Ensemble Methods: Bagging & Random Forests

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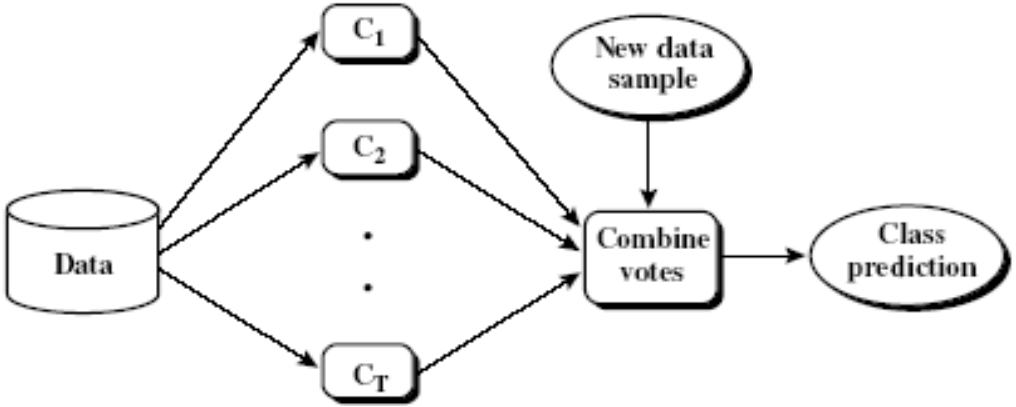
What are Ensemble Methods?

- Real - world problems often do not have a unique “correct” solution
- Multiple thought processes and teams and approaches often yield equally valid but completely different solutions.
- Combining different approaches using some heuristic could lead to a meta-learning method that utilizes the best of different approaches.
- Such a set of methods for combining many solutions (classifiers, regressors etc.) into one “better” solution are known as “**Ensemble Methods”**

Ensemble methods

- Uses a combination of N learned models: C_1, C_2, … C_N with the aim of creating an improved model C*
- Ensemble learning, more often than not, decreases variance of the predictors and allows better generalization



Paradigms of Ensemble Learning

Parallel Ensembles

- Combines several models, built separately to fit the data
- Allows naive parallelisation (many parallel models)
- Example: **Bagging** etc.

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Sequential Ensembles

- Each model built, explicitly uses other model predictions sequentially
- Every model improves upon the weaknesses of previous models
- Example: **Boosting** etc.

Committee Methods

- Individual learners are often “high capacity”, with a tendency to overfit
- High variance in such learners reduces their generalization capability
- Ensemble methods aim to reduce variance → counter overfitting

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- **Committees:**
  - Group of N individual models: C_1, C_2, … C_N
  - makes predictions by averaging over predictions of individual models
  - Motivated by frequentist perspective of bias and variance
- How does averaging predictions reduce variance?

Error Reduction

- Regression: Predict real-valued function **h(x)**
- Input: **x** = $(x_1, \ldots, x_p)^T$ where each $x_i \in \mathbb{R}$
- N models predicting outputs $\mathbf{y_i(x)}$ for i=1,...,N

$$y_i(\mathbf{x}) = h(\mathbf{x}) + \epsilon_i(\mathbf{x})$$

- Committee prediction: averaging

$$y_{\mathrm{COM}}(\mathbf{x}) = \sum_{i=1}^{N} y_i(\mathbf{x})$$

Error Reduction

The average sum-of-squares error of all N models:

$$E_{\text{avg}} = \frac{1}{N} \sum_{i=1}^{N} \mathbb{E}_x \left[\{ h(\mathbf{x}) - y_i(\mathbf{x}) \}^2 \right]$$

$$= \frac{1}{N} \sum_{i=1}^{N} \mathbb{E}_x \left[\epsilon_i(\mathbf{x})^2 \right]$$

Error Reduction

The sum-of-squares error for the committee prediction is:

$$E_{\mathrm{COM}} = \mathbb{E}_x\left[\left\{h(\mathbf{x}) - \frac{1}{N}\sum_{i=1}^{N} y_i(\mathbf{x})\right\}^2\right]$$

$$= \mathbb{E}_x\left[\left\{\frac{1}{N}\sum_{i=1}^{N} h(\mathbf{x}) - y_i(\mathbf{x})\right\}^2\right]$$

$$= \mathbb{E}_x\left[\left\{\frac{1}{N}\sum_{i=1}^{N} \epsilon_i(\mathbf{x})\right\}^2\right]$$

