Lecture 6 – Tree-based methods, Bagging and Random Forests

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Summary of Lecture 5 (I/IV)

When **choosing models/methods**, we are interested in how well they will perform when **faced with new unseen data**.

The new data error

$$E_{\text{new}} \triangleq \mathbb{E}_\star \left[E(\widehat{y}(\mathbf{x}_\star; \mathcal{T}), y_\star) \right]$$

describes how well a method (which is trained using data set $\mathcal{T}$) will perform "in production".

E is for instance mean squared error (regression) or misclassification (classification).

The overall goal in supervised machine learning is to achieve small E_{new}.

$E_{\text{train}} \triangleq \frac{1}{n} \sum_{i=1}^{n} E(\widehat{y}(\mathbf{x}_i; \mathcal{T}), y_i)$ is the training data error.
Not a good estimate of E_{new}.

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Summary of Lecture 5 (II/IV)

Two methods for estimating E_{new}:

1. **Test data approach:** Randomly split the data into a **training set** and a **test set**. Learn the model using the training set. Estimate E_{new} using the test set.
2. **c-fold cross-validation:** Randomly split the data into c parts (or **folds**) of roughly equal size.
   a) The first fold is kept aside as a validation set and the model is learned using only the remaining $c-1$ folds. E_{new} is estimated on the validation set.
   b) The procedure is repeated c times, each time a different fold is treated as the validation set.
   c) The average of all c estimates is taken as the final estimate of E_{new}.

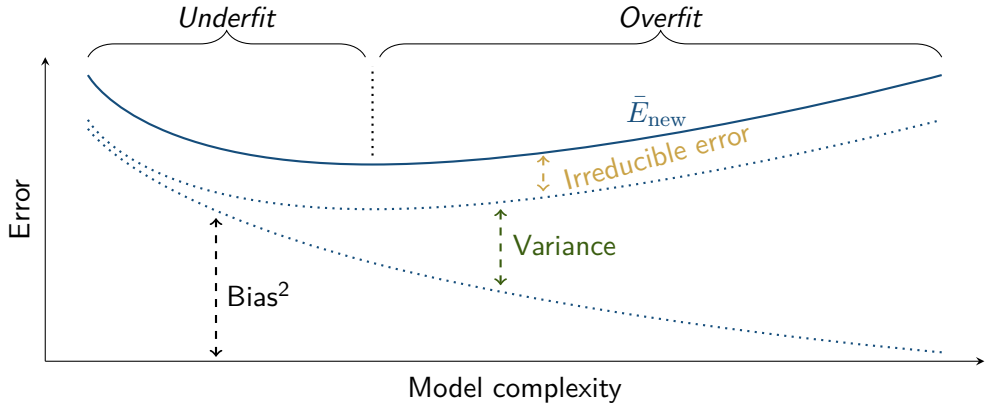
Summary of Lecture 5 (III/IV)

$$\bar{E}_{\text{new}} = \underbrace{\mathbb{E}_\star\left[(g(\mathbf{x}_\star) - f(\mathbf{x}_\star))^2\right]}_{\text{Bias}^2} + \underbrace{\mathbb{E}_\star\left[\mathbb{E}_\mathcal{T}\left[(\widehat{y}(\mathbf{x}_\star;\mathcal{T}))^2\right] - (g(\mathbf{x}_\star))^2\right]}_{\text{Variance}} + \underbrace{\sigma^2}_{\substack{\text{Irreducible} \\ \text{error}}}$$

- **Bias**: The inability of a method to describe the complicated patterns we would like it to describe.
- **Variance**: How sensitive a method is to the training data.

The more prone a model is to adapt to complicated pattern in the data, the higher the **model complexity** (or model flexibility).

Summary of Lecture 5 (IV/IV)



Finding a balanced fit (neither over- nor underfit) is called the **the bias-variance tradeoff**.

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Contents – Lecture 6

1. Classification and regression trees (CART)
2. Bagging – *a general variance reduction technique*
3. Random forests

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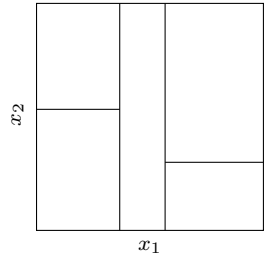
The idea behind tree-based methods

In both regression and classification settings we seek a function $\widehat{y}(\mathbf{x})$ which maps the input $\mathbf{x}$ into a prediction.

