MATH60026/MATH70026
Methods for Data Science
Lecture 3

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Department of Mathematics, Academic year 2024-2025

IMPERIAL

Naive Bayes

One of the simplest multi-class classifier. It essentially relies upon:

Bayes' theorem + *naive* assumption

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Setup:

$$\mathbf{x}^{(i)} = (x_1^{(i)}, \ldots, x_p^{(i)}) \qquad i = 1, \ldots, N$$

$$y^{(i)} \in \mathcal{C}_q = \{c_1, \ldots, c_Q\}$$

Bayes' theorem:

$$P(Y = c_q \mid X = \mathbf{x}) = \frac{\overbrace{P(X = \mathbf{x} \mid Y = c_q)}^{\spadesuit}\overbrace{P(Y = c_q)}^{\clubsuit}}{\underbrace{P(X = \mathbf{x})}_{\bigstar}}, \quad q = 1, \ldots, Q$$

Likelihood ♠ Prior ♣ Evidence (normalisation) ★

Key quantity: probability of belonging to a class conditional on the predictors (posterior)

Naive Bayes

Let's look each term:

'Prior' (♣): reflects a priori knowledge on the class distribution.
A simple, agnostic choice is a prior based on class frequency:

Indicator function

$$P(Y = c_q) = \frac{\sum_{i=1}^{N} I(y^{(i)} = c_q)}{N}$$

Fraction of training data in each class

Naive Bayes

$\mathbf{`Likelihood'}$ $(\spadesuit)$: this is where the naive assumption enters.

Naive assumption = class-conditional independence of data features

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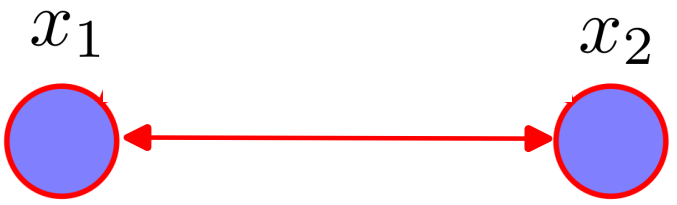

Two data features correlated

Naive Bayes

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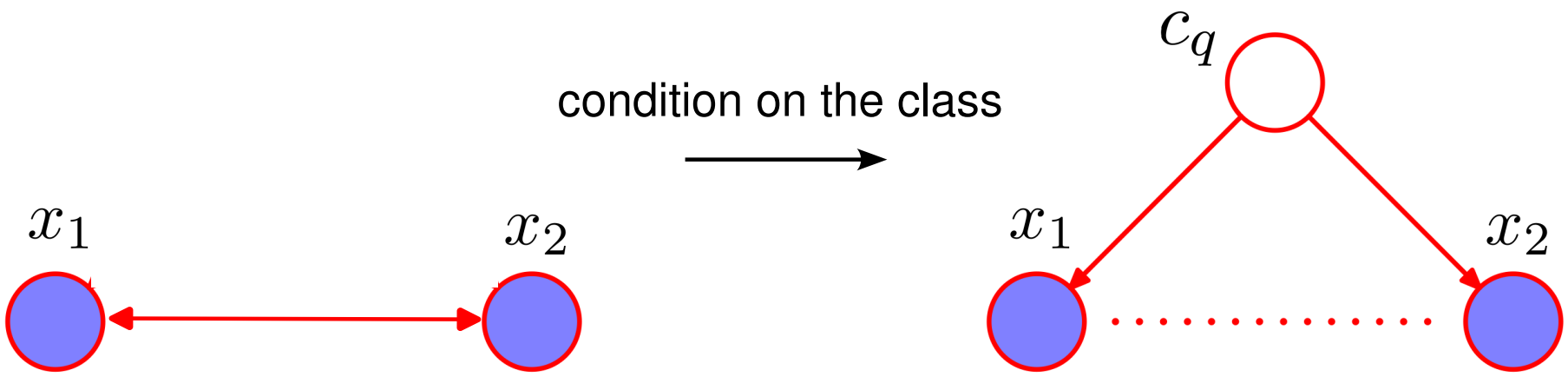

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Assume they are independent when conditioned on the class

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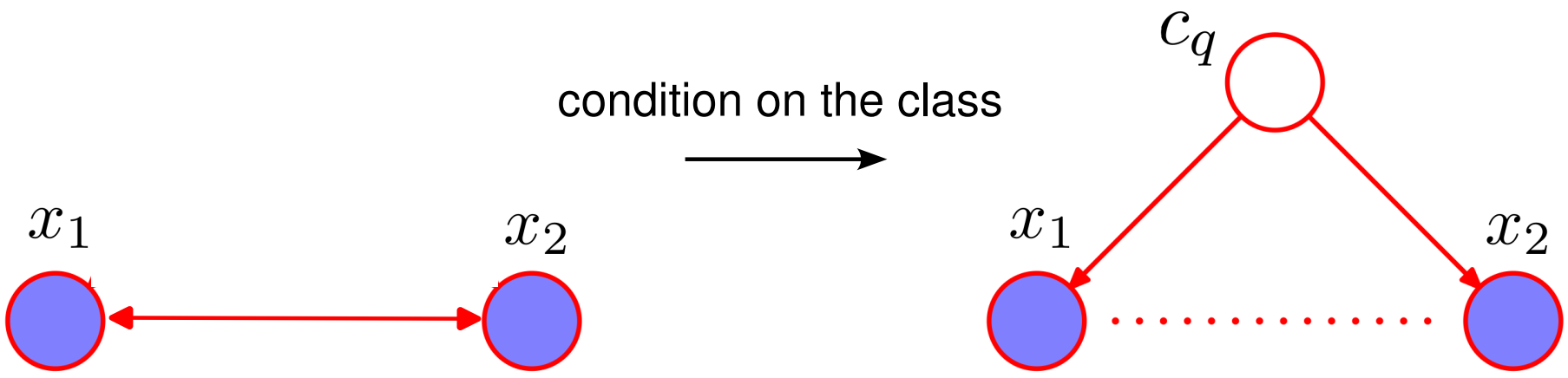

Two data features correlated

Assume they are independent when conditioned on the class

Naive assumption:
class-conditional feature probabilities factorise

$$P(X = \mathbf{x} \mid Y = c_q) = P(X_1 = x_1, X_2 = x_2, \ldots, X_p = x_p \mid Y = c_q)$$
$$= \prod_{j=1}^{p} P(X_j = x_j \mid Y = c_q)$$

Naive Bayes

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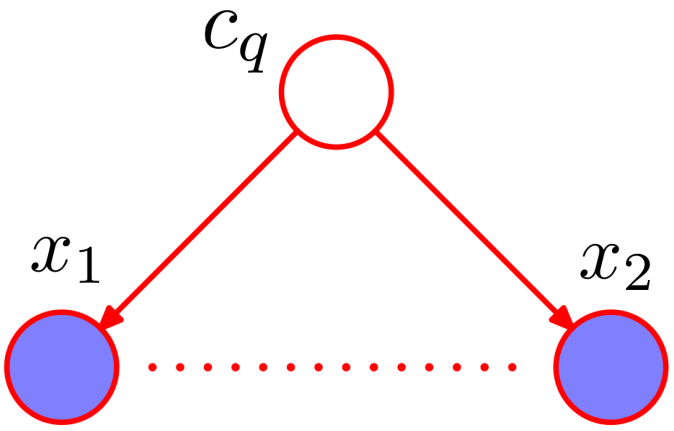
Naive assumption = class-conditional independence of data features

Advantages:

1. **Scalability**: estimation for each descriptor computed *separately* (fitting correlations is expensive and requires many data points).

2. Simple to deal with **mixed-type** data (continuous and discrete features).



Assume they are independent when conditioned on the class

Just an approximation!

Naive Bayes

'Likelihood' (♠): this is where the naive assumption enters.

What distributions? Standard options:

Discrete predictors: Count-based estimate

Boolean 'and'

$$P(X_j = x_j \mid Y = c_q) \approx \frac{\sum_{i=1}^{N} I(x_j^{(i)} = x_j \wedge y^{(i)} = c_q)}{\sum_{i=1}^{N} I(y^{(i)} = c_q)}, \quad j = 1, \ldots, p$$

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Problem of empty entries:
Laplace smoothing, see notebook

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Continuous predictors: Gaussian distribution

$$P(X_j = x_j \mid Y = c_q) \approx \frac{1}{\sqrt{2\pi\sigma_{j,q}^2}} e^{\frac{-(x_j - \mu_{j,q})^2}{2\sigma_{j,q}^2}}$$

$$\mu_{j,q} = \frac{1}{N_q} \sum_{y^{(i)} \in c_q} x_j^{(i)}$$

$$\sigma_{j,q}^2 = \frac{1}{N_q} \sum_{y^{(i)} \in c_q} (x_j^{(i)} - \mu_{j,q})^2$$

Sample estimator of mean
and variance in each class

Naive Bayes

Normalisation factor ($\bigstar$): sum of previous terms over classes.

$$P(X = \mathbf{x}) = \sum_{q=1}^{Q} P(X = \mathbf{x} \mid Y = c_q) P(Y = c_q)$$

$$= \sum_{q=1}^{Q} [\clubsuit \cdot \spadesuit]_q$$

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Final Naive Bayes classifier prediction:

$$P(Y = c_q \mid X = \mathbf{x}) = \frac{P(Y = c_q) \prod_{j=1}^{p} P(X_j = x_j \mid Y = c_q)}{\sum_{q=1}^{Q} [\clubsuit \cdot \spadesuit]_q} = \frac{[\clubsuit \cdot \spadesuit]_q}{\sum_{q=1}^{Q} [\clubsuit \cdot \spadesuit]_q}$$

Naive Bayes

The prediction is a vector of probabilistic class assignments (soft classification):

$$\boldsymbol{\pi}^{(\mathrm{NB})} = \begin{bmatrix} \pi_1^{(\mathrm{NB})} \\ \vdots \\ \pi_Q^{(\mathrm{NB})} \end{bmatrix}, \text{ where each component is:}$$

$$\pi_q^{(\mathrm{NB})} = P(Y = c_q \mid X = \mathbf{x}^{\mathrm{in}}) = \frac{[\clubsuit \cdot \spadesuit]_q}{\sum_{q=1}^{Q} [\clubsuit \cdot \spadesuit]_q}$$

New sample to classify

Normalised by construction:

$$\sum_{q=1}^{Q} \pi_q^{(\mathrm{NB})} = 1$$

Naive Bayes

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As usual, the hard classification version is obtained by:

$$\hat{y}^{(\mathrm{NB})} = \underset{q}{\operatorname{argmax}}\, \boldsymbol{\pi}^{(\mathrm{NB})}$$

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4. The naive assumption leads to a drastic simplification of model construction, making it scalable and amenable to mixed-type data.

5. Standard choices for the factorised likelihood term (the count-based estimate for discrete, the gaussian distribution for continuous) help spare model calibration efforts (no learning by loss minimisation, no hyper-parameters to set).