Error Reduction

- Assumption 1: Classifiers have zero bias

$$\mathbb{E}_x[y_i(\mathbf{x})] = h(\mathbf{x}) \implies \mathbb{E}_x[\epsilon_i(\mathbf{x})] = 0$$

- Assumption 2: Classifiers are uncorrelated

$$\mathbb{E}_x\left[\epsilon_i(\mathbf{x})\epsilon_j(\mathbf{x})\right] = 0 \quad \text{for all } i \neq j$$

Error Reduction

The committee sum-of-squares error is reduced to:

$$
\begin{aligned}
E_{\mathrm{COM}} &= \mathbb{E}_x\left[\left\{\frac{1}{N}\sum_{i=1}^{N}\epsilon_i(\mathbf{x})\right\}^2\right] \\
&= \mathbb{E}_x\left[\frac{1}{N^2}\cdot\left\{\sum_{i=1}^{N}\epsilon_i(\mathbf{x})^2 + \sum_{i\neq j}\epsilon_i(\mathbf{x})\epsilon_j(\mathbf{x})\right\}\right] \\
&= \frac{1}{N}\cdot\mathbb{E}_x\left[\frac{1}{N}\sum_{i=1}^{N}\epsilon_i(\mathbf{x})^2\right] \\
&= \frac{1}{N}\cdot E_{\mathrm{avg}}
\end{aligned}
$$

Error Reduction

This shows us that committees reduce variance in an ideal world using uncorrelated learners.

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This shows us that committees reduce variance in an ideal world using uncorrelated learners.

What if we introduce correlation? (real world)

Recall, correlation from statistics:

$$\text{corr}(X, Y) = \frac{\text{cov}(X, Y)}{\sqrt{\text{var}(X) \cdot \text{var}(Y)}}$$

where: cov() and var() refer to the covariance and variance respectively

Error Reduction

The variance of classifier $\mathbf{y_i(x)}$ is given by:

$$\begin{aligned}\mathrm{var}(y_i(\mathbf{x})) &= \mathbb{E}_x\left[\left\{y_i(\mathbf{x}) - \mathbb{E}_x\left[y_i(\mathbf{x})\right]\right\}^2\right] \\ &= \mathbb{E}_x\left[\left\{y_i(\mathbf{x}) - h(\mathbf{x})\right\}^2\right] \\ &= \mathbb{E}_x\left[\epsilon_i(\mathbf{x})^2\right]\end{aligned}$$

Error Reduction

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Similarly, we have covariance between two classifiers:

$$\text{cov}(y_i(\mathbf{x}), y_j(\mathbf{x})) = \mathbb{E}_x\left[\epsilon_i(\mathbf{x})\ \epsilon_j(\mathbf{x})\right]$$

Error Reduction

Discard Assumption 2 (no correlation). However we make the simplifying assumption that each classifier is equivariate.

Let pairwise correlation between 2 classifiers be denoted by $\boldsymbol{\rho}$>0. Then rearranging the correlation equation we get:

$$\mathbb{E}_x\left[\epsilon_i(\mathbf{x})\ \epsilon_j(\mathbf{x})\right] = \rho \cdot \mathbb{E}_x\left[\epsilon_i(\mathbf{x})^2\right]$$

Error Reduction

Reducing the sum-of-squares error for the committee predictions:

$$
\begin{aligned}
E_{\mathrm{COM}} &= \mathbb{E}_x\left[\frac{1}{N^2}\cdot\left\{\sum_{i=1}^{N}\epsilon_i(\mathbf{x})^2+\sum_{i\neq j}\epsilon_i(\mathbf{x})\epsilon_j(\mathbf{x})\right\}\right] \\
&= \mathbb{E}_x\left[\frac{1}{N^2}\cdot\left\{\sum_{i=1}^{N}\epsilon_i(\mathbf{x})^2+\rho\cdot\sum_{i\neq j}\epsilon_i(\mathbf{x})^2\right\}\right] \\
&= \frac{1}{N}\cdot\mathbb{E}_x\left[\frac{1}{N}\sum_{i=1}^{N}\epsilon_i(\mathbf{x})^2\right]+\rho\cdot\frac{N-1}{N}\cdot\mathbb{E}_x\left[\frac{1}{N}\sum_{i=1}^{N}\epsilon_i(\mathbf{x})^2\right] \\
&= \frac{1}{N}\cdot E_{\mathrm{avg}}+\frac{N-1}{N}\cdot\rho\cdot E_{\mathrm{avg}} \\
&= \left(\rho+\frac{1-\rho}{N}\right)\cdot E_{\mathrm{avg}}
\end{aligned}
$$

