# Lecture 19: Ensemble Learning

**COMP90049**

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# 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**

- Ensembles: combining multiple (weak/unstable) models into one strong model!

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

# Aside I: linear vs. non-linear classification

## Linear classifiers

$\theta_1 x_1 + \theta_2 x_2 + \dots$

- 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 $x$).

## 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.

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# 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 $\boxed{y = f(x; \theta)}$ which holds true no matter what $x$. We fit parameters to a **given model**.

$\sigma(\theta^T x)$

## 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?

# Now, on to ensembles

# Ensembles: Intuition & Guarantees

- **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: Toy example

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

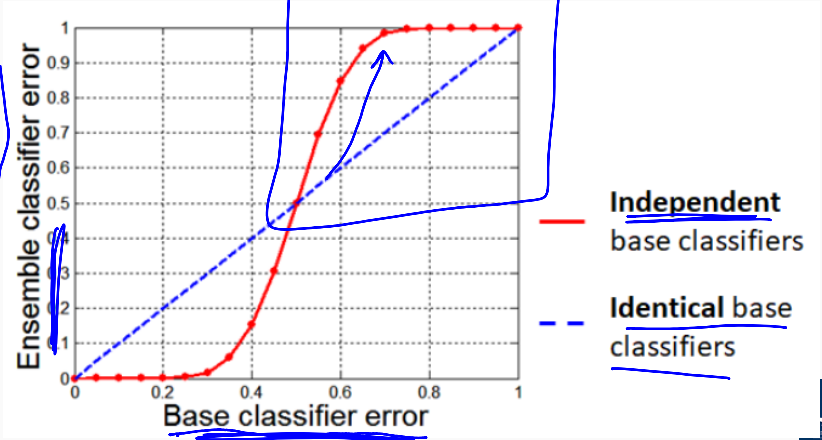
| | $t_1$ | $t_2$ | $t_3$ |
|---|---|---|---|
| $C_1$ | √ | √ | x |
| $C_2$ | x | √ | √ |
| $C_3$ | √ | x | √ |
| $C^*$ | √ | √ | √ |

| | $t_1$ | $t_2$ | $t_3$ |
|---|---|---|---|
| $C_1$ | √ | √ | 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: Error rate of base classifiers

- When does ensemble learning work?



# Ensembles: Reduction of error rates of base classifiers

p(wrong) = 0.35

**Let's assume that:**

- We have a set of 25 binary base classifiers
- Each has an error rate of $\epsilon = 0.35$
- The base classifiers are independent (that's usually false)
- We perform classifier combination by voting

**The error rate of the combined classifier is:**

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

- The simplest means of classification over multiple base classifiers is simple **voting**:
  - **Classification**: run multiple base classifiers over the test data and select the class predicted by the most base classifiers (e.g. k-NN)
  - **Regression**: 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
- **Algorithm manipulation**: semi-randomly “tweak” internal parameters within a given algorithm to generate multiple base classifiers over a given dataset
- **Class label manipulation**: generate multiple training datasets by manipulating the class labels in a reversible manner

[1,2,3,4,5]

[1 | 2345]

[12 | 345] ...

# Stacking

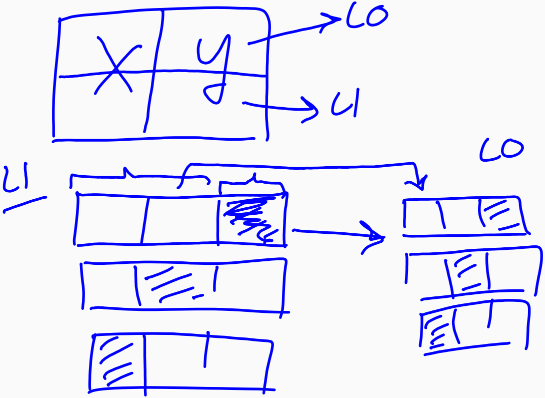
# Stacking: Intuition

- **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: Meta classification

- **Level 0**: 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 of the classifiers above
  - other data as available (NB scores etc.)
- **Level 1**: Train meta-classifier. Usually Logistic Regression or Neural Network

## Nested Cross-validation



# Stacking: Summary

- 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)

Quiz!

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# Bagging

## Bagging: Intuition

- **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 $\boxed{N}$ times, **with replacement** (bootstrap)
  - Thus, we get a new dataset of the same size, where any individual instance is absent with probability $\underline{(1 - \frac{1}{N})^N}$ $\sim 0.37$
  - construct $k$ random datasets for k base classifiers, and arrive at prediction via voting

# Bagging: Example

- 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: Use cases I

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

# Bagging: Use cases II

- 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 $\tau$ 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

This is an instance of **Feature Manipulation**.

# 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

This is an instance of **Instance Manipulation**.

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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: ???

**Practical Properties of Random Forests**:

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

# Boosting

# Boosting: Intuition

- **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: Example

- 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 |

⋮

# Adaptive Boosting: AdaBoost

# AdaBoost I

**AdaBoost** (Adaptive Boosting) is a *sequential* ensembling algorithm.

**Basic idea**:

- Base classifier: $C_0$
- Training instances $(x_j, y_j)|j = 1, 2, \ldots, N$
- Initial instance weights $w_j^{(0)} = \frac{1}{N}|j = 1, 2, \ldots, N$
- In iteration $i$:
    - Construct classifier $C_i$ and compute error rate $\epsilon_i$

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

0

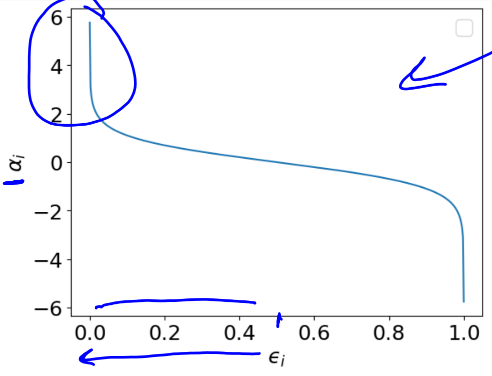
1

- Use $\epsilon_i$ to compute the classifier weight $\alpha_i$ (importance of $C_i$)
- Use $\alpha_i$ to update instance weights
- Add weighted $C_i$ to ensemble

**Output**: Weighted set of base classifiers: $\{(\alpha_1, C_1), (\alpha_2, C_2), \ldots, (\alpha_T, C_T)\}$

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

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

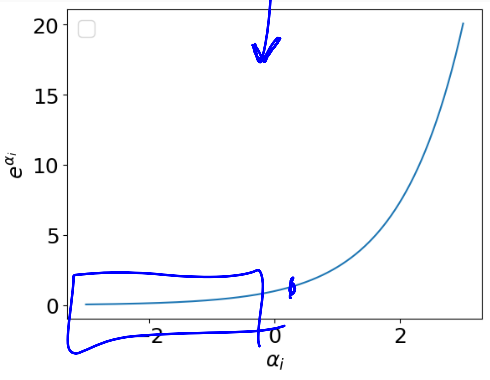


# AdaBoost III: Updating $w$

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

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

0




(recall that the $\alpha_i$s are always positive)

- Continue iterating for $i = 1, 2, \ldots, T$ , but re-initialise the instance weights whenever $\epsilon_i > 0.5$
- As long as each base classifier is better than random, convergence to a stronger model is **guaranteed**
- **Classification:** weighted voting

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

- **Typical base classifiers**: decision stumps (OneR) or decision trees. (Possibly the world's favorite classifier!)

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# Boosting: Summary

- 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 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?

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