Decision Trees

Building blocks of Random Forests, a powerful method used for classification and regression.

Let's start with classification: $\mathbf{x} = (x_1, ..., x_p) \rightarrow y \;\; y \in \mathcal{C}_q = \{c_1, \ldots, c_Q\}$

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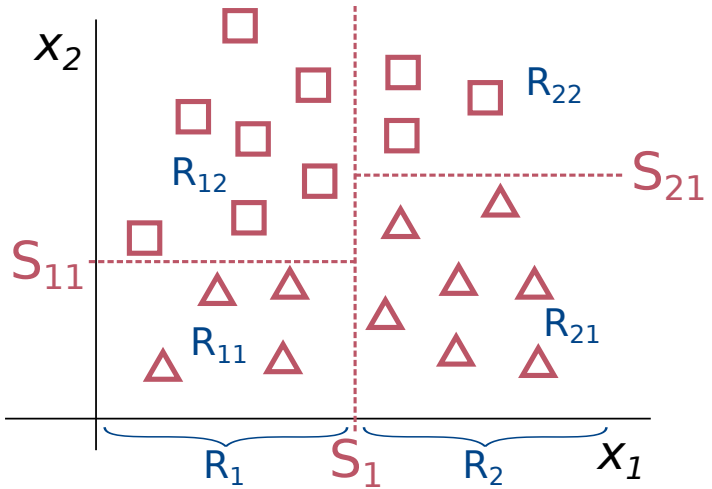

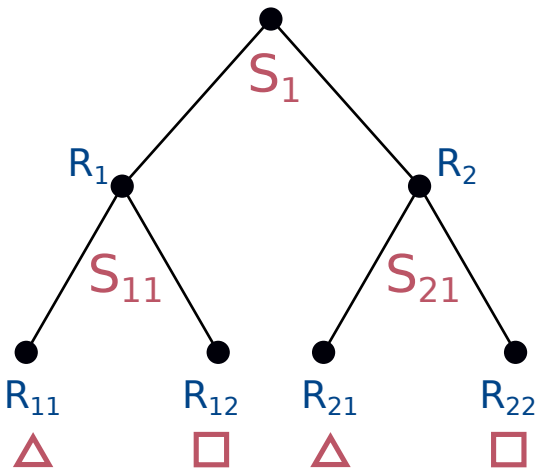

Tree = set of splits

$$\text{split } (j,s) = \left\{ \begin{array}{l} \{x_j : x_j < s\} =: R_1(j,s) \} \\ \{x_j : x_j \geq s\} =: R_2(j,s) \} \end{array} \right\}$$

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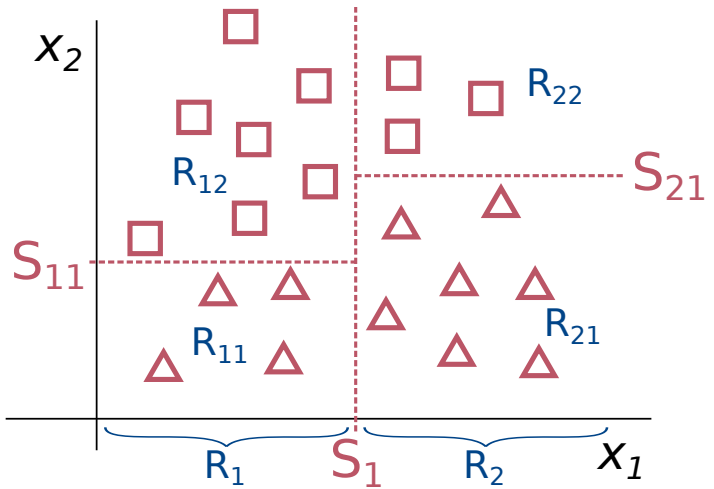

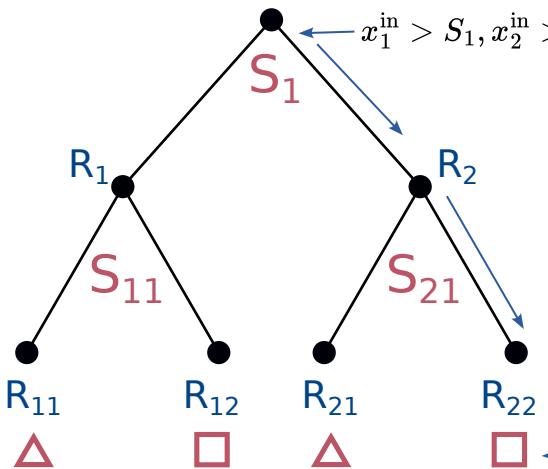

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Prediction = majority class in the region

Example: spam data

- Classifier of ‘spam’/’e-mail’ messages
- 57 continuous predictors (words, special characters, sequences of capital letters)
- Training set (3065) and Test set (1536)

Class	Features				
	CAPTOT	ch$	remove	business	
email	0.11	0.053	0.21	0.003	...
spam	0.10	0.015	0.25	0.081	...
email	0.21	0.012	0.32	0.001	...
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Example discussed in Hastie, Tibshirani, Friedman, Elements of statistical learning, chap. 9, 15

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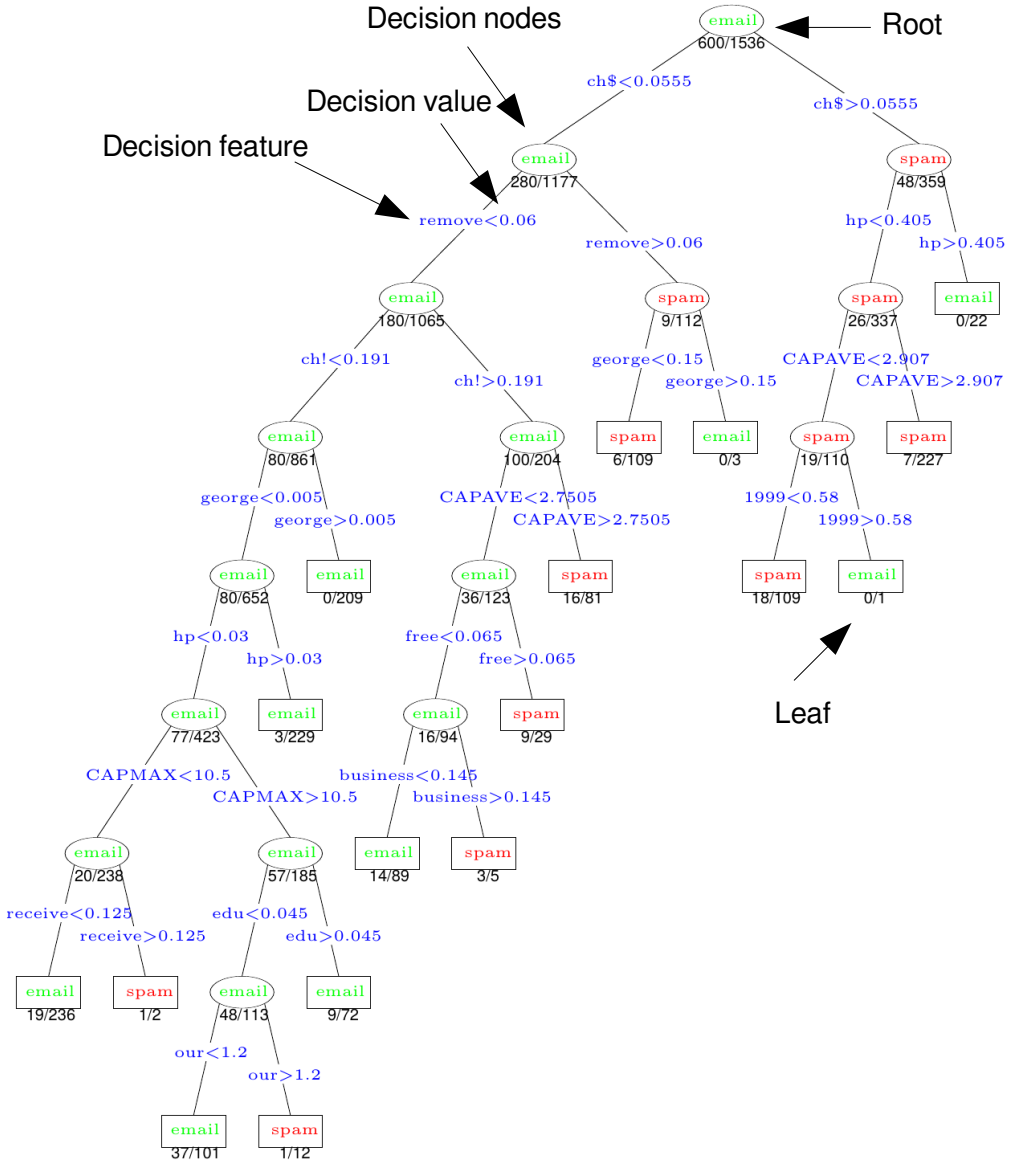

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Decision Trees

Algorithm: it proceeds *greedily*, i.e., it computes the optimal split one level at a time.

To obtain optimal splits, we a need **loss/cost function**: here taken from **information theory**.

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Node impurity: proportion of data in each class:

$$\pi_q(R_{\boldsymbol{\alpha}}) = \frac{\sum_{i=1}^{N} I\left(\mathbf{x}^{(i)} \in R_{\boldsymbol{\alpha}} \wedge y^{(i)} \in c_q\right)}{\sum_{i=1}^{N} I(\mathbf{x}^{(i)} \in R_{\boldsymbol{\alpha}})}$$

Number of data in the region belonging to *q*

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Gini index

$$\mathrm{GI}\left[\boldsymbol{\pi}(R_{\boldsymbol{\alpha}})\right] = \sum_{q=1}^{Q} \pi_q(R_{\boldsymbol{\alpha}})\left(1 - \pi_q(R_{\boldsymbol{\alpha}})\right)$$

Cross-entropy

$$\mathrm{CE}\left[\boldsymbol{\pi}(R_{\boldsymbol{\alpha}})\right] = -\sum_{q=1}^{Q} \pi_q(R_{\boldsymbol{\alpha}}) \log \pi_q(R_{\boldsymbol{\alpha}})$$ *

They both measure the **deviation wrt to a homogeneous distribution** into classes, i.e. , they measure the **information** about classes carried by $\boldsymbol{\pi}(R_{\boldsymbol{\alpha}})$ at a given split

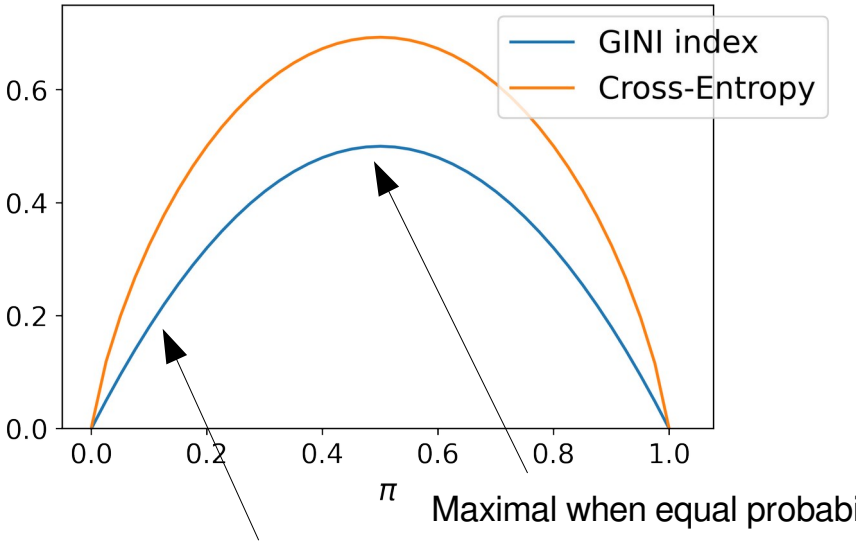
*We call it 'Cross-Entropy' because it can be derived as the cross-entropy between data and model-predicted distribution, see the Lecture Notes!