Error Reduction

The sum-of-squares error in committee predictions $\mathbf{E_{COM}}$ based on N unbiased learners with average sum-of-squares error $\mathbf{E_{avg}}$ and a pairwise correlation $\boldsymbol{\rho}$>0 is:

$$E_{\mathrm{COM}} = \rho\, E_{\mathrm{avg}} + (1-\rho)\frac{E_{\mathrm{avg}}}{N}$$

- $\boldsymbol{\rho}$ = 0 : Fully uncorrelated ⇒ $\boldsymbol{\sigma}^2$/N **(Maximum Error Reduction)**
- $\boldsymbol{\rho}$ = 1 : Fully correlated ⇒ $\boldsymbol{\sigma}^2$ **(No Error Reduction)**

As N → ∞, only the first term (due to correlation) remains.

Note that for any $\boldsymbol{\rho}$:

$$E_{\mathrm{COM}} \leq E_{\mathrm{avg}}$$

Parallel Ensembles: Bagging

Modification of committee methods that uses copies of the same learner each trained on multiple bootstrapped datasets to introduce variability.

The name of this method comes from its steps: **B**ootstrap **Agg**regat**ing**

Bootstrapping + Aggregating = Bagging

- **Bootstrapping:** refers to bootstrap sampling ie. **sampling with replacement**
- **Aggregating:** refers to the aggregation of individual learner predictions into a composite prediction

Bagging

- **Bootstrapping**
  - Create a new set of N datasets: $\mathbb{D}_1$, $\mathbb{D}_2$, … $\mathbb{D}_N$ each of size n’ = n,
  - sampled randomly with replacement from the original dataset
  - Why replacement ? - Allows $\mathbb{D}_1$, … $\mathbb{D}_N$ to be independent of previous sampling

Bagging

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- **Training:** Each model C_i is trained independently on bootstrapped datasets $\mathbb{D}_i$
- **Aggregation**
  - Classify a data point: it is independently classified by every C_i to give a prediction
  - C* then aggregates these predictions into a single prediction
  - Aggregating predictions: Majority voting, averaging class probabilities etc.

Bagging

- For noisy data → significantly more robust
- More **stable classification**
- **Caveat:** Bagging poor classifiers (high bias) could cause performance to become arbitrarily worse!
- Works especially well for:
  - High capacity (low bias) learners with a tendency to overfit (high variance)
  - Unstable learners which are very data-dependent
- **Examples: ?**

Bagging

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  - Unstable learners which are very data-dependent
- **Examples:** DECISION TREES

Why Decision trees?

- Are high capacity learners
- Have a tendency to overfit on data
- Are difficult to regularize
- Are highly unstable learners

Bagged decision trees are themselves very useful. However, they can be improved further!

How?

Random Forests

- We have established that decision trees are naturally very good learners for use in bagging
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Random Forests

- We have established that decision trees are naturally very good learners for use in bagging
- Bagging reduces variance ⇒ When is this most effective?
- **When learners are not very correlated!**
- Highly correlated learners will often learn similar things and give similar predictions - bagged classifier will often also have similar predictions

Random Forests

We need to bag decision trees and attempt to reduce correlation at the same time!

Recall that we use p-dimensional data. For every data point, there are p features.

How can we reduce correlation between classifiers?

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We need to bag decision trees and attempt to reduce correlation at the same time!

Recall that we use *p*-dimensional data. For every data point, there are *p* features.

How can we reduce correlation between classifiers?

- At every step of growing the decision tree do the following:
  - Randomly pick only *t* out of the *p* features available
  - Pick the feature out of these *t* which offers the best split
  - Use it to grow the tree.
  - Repeat again with a new randomly picked set of *t* features
  - Break when further refinement is not possible

- Typical values of *t* could be: $p/2$, $\sqrt{p}$ etc.