One **flexible** way of designing this function is to partition the input space into disjoint regions and fit a simple model in each region.



- **Classification:** Majority vote within the region.
- **Regression:** Mean of training data within the region.

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Finding the partition

The key challenge in using this strategy is to find a good partition.

Even if we restrict our attention to seemingly simple regions (e.g. "boxes"), finding an ***optimal*** partition w.r.t. minimizing the training error is ***computationally infeasible!***

Instead, we use a "greedy" approach: **recursive binary splitting**.

1. Select one of the inputs x_j and a cut-point s. Partition the input space into two half-spaces,

$$\{\mathbf{x} : x_j < s\} \qquad\qquad \{\mathbf{x} : x_j \geq s\}.$$

2. Repeat this splitting for each region until some stopping criterion is met (e.g., no region contains more than 5 training data points).

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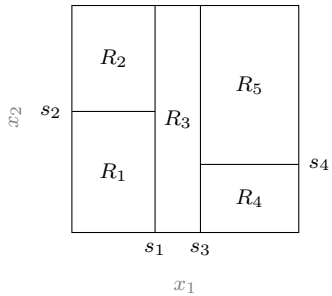
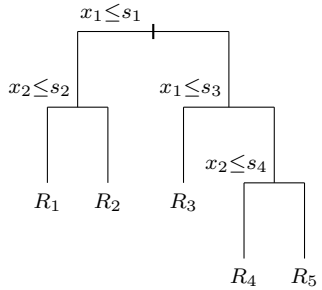
Recursive binary splitting

Partitioning of input space



Tree representation



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Classification trees

Classification trees are constructed similarly to regression trees, but with *two differences*.

Firstly, the class prediction for each region is based on the proportion of data points from each class in that region. Let

$$\widehat{\pi}_{mk} = \frac{1}{n_m} \sum_{i:\mathbf{x}_i \in R_m} \mathbb{I}\{y_i = k\}$$

be the proportion of training observations in the mth region that belong to the kth class. Then we approximate

$$p(y = k \,|\, \mathbf{x}) \approx \sum_{m=1}^{M} \widehat{\pi}_{mk} \mathbb{I}\{\mathbf{x} \in R_m\}$$

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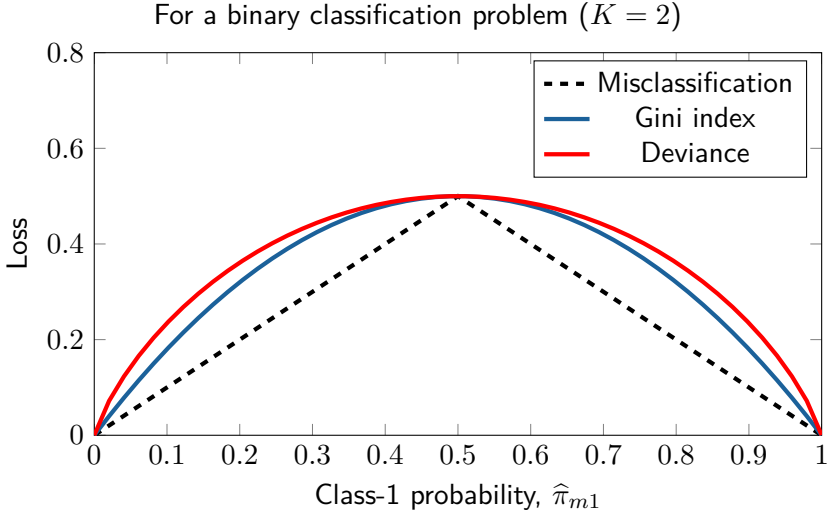
Classification trees

Secondly, the squared loss used to construct the tree needs to be replaced by a measure suitable to qualitative outputs.

Three common error measures are,

$$\begin{aligned} \text{Misclassification error:} \quad & 1 - \max_k \widehat{\pi}_{mk} \\ \text{Entropy/deviance:} \quad & -\sum_{k=1}^{K} \widehat{\pi}_{mk} \log \widehat{\pi}_{mk} \\ \text{Gini index:} \quad & \sum_{k=1}^{K} \widehat{\pi}_{mk}(1 - \widehat{\pi}_{mk}) \end{aligned}$$