Decision Trees

Simple example: 1 splitting, 2 classes

$$\mathrm{GI}[\pi] = 2\pi(1-\pi)$$

$$\mathrm{CE}[\pi] = -\pi\log\pi - (1-\pi)\log(1-\pi)$$



Maximal when equal probability

Decreases probabilities are dissimilar

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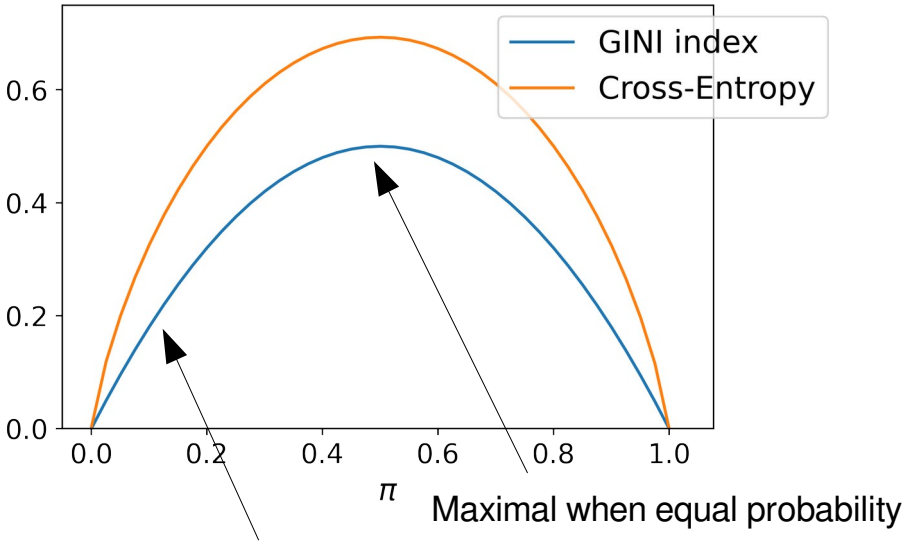

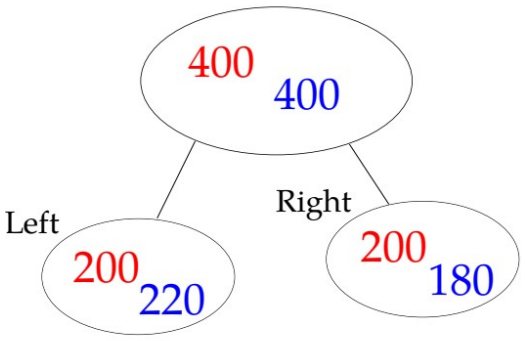

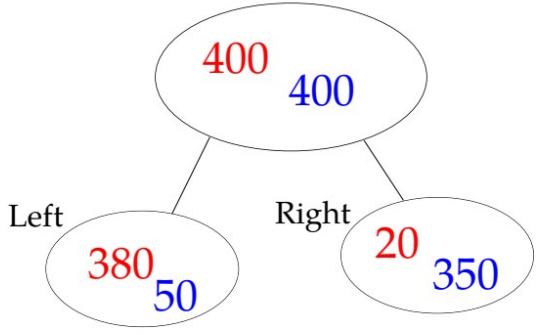

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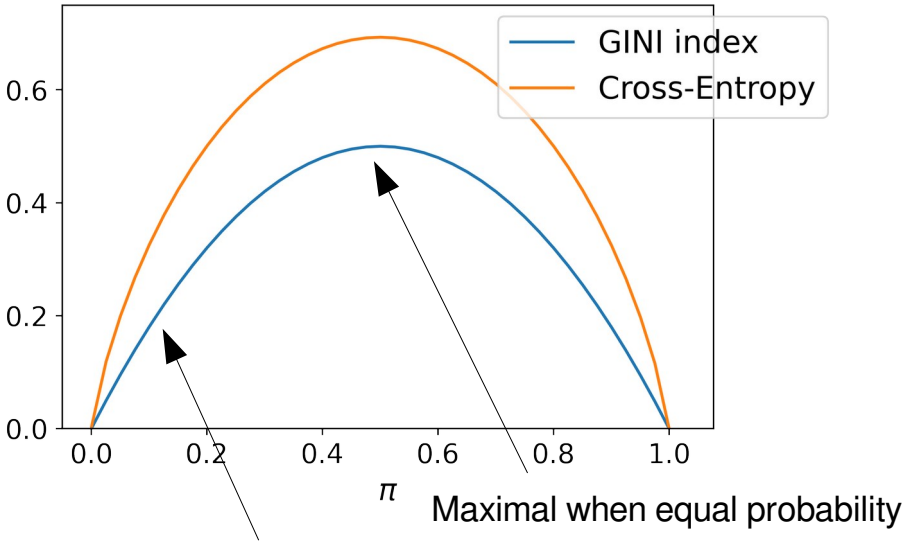
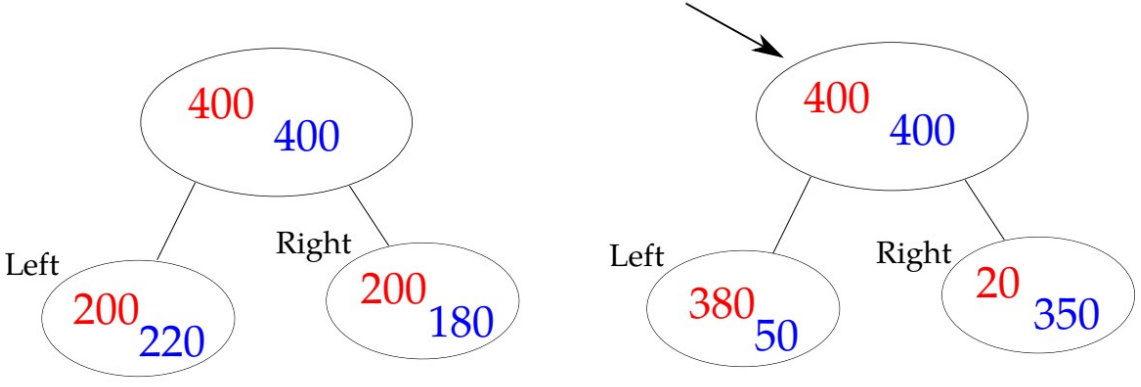


This split provides more 'information' about the data separation into classes



$GI = 0.525\, GI^L + 0.475\, G^R = 0.5$

$GI = 0.5375\, GI^L + 0.4625\, G^R = 0.16$

The splitting that minimizes the Gini index or the cross-entropy leads to regions dominated by 1 class

Decision Trees

GI and CE are therefore functions to minimise to achieve a classification task.

*

Decision Trees

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Recall that a tree = set of splits

$$\text{split } (j,s) = \left\{ \begin{array}{l} \{x_j : x_j < s\} =: R_1(j,s)\} \\ \{x_j : x_j \geq s\} =: R_2(j,s)\} \end{array} \right\}$$

A given split is chosen by:

$$\min_{j,s} \left[\mathbb{p}_{R_1} \mathrm{GI}\big(\boldsymbol{\pi}(R_1), j, s\big) + \mathbb{p}_{R_2} \mathrm{GI}\big(\boldsymbol{\pi}(R_2), j, s\big) \right]^*$$

Fraction of samples ending up in that region

To repeat until a stopping criterion is met.

Example: spam data

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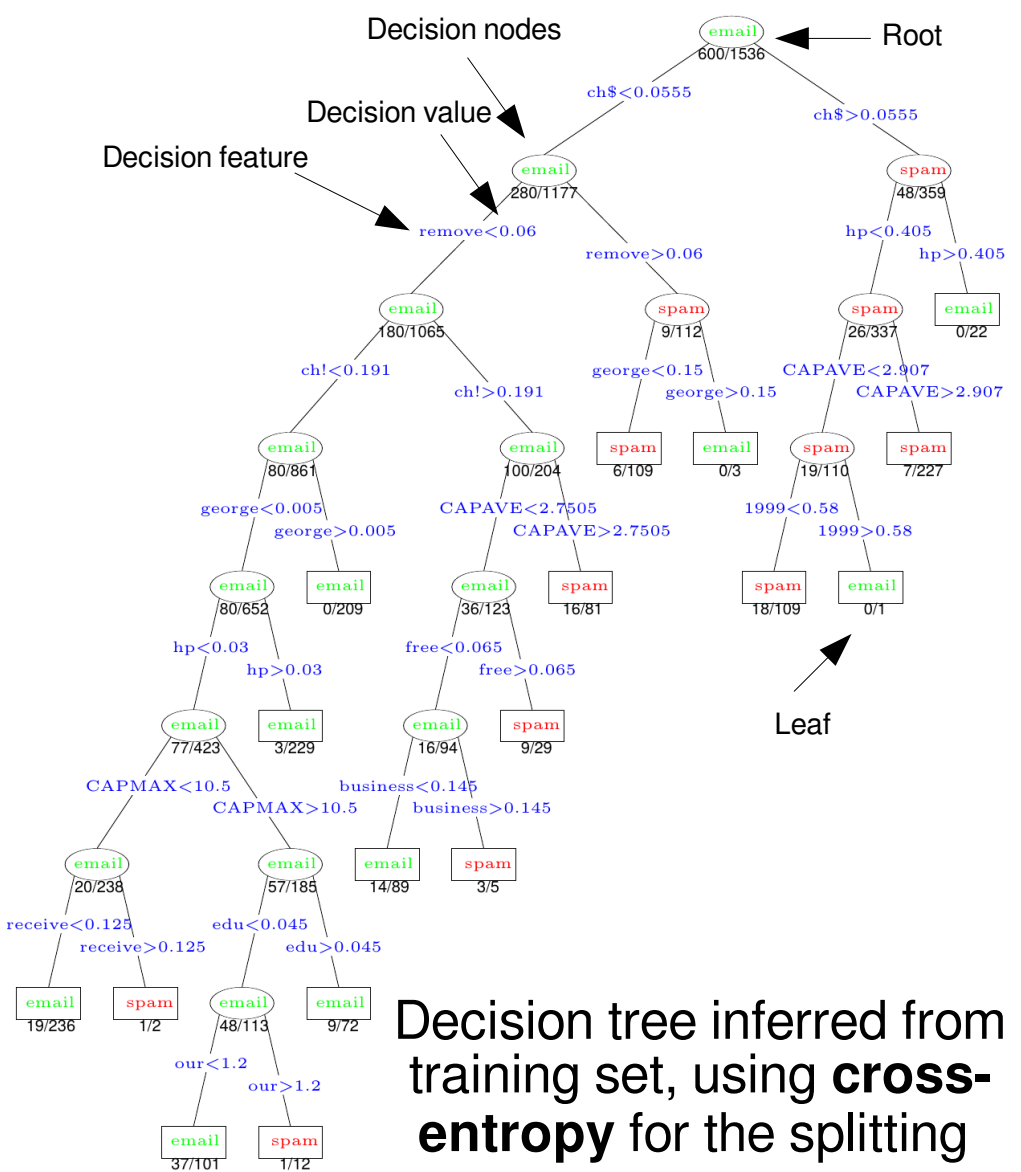

Decision tree inferred from training set, using **cross-entropy** for the splitting

Which stopping criterion to use?

