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

Boosting

Boosting I

- Intuition: tune base classifiers to focus on the “hard to classify” instances
- Approach: 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 probability of $\frac{1}{N}$ 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 II

- Original dataset:

1	2	3	4	5	6	7	8	9	10

- Boosting samples:

Iteration 1:	7	2	6	7	5	4	8	8	1	10
Iteration 2:	1	3	8	4	3	5	4	10	1	4
Iteration 3:	4	9	4	2	4	4	3	10	1	4

$\vdots$

AdaBoost I

- Base classifiers: $C_1, C_2, \ldots, C_T$
- Training instances $(x_j, y_j) | j = 1, 2, \ldots, N$
- Initial instance weights $w_j^{(0)} = \frac{1}{N} | j = 1, 2, \ldots, N$
- Construct classifier C_i in iteration i:

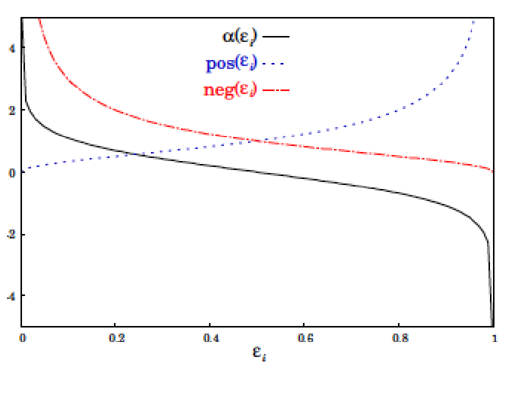
Error rate for C_i:

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

AdaBoost II

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

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



AdaBoost III

- Weights for instance j ($i > 0$):

$$w_j^{(i+1)} = \frac{w_j^{(i)}}{Z_i} \times \begin{cases} e^{-\alpha_i} & \textit{if} \quad C_i(x_j) = y_j \\ e^{\alpha_i} & \textit{if} \quad C_i(x_j) \neq y_j \end{cases}$$

AdaBoost VI

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

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

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

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Boosting III

- 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

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Bagging vs. Boosting

Bagging

- Parallel sampling
- Simple voting
- Single classification algorithm
- Minimise variance
- Not prone to overfitting

Boosting

- Iterative sampling
- Weighted voting
- Single classification algorithm
- Minimise (instance) bias
- Prone to overfitting

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

- 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.