Classification error measures



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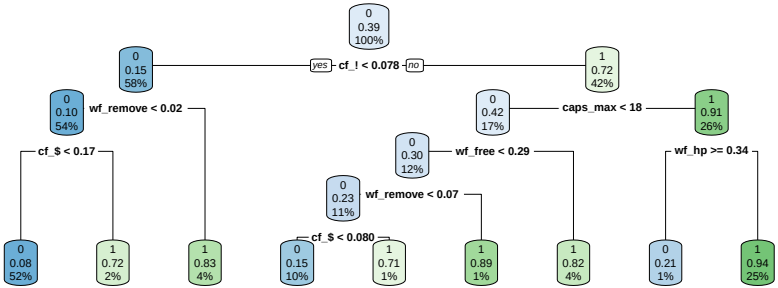
ex) Spam data

Classification tree for spam data:



	Tree	**LDA**
Test error:	11.3 %	10.9 %

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Improving CART

The flexibility/complexity of classification and regression trees (CART) is decided by the tree depth.

- ***!*** To obtain a **small bias** the tree need to be grown deep,
- ***!*** but this results in a **high variance!**

The performance of (simple) CARTs is often unsatisfactory!

To improve the practical performance:

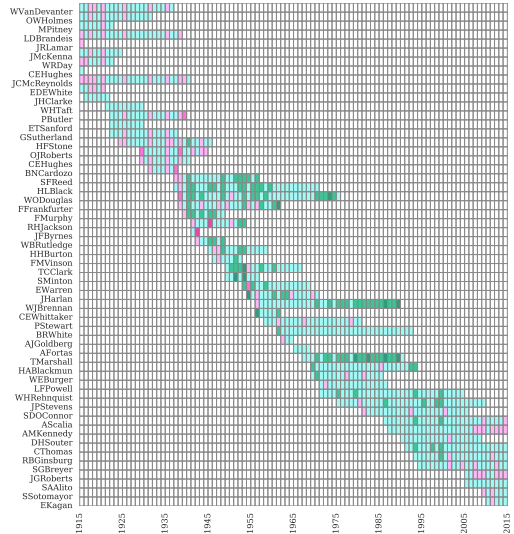
- **Pruning** – grow a deep tree (small bias) which is then pruned into a smaller one (reduce variance).
- **Ensemble methods** – average or combine multiple trees.
  - Bagging and Random Forests (this lecture)
  - Boosted trees (next lecture)

ex) Predicting US Supreme Court behavior

Random forest classifier built on SCDB data[1] to predict the votes of Supreme Court justices:

$$Y \in \{\texttt{affirm}, \texttt{reverse}, \texttt{other}\}$$

Result: 70% correct classifications



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ex) Predicting US Supreme Court behavior

> *Not only have random forests proven to be "unreasonably effective" in a wide array of supervised learning contexts, but in our testing, random forests outperformed other common approaches including support vector machines [. . .] and feedforward artificial neural network models such as multi-layer perceptron*
>
> — Katz, Bommarito II and Blackman (arXiv:1612.03473v2)

Random forests

Bagging can drastically improve the performance of CART!

However, the B bootstrapped dataset are ***correlated***
$\Rightarrow$ the variance reduction due to averaging is diminished.

Idea: De-correlate the B trees by randomly perturbing each tree.

A **random forest** is constructed by bagging, but for each split in each tree only a ***random subset*** of $q \leq p$ inputs are considered as splitting variables.

Rule of thumb: $q = \sqrt{p}$ for classification trees and $q = p/3$ for regression trees.[2]

[2] Proposed by Leo Breiman, inventor of random forests.

Random forest pseudo-code

Algorithm Random forest for regression

1. For $b = 1$ to B *(can run in parallel)*
   (a) Draw a bootstrap data set $\widetilde{\mathcal{T}}$ of size n from $\mathcal{T}$.
   (b) Grow a regression tree by repeating the following steps until a minimum node size is reached:
      i. Select q out of the p input variables uniformly at random.
      ii. Find the variable x_j among the q selected, and the corresponding split point s, that minimizes the squared error.
      iii. Split the node into two children with $\{x_j \leq s\}$ and $\{x_j > s\}$.
2. Final model is the average the B ensemble members,

$$\widehat{y}_\star^{\text{rf}} = \frac{1}{B} \sum_{b=1}^{B} \widetilde{y}_\star^b.$$

Random forests

Recall: For i.d. random variables $\{Z_i\}_{i=1}^n$

$$\text{Var}\left(\frac{1}{n}\sum_{i=1}^{n} Z_i\right) = \frac{1-\rho}{n}\sigma^2 + \rho\sigma^2$$