How much should we grow the tree?

1. **Setting constraints on tree size**: minimum node size, minimum number of samples for a leaf, maximum number of leaves, maximum depth.

Example: spam data

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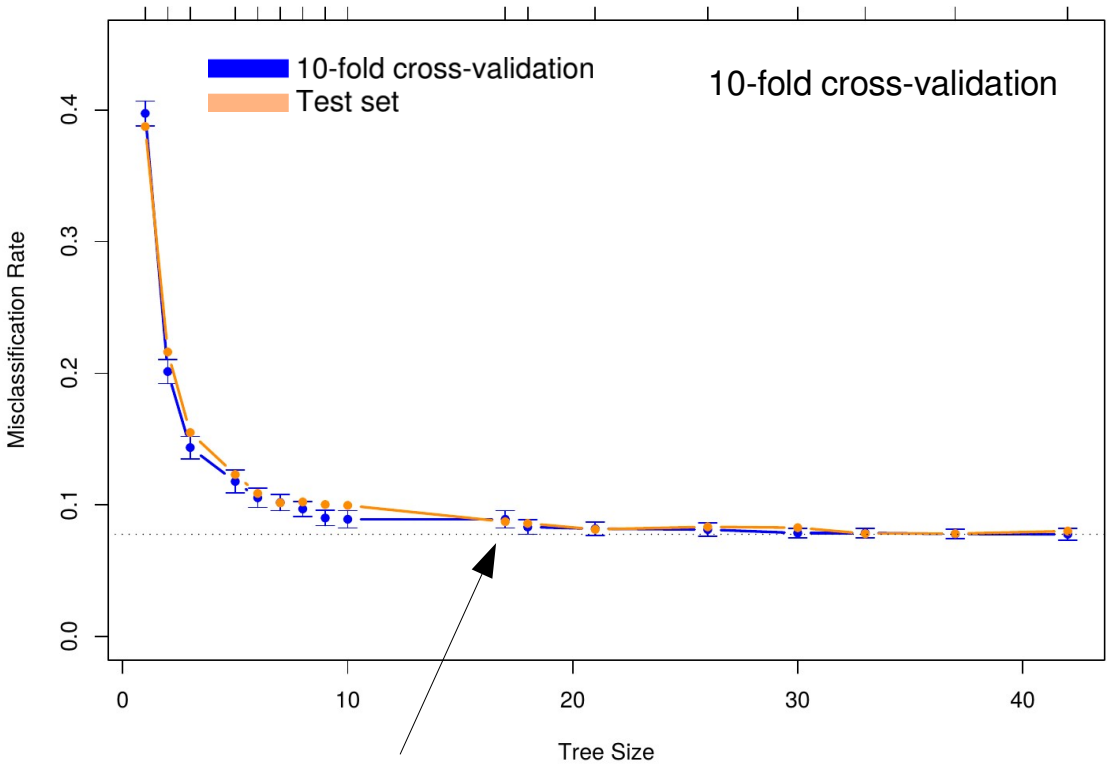
They stop when there is a plateau in performance on the validation set.



17-nodes tree chosen by cross-validation

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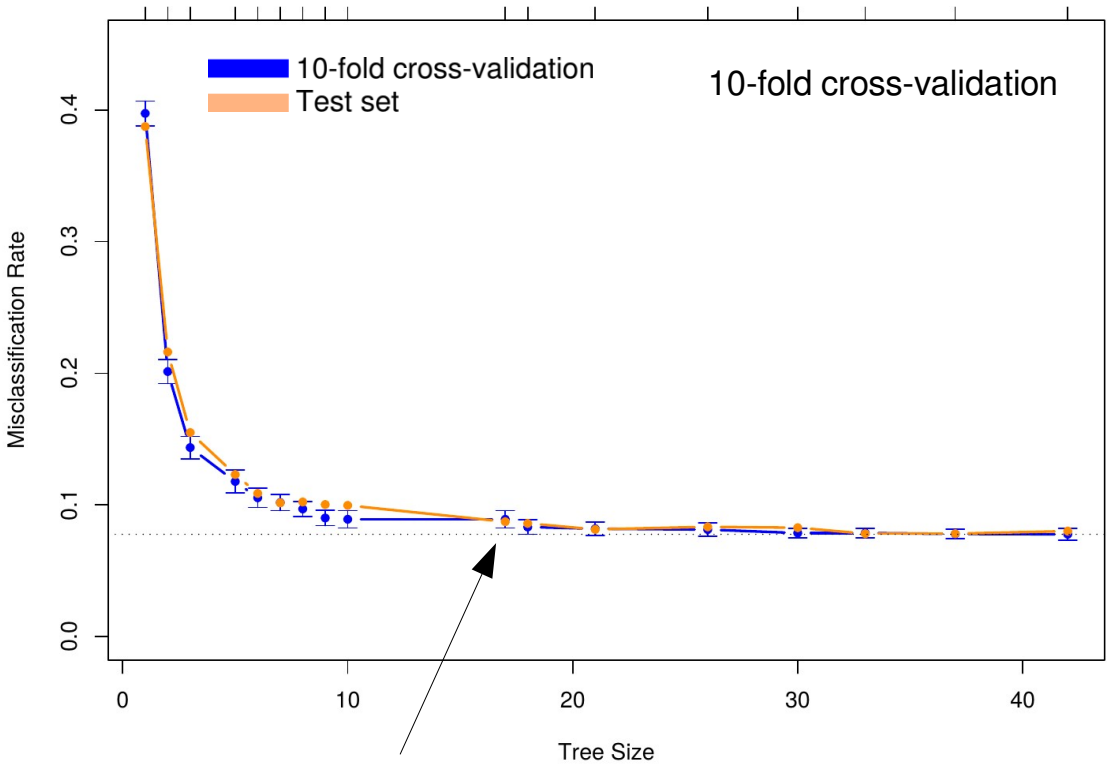


17-nodes tree chosen by cross-validation

Confusion matrix

	Predicted	
True	email	spam
email	57.3%	4.0%
spam	5.3%	33.4%

Misclassification rate = 9.3%

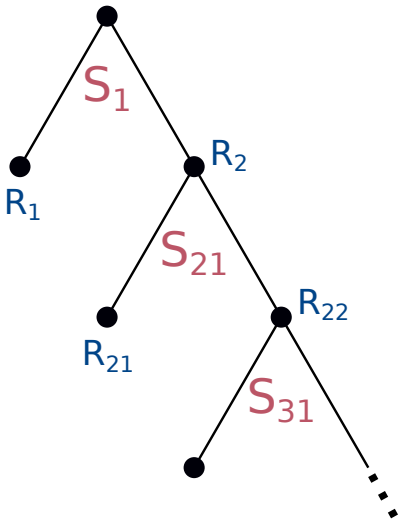
Example discussed in Hastie, Tibshirani, Friedman, Elements of statistical learning, chap. 9, 15

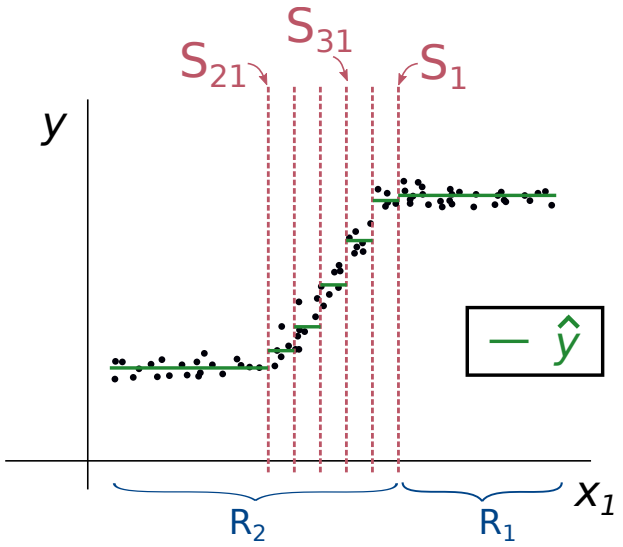
Decision Trees

Decision trees are also applied to regression. The only change is in the cost function:

$$\min_{j,s} RSS(\mathbf{y}; j, s), \qquad RSS(\mathbf{y}; j, s) = \left[\sum_{\mathbf{x}^{(i)} \in R_1(j,s)} (y^{(i)} - \overline{y}_{R_1})^2 + \sum_{\mathbf{x}^{(i)} \in R_2(j,s)} (y^{(i)} - \overline{y}_{R_2})^2 \right]$$

Mean of output variable in that region





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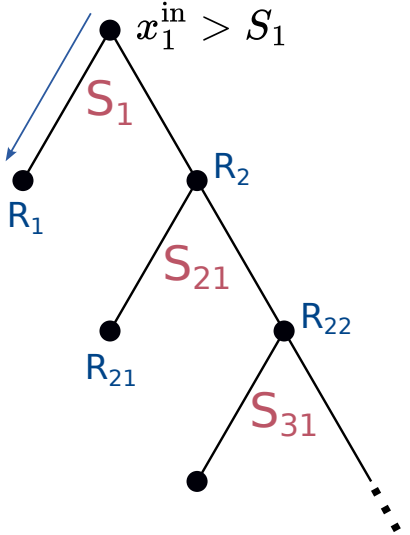
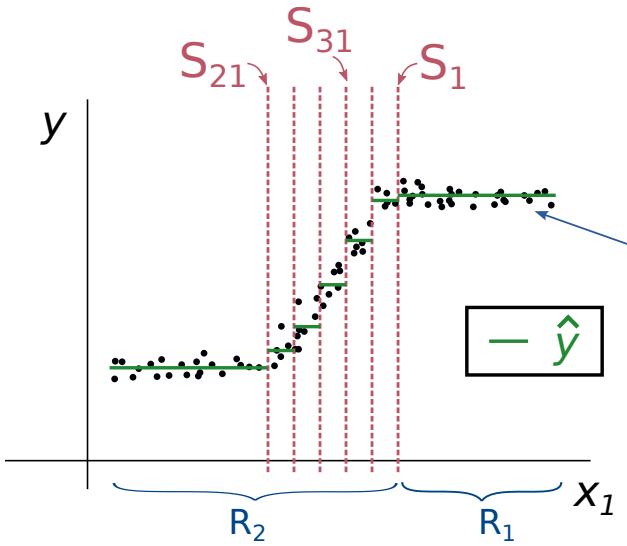
Mean of output variable in that region