Random Forests

The two important parameters of the RF algorithm are:

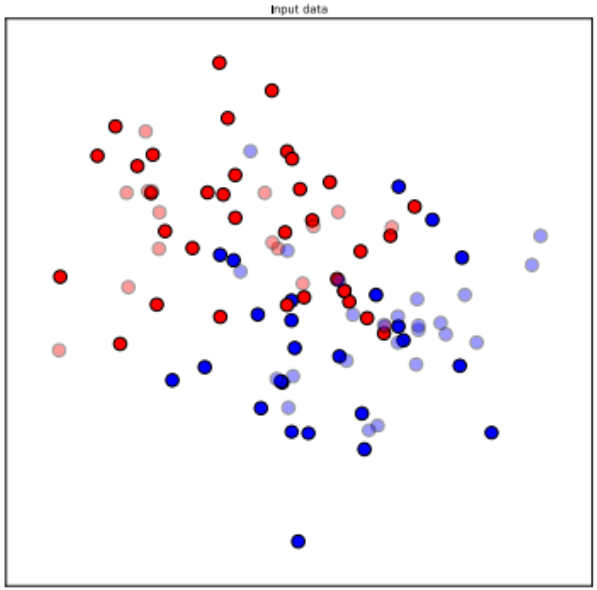
- **Number of trees (n_est)**

  RF builds a number of decision trees and fits them onto the different sampled datasets. As the number of learners used increases, the variance tends to decrease until it saturates.

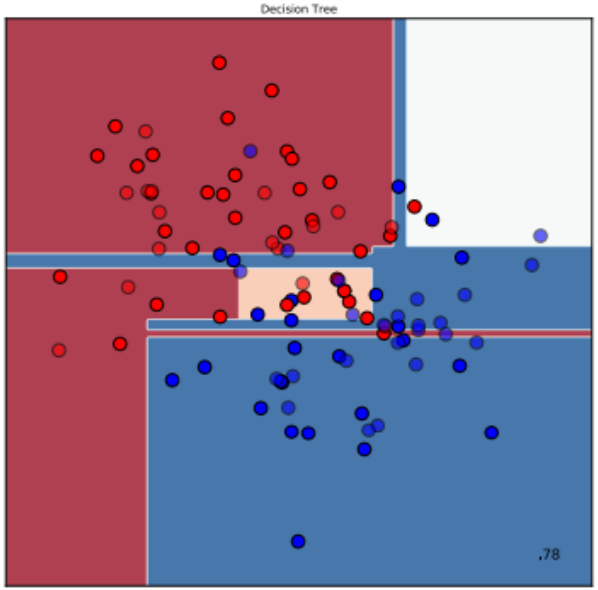
- **Maximum features at a node (t)**

  As discussed in previous slide, the reduction in number of features used for splitting the decision tree at every node leads to uncorrelated trees. Very large values of t ($t \rightarrow p$) tends to give very similar (correlated) trees.

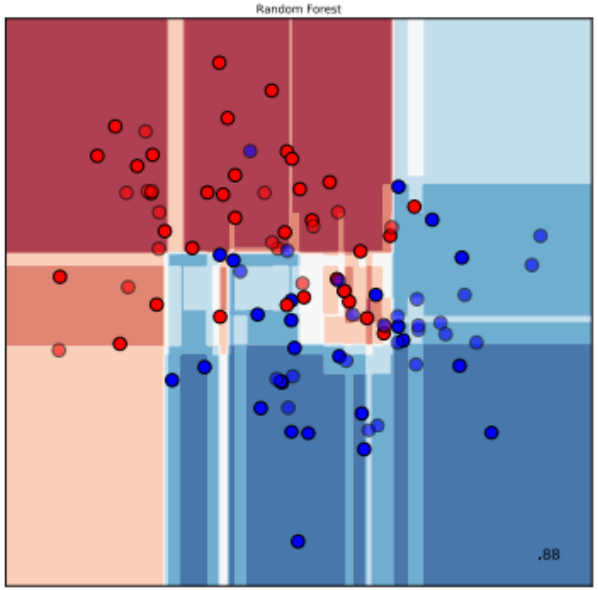
Random Forests



Decision tree



Random forest



Accuracy: **78%** **88%**

Random Forests

- RF can give competitive results with gradient boosted trees
- Number of high performance libraries made it a very popular algorithm!
- In recent years however, there is an advent of high performance gradient boosting algorithms: XGBOOST, LightGBM etc.
- Try a combination of these to see which works best for your application!

Summary

- Ensemble methods - Types - Why are they used
- Committee Methods
  - Error reduction by averaging predictions
  - Effect of correlation between learners on error reduction
- Bagging (Bootstrap Aggregating)
  - Bootstrapping to generate multiple slightly different datasets from same data
  - Aggregating classifiers trained on different to give a single prediction
  - Useful for low bias, high variance unstable learners - Decision Trees
- Random Forests
  - Bagged Decision trees with random feature selection at nodes!
  - Random Forests algorithm - building a forest of trees with less correlation