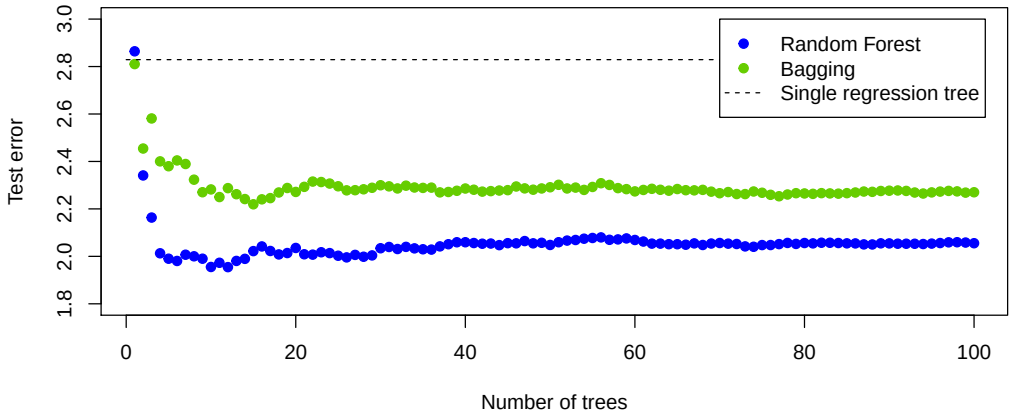
The random input selection used in random forests:

- ▼ increases the bias, but often very slowly
- ▼ adds to the variance (σ^2) of each tree
- ▲ reduces the correlation (ρ) of the trees

The reduction in correlation is typically the dominant effect $\Rightarrow$ there is an overall reduction in MSE!

ex) Toy regression model

For the toy model previously considered...



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Overfitting?

The complexity of a bagging/random forest model increases with an increasing number of trees B.

Will this lead to overfitting as B increases?

No – more ensemble members ***does not*** increase the ***flexibility*** of the model!

Regression case:

$$\widehat{y}_\star^{\mathsf{rf}} = \frac{1}{B}\sum_{b=1}^{B} \widehat{y}_\star^b \to \mathbb{E}\left[\widetilde{y}_\star \,|\, \mathcal{T}\right], \qquad \text{as } B \to \infty,$$

where the expectation is w.r.t. the randomness in the data bootstrapping and input selection.

Advantages of random forests

Random forests have several **computational advantages**:

- Embarrassingly parallelizable!
- Using $q < p$ potential split variables reduces the computational cost of each split.
- We ***could*** bootstrap fewer than n, say $\sqrt{n}$, data points when creating $\widetilde{\mathcal{T}}^b$ — very useful for "big data" problems.

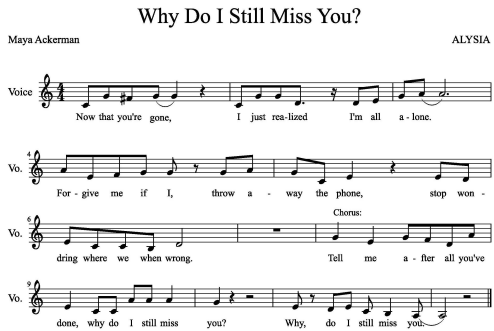
. . . and they also come with some other benefits:

- Often works well off-the-shelf – few tuning parameters
- Requires little or no input preparation
- Implicit input selection

ex) Automatic music generation

ALYSIA: automated music generati on using random forests.

- User specifies the lyrics
- ALYSIA generates accompanying music via
  - *rythm model*
  - *melody model*
- Trained on a corpus of pop songs.



http://www.cs.sjsu.edu/~ackerman/ALYSIA_songs.html

M. Ackerman and D. Loker. **Algorithmic Songwriting with ALYSIA**. *In: Correia J., Ciesielski V., Liapis A. (eds) Computational Intelligence in Music, Sound, Art and Design. EvoMUSART*, 2017.

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A few concepts to summarize lecture 6

CART: Classification and regression trees. A class of nonparametric methods based on partitioning the input space into regions and fitting a simple model for each region.

Recursive binary splitting: A greedy method for partitioning the input space into "boxes" aligned with the coordinate axes.

Gini index and deviance: Commonly used error measures for constructing classification trees.

Ensemble methods: Umbrella term for methods that average or combine multiple models.

Bagging: Bootstrap aggregating. An ensemble method based on the statistical bootstrap.

Random forests: Bagging of trees, combined with random feature selection for further variance reduction (and computational gains).