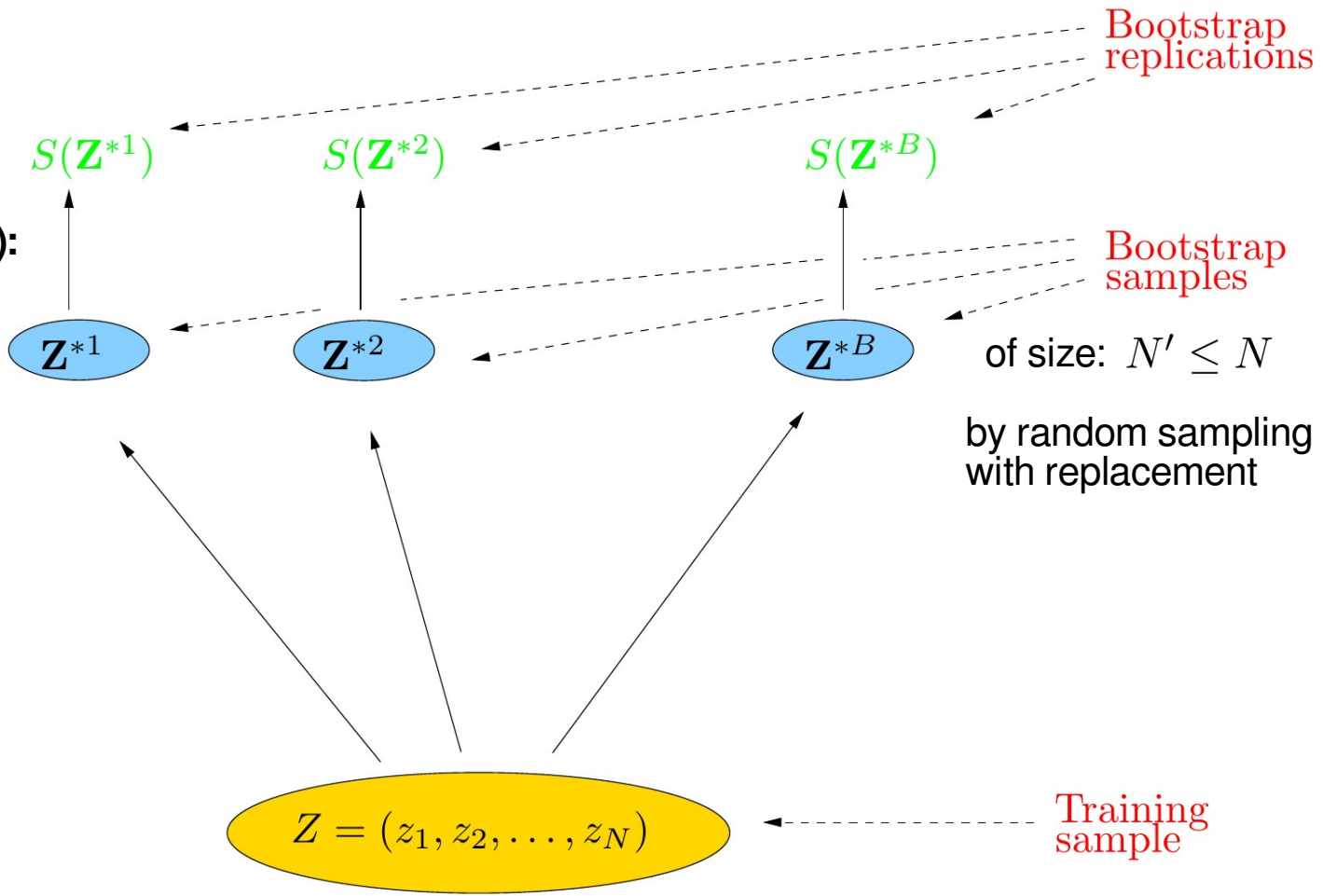
Prediction = average output in the region where the input lies

$$\hat{y}^{\text{DT}}(\mathbf{x}^{\text{in}}) = \overline{y}_{R_\alpha} \text{ with } \mathbf{x}^{\text{in}} \in R_\alpha$$

Pros and Cons

- **Flexible:** They can easily handle both continuous and categorical data multi-class classification, regression. ✓
- **Powerful:** perform well with nonlinear relationships among features ✓
- **Prone to overfitting** - need to reduce the variance ✗

Bootstrap Aggregation (Bagging):
average over many trees to reduce the variance of the DT estimator.

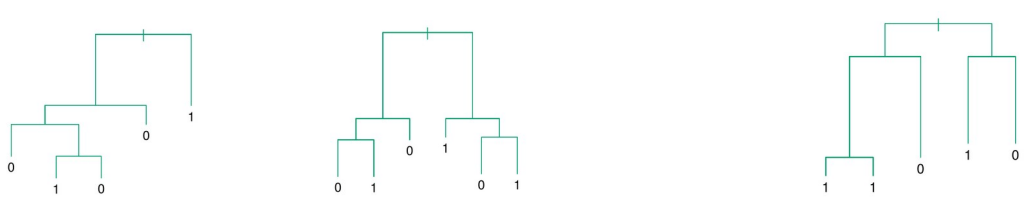


From Hastie, Tibshirani, Friedman,

Elements of statistical learning, chap. 7

For each bootstrap sample grow a tree, giving the ensemble

$$\left\{ \hat{f}_b^{\mathrm{DT}} \right\}_{b=1}^{B}$$



Bootstrap replications

$S(\mathbf{Z}^{*1})$ $S(\mathbf{Z}^{*2})$ $S(\mathbf{Z}^{*B})$

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Bootstrap samples

$\mathbf{Z}^{*1}$ $\mathbf{Z}^{*2}$ $\mathbf{Z}^{*B}$

of size: $N' \leq N$

by random sampling with replacement

$Z = (z_1, z_2, \ldots, z_N)$

Training sample

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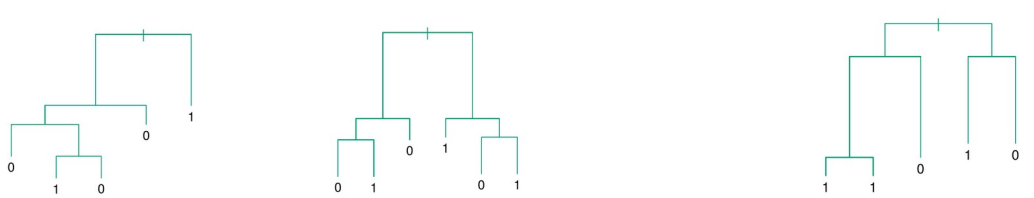

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*Note: it's a **general procedure** for variance reduction by averaging over ensembles of models*

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From Hastie, Tibshirani, Friedman, Elements of statistical learning, chap. 7

If there are correlations between variables, one can't reduce the variance beyond a certain limit...

B random variables (in this case, the trees), that are simply i.d. (identically distributed, but not necessarily independent), with positive pairwise correlation ρ and each of them with variance σ^2, the variance of their average as an estimator is:

$$\rho\sigma^2 + \frac{1-\rho}{B}\sigma^2$$

Random forests (Breiman, 2001) attempt further variance reduction by decreasing the correlation

Random Forests:

Key idea: before each split, select at random $m \leq p$ features as candidates for splitting

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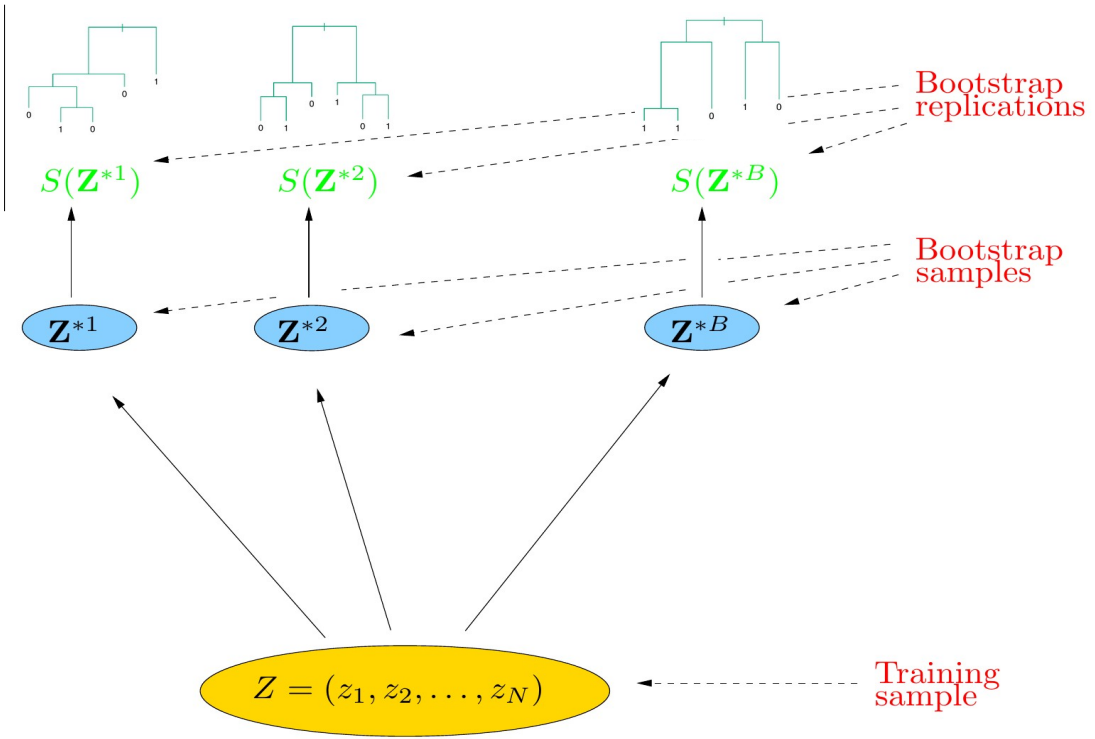
For each bootstrap sample grow a tree (bagging)

+

random selection of predictors at each splitting



Random Forests:

Algorithm: Random Forests for Regression and Classification

Training.
For $b = 1$ to B:

(1) Draw a bootstrap sample $\mathbf{Z}^{*b}$ from the training data.

(2) Train a tree $\hat{f}_b^{\mathrm{DT}}$ on the bootstrapped sample as follows.
For each terminal node at the current level, repeat:
(i): Draw at random a subset of m features from the p features.
(ii): Find the optimal split (j, s) (according to the relevant cost function), choosing j only among the m features randomly sampled in *(i)*.
(iii) Perform the split into two daughter nodes.
Until the stopping criterion is reached.

Making predictions (aggregating). Given a new data point $\mathbf{x}^{\mathrm{in}}$:

(1) *Regression:*

$$\hat{y} = \hat{f}(\mathbf{x}^{\mathrm{in}}) = \frac{1}{B} \sum_{b=1}^{B} \hat{f}_b^{\mathrm{DT}}(\mathbf{x}^{\mathrm{in}})$$

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$$\hat{y} = \underset{q}{\operatorname{argmax}}\, \boldsymbol{\pi}, \text{ with } \boldsymbol{\pi} = \frac{1}{B} \sum_{b=1}^{B} \boldsymbol{\pi}_b^{\mathrm{DT}}$$

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Additional hyper-parameters to choose!

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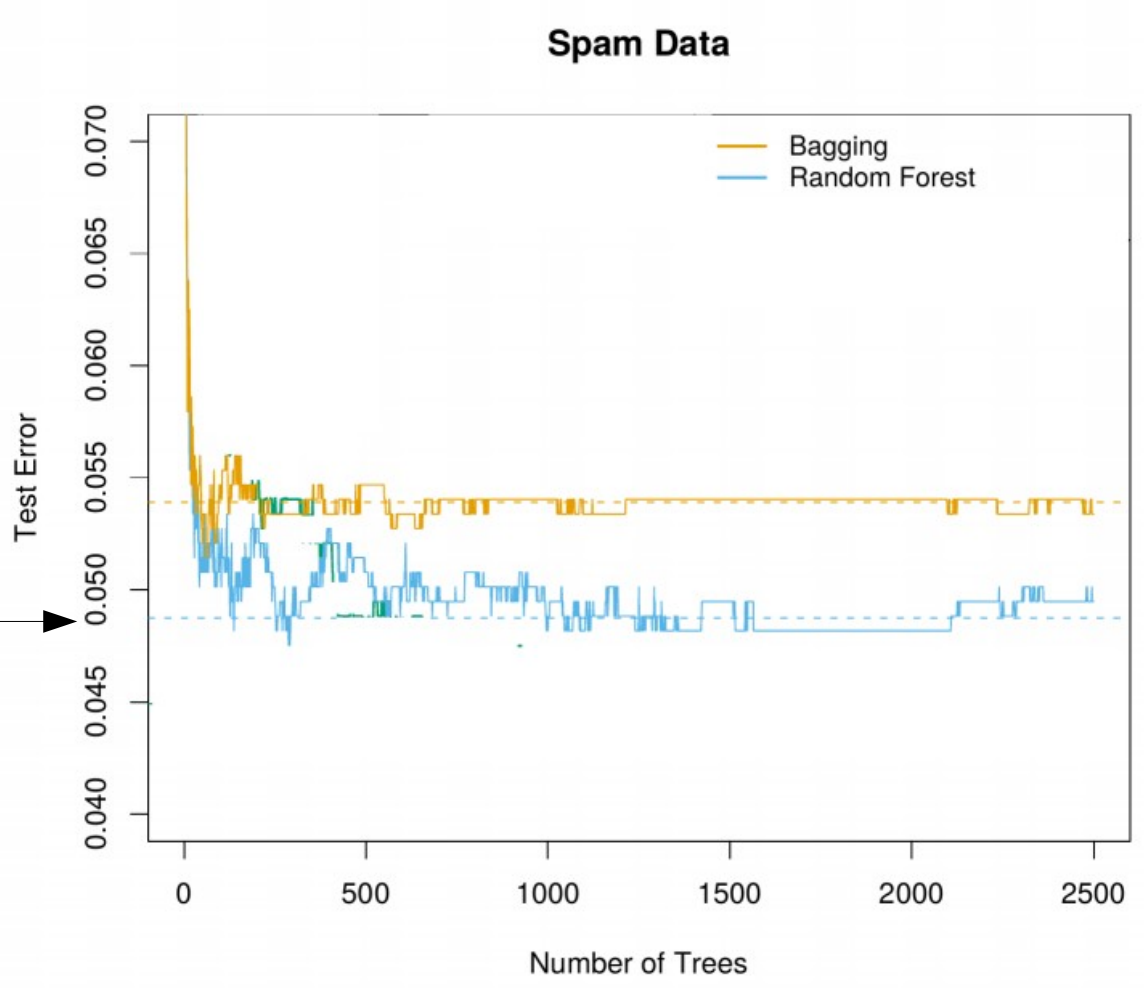
The spam example data illustrates:
1. Bagging improves over decision tree: reducing variance by averaging
2. Random forests improve over bagging alone by de-correlating the bagging trees

Bagging: error rate 5.4%

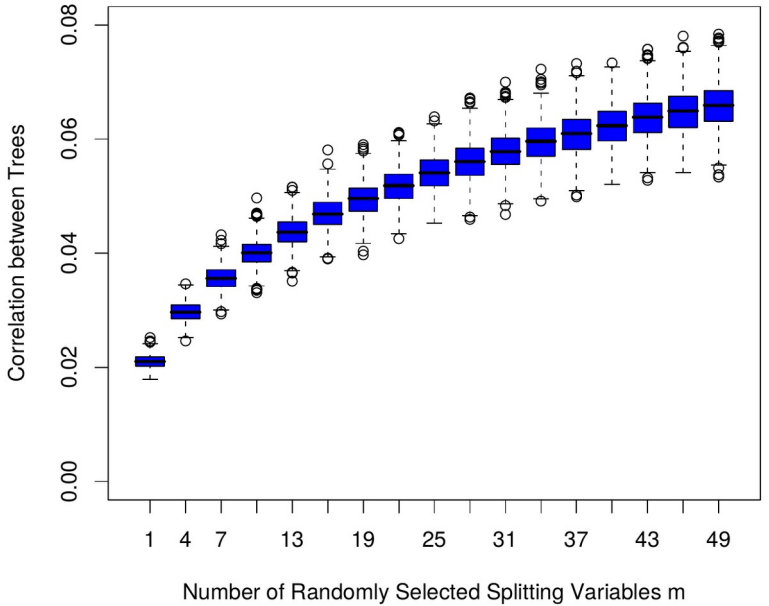
Random Forest: error rate 4.9%

As a comparison:

Simple Decision tree: 9.3%
Logistic regression: 7.6%



Number of splitting variables *m*



Less splitting variables lead to more dissimilar trees

*Simulated data for **regression task**, from Hastie, Tibshirani, Friedman, Elements of statistical learning, chap.15*

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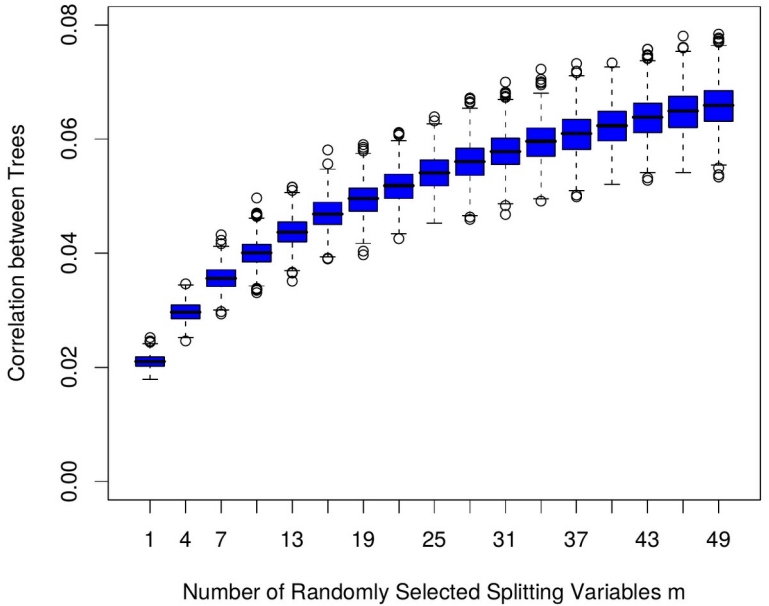

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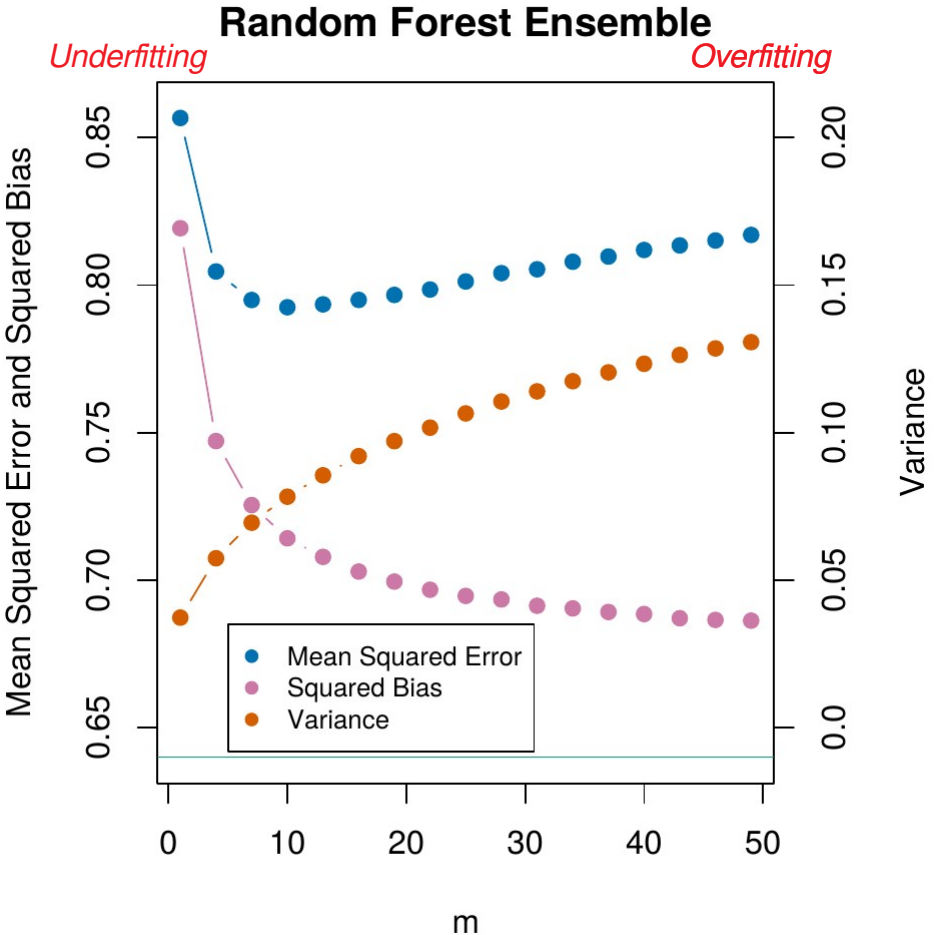

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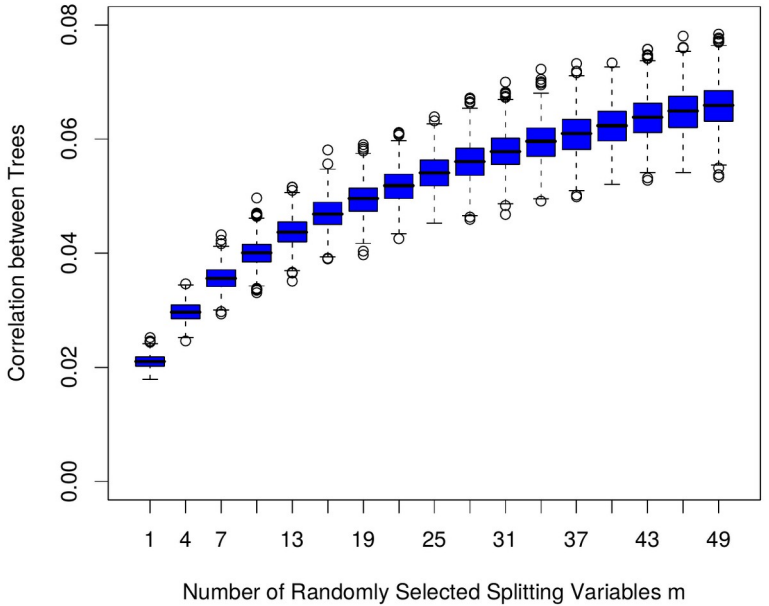
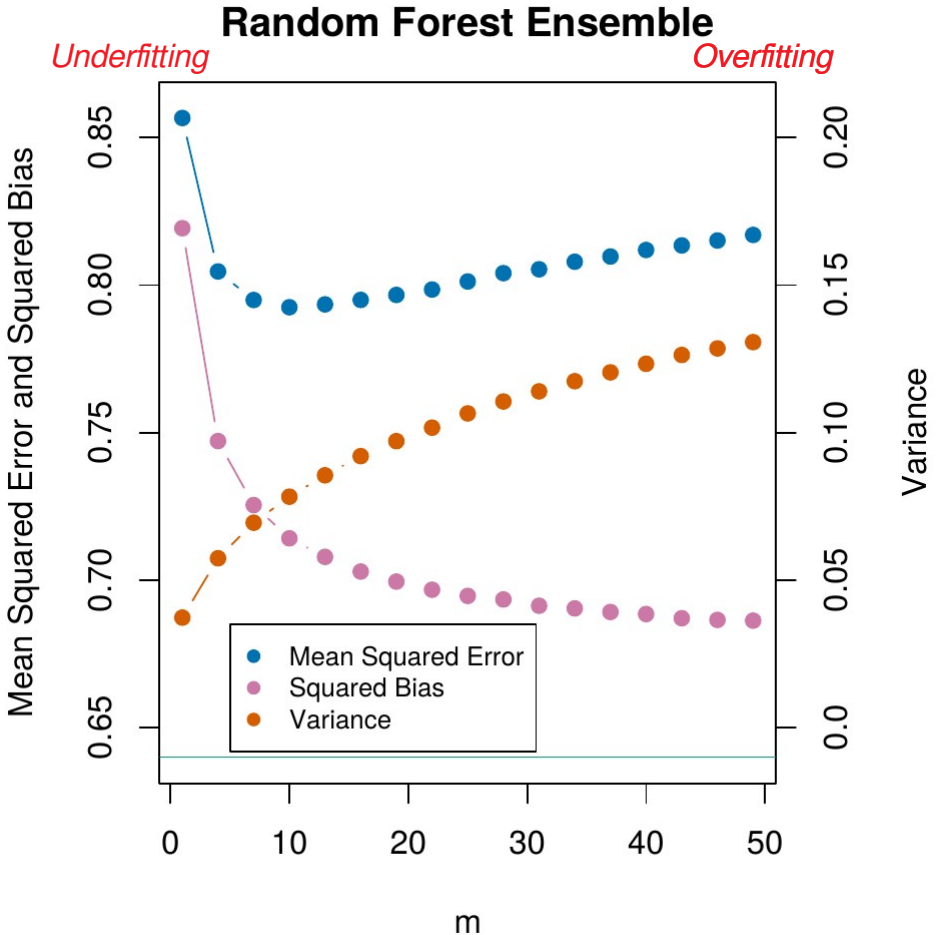


Less splitting variables lead to more dissimilar trees

Default choice (authors' recommendation):

- Regression $m \sim p/3$
- Classification $m \sim \sqrt{p}$



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Samples that were *not* picked in a certain bootstrap sample. For the corresponding tree, OOB samples are *unseen* samples, thus can be used the OOB validation (hyper-parametric search)

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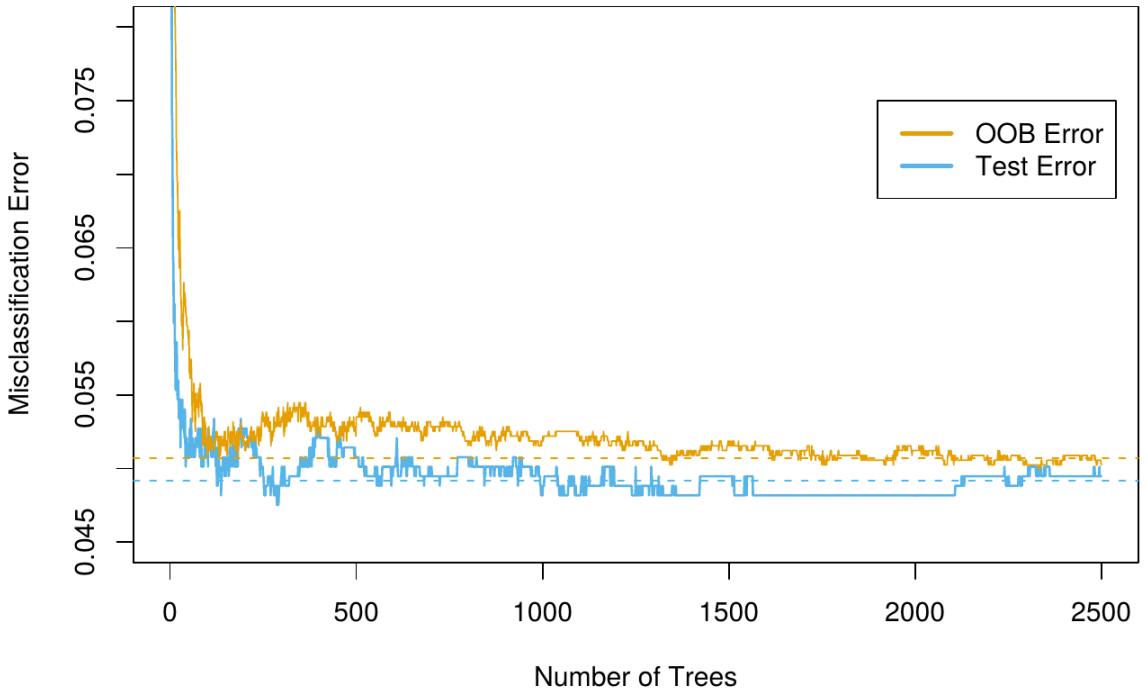

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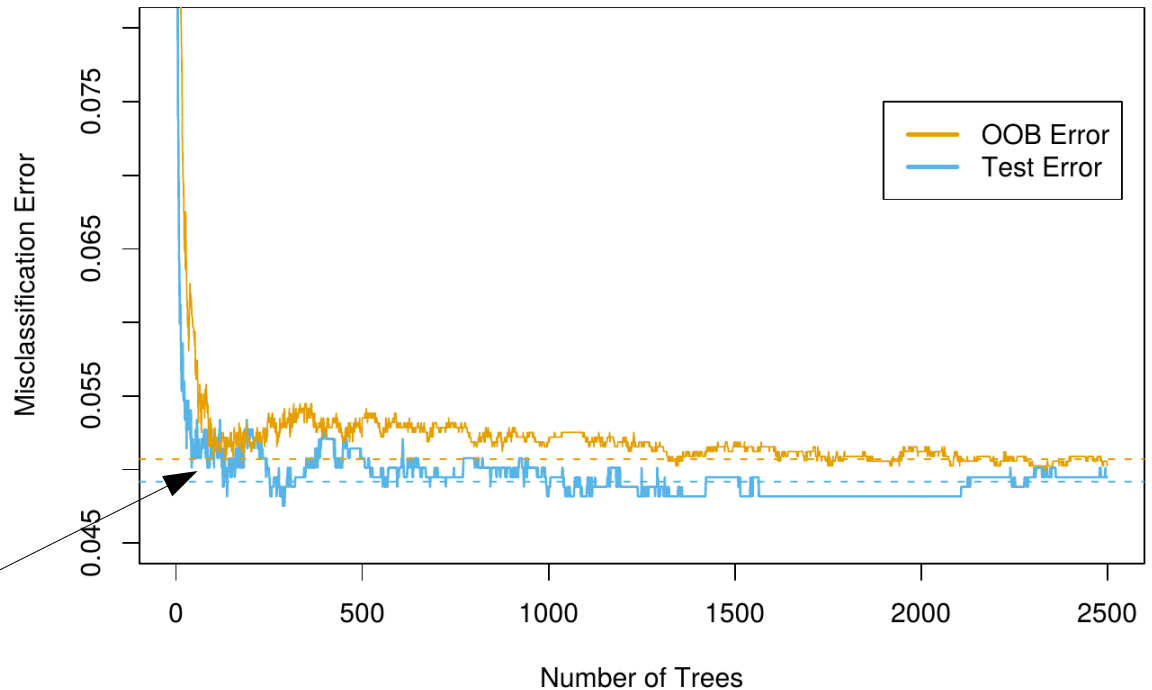

About 200 trees are already sufficient

OOB error is equivalent to the one obtained by cross-validation, hence when the OOB error stabilizes one can stop increasing B

A way to gain interpretability: Variable Importance

For each tree:

OOB samples

Class	Features				
	CAPTOT	ch$	remove	business	
email	0.11	0.053	0.21	0.003	...
spam	0.10	0.015	0.25	0.081	...
email	0.21	0.012	0.32	0.001	...
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Importance of variable *k* = |OOB accuracy - OOB accuracy with variable *k* permuted|

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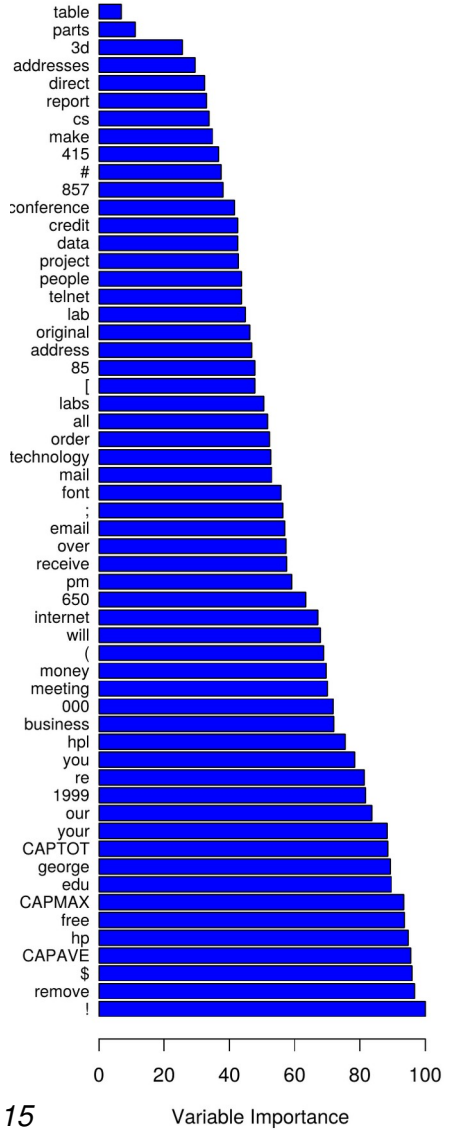

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1. Some predictors are more important than others in separating spam from e-mail

2. In general, it's important to identify what is the predictive power of each feature (e.g. get insights into the main determinants of a given outcome).

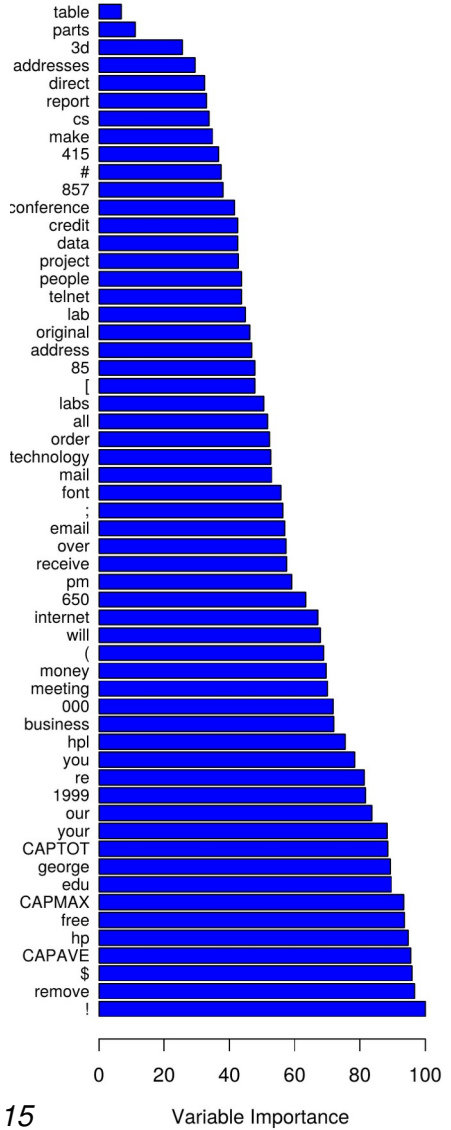

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Table 6. Mean-squared test set error.

Data set	Bagging	Adapt. bag	Forest
Boston Housing	11.4	9.7	10.2
Ozone	17.8	17.8	16.3
Servo $\times 10 - 2$	24.5	25.1	24.6
Abalone	4.9	4.9	4.6
Robot Arm $\times 10 - 2$	4.7	2.8	4.2
Friedman #1	6.3	4.1	5.7
Friedman #2 $\times 10 + 3$	21.5	21.5	19.6
Friedman #3 $\times 10 - 3$	24.8	24.8	21.6

See additional reading for other examples and comparisons

Table 8. Mean-squared test set error.

Random feature selection + noise on the output works better than bagging alone →

Data set	With bagging	With Noise
Boston Housing	10.2	9.1
Ozone	17.8	16.3
Servo $\times 10 - 2$	24.6	23.2
Abalone	4.6	4.7
Robot Arm $\times 10 - 2$	4.2	3.9
Friedman #1	5.7	5.1
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Examples of RF for regression, from Breiman 2001

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Given a *strong* model (like DT): it's the iterative addition of *weak* models to reduce the error of the strong one.

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Shrinkage: controls the rate of update

$$S_{t+1} = S_t - \nu w_t$$

Strong model prediction at iteration t+1

Weak model prediction at t

*Weak model is trained to predict the **error** of the strong model at iteration t*

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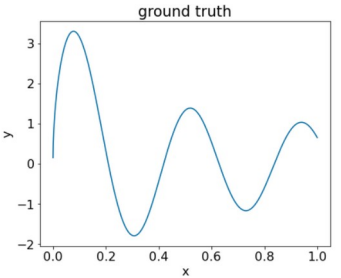

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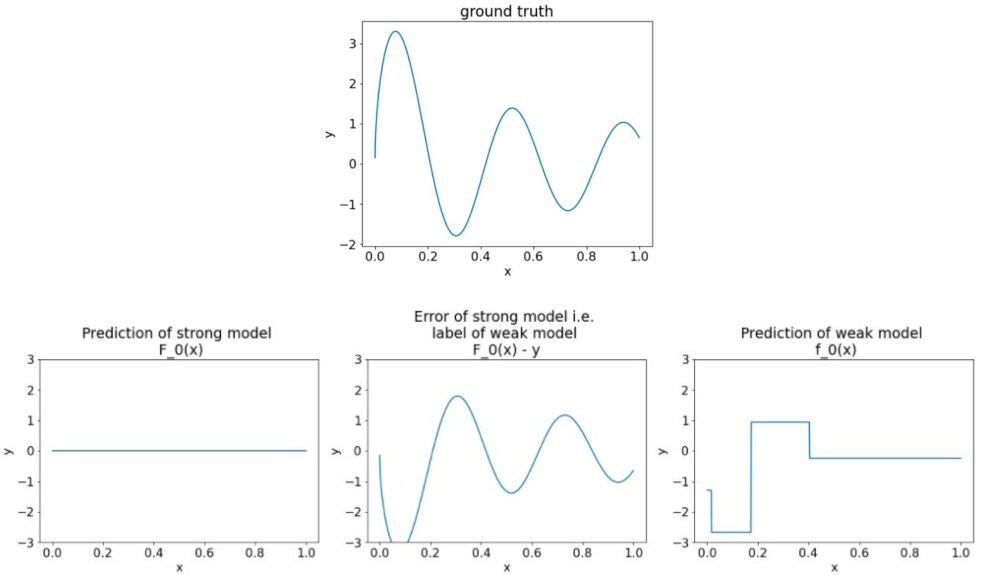

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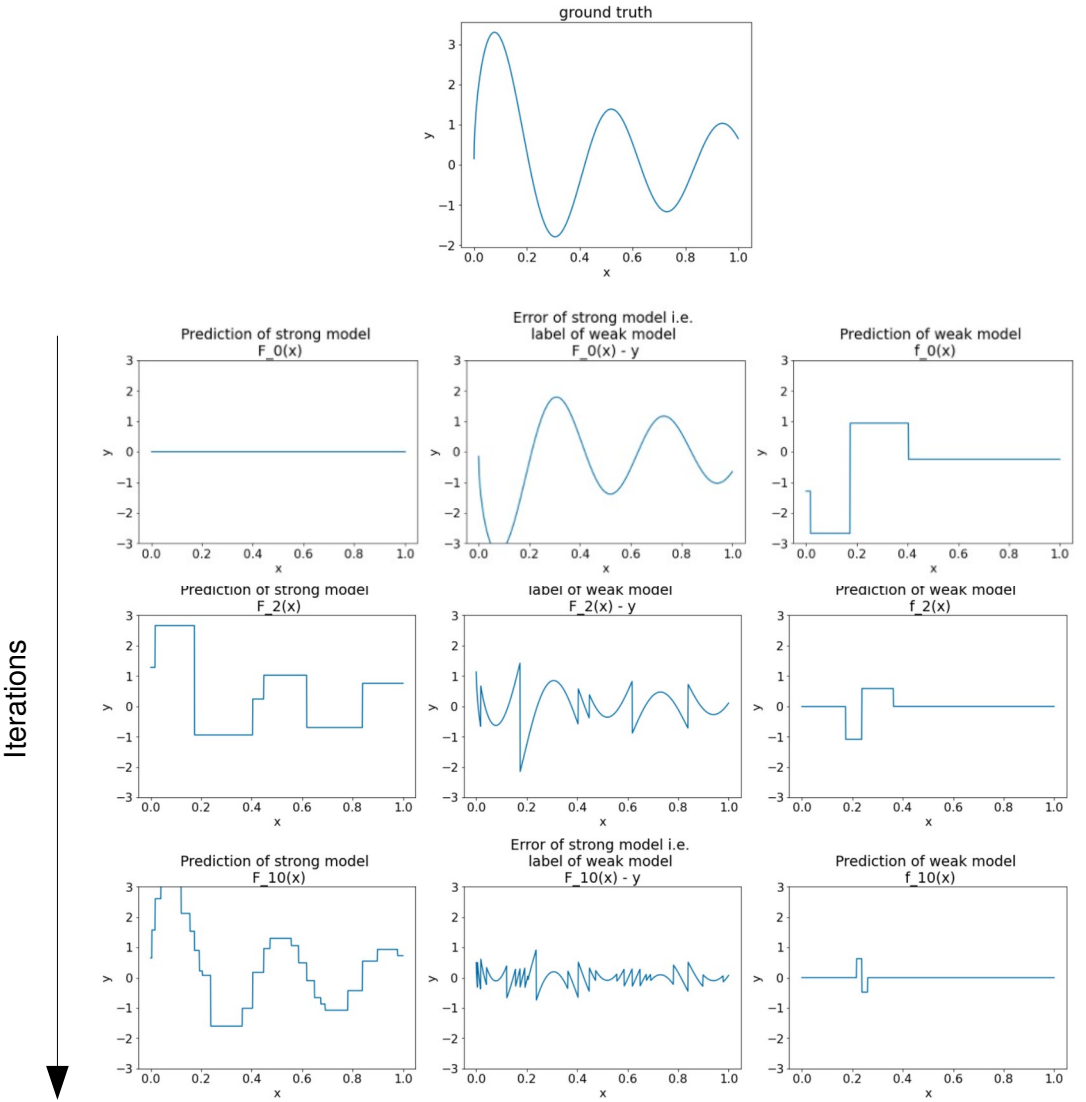

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With a squared error loss, one recovers the strong ***signed error*** *as learning target for the weak model*

$$L(y, S_t) = (y - S_t)^2$$

$$\frac{\partial L(y, S_t)}{\partial S_t} = -2(y - S_t)$$

Summary:

1. Decision trees:

- Minimising CE and GINI index produces regions dominated by 1 class
- Tree size: one can set constraints or use cross-validation (see spam example)
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- Number of decision trees and splitting features needs to be selected
- OOB estimates can be used for: hyper-parametric search, variable importance