Classification: Support vector machines and random forests

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Learning goals

At the end of this lecture you will:

- Explain the formulation support vector machines (SVM) for classification problems.
- Explain the formulation of tree based methods for classification (and regression) problems.
- Illustrate the application of SVM and tree based methods to some case studies and interpret the results.

Materials:

- Chapters 9, 12 and 15 from Friedman et al., *The Elements of Statistical Learning*

Maximal margin classifier

Classification problem: find a hyperplane that separates the classes in feature space.

In p dimensions a hyperplane is a flat affine subspace of dimension $p-1$, with general equation.

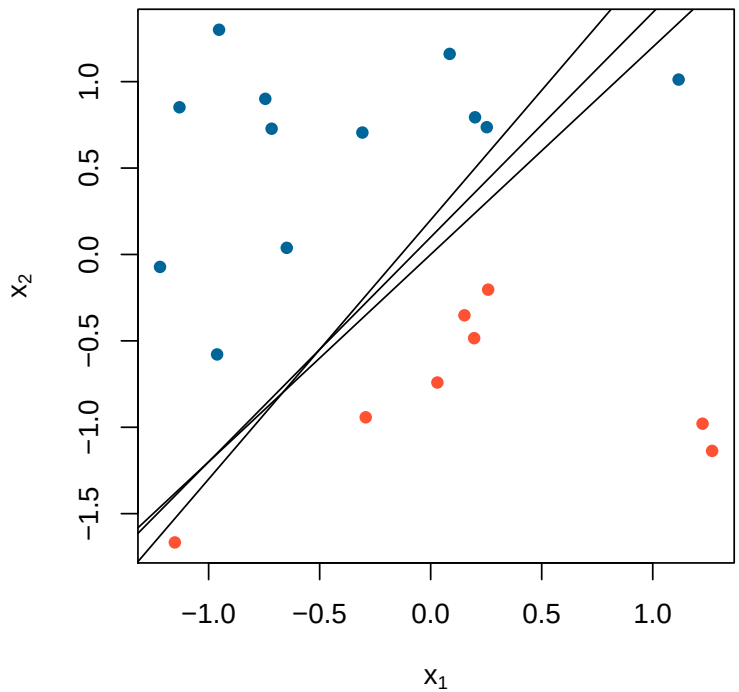
$$f(x) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p = x^T \beta + \beta_0 = 0 \qquad (1)$$

Where:

- $\beta_0 = 0$ only if the hyperplane goes through the origin
- the vector $\beta = (\beta_1, \beta_2, \ldots, \beta_p)$ is a unit vector ($\|\beta\| = 1$) orthogonal to the surface of the hyperplane

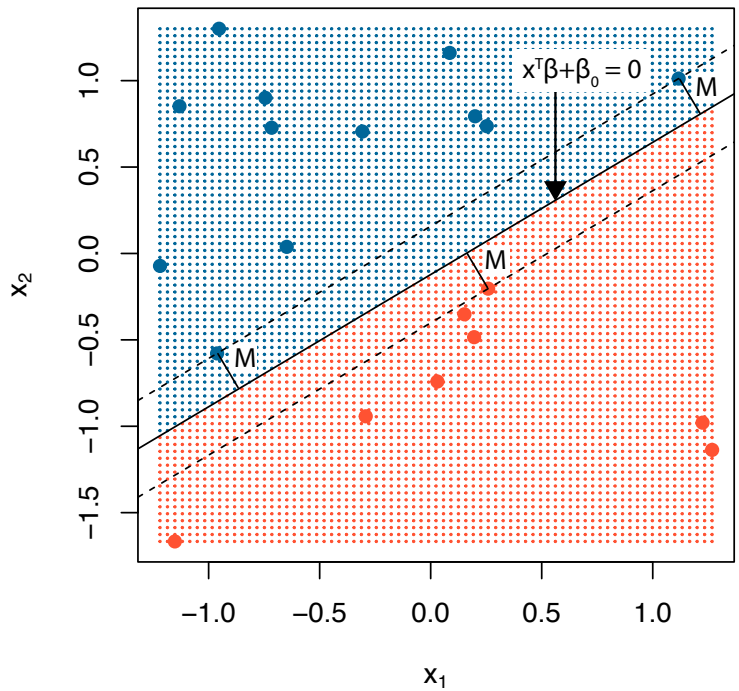
Maximal margin classifier

Imagine to have a training data of N pairs:
$\{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\}$, with $x_i \in \mathbb{R}^p$ and $y_i \in \{-1, 1\}$.
If the classes are perfectly separable, there are generally multiple hyperplanes that can separate them.



Maximal margin classifier

The *maximal margin classifier* is the one with biggest margin between the two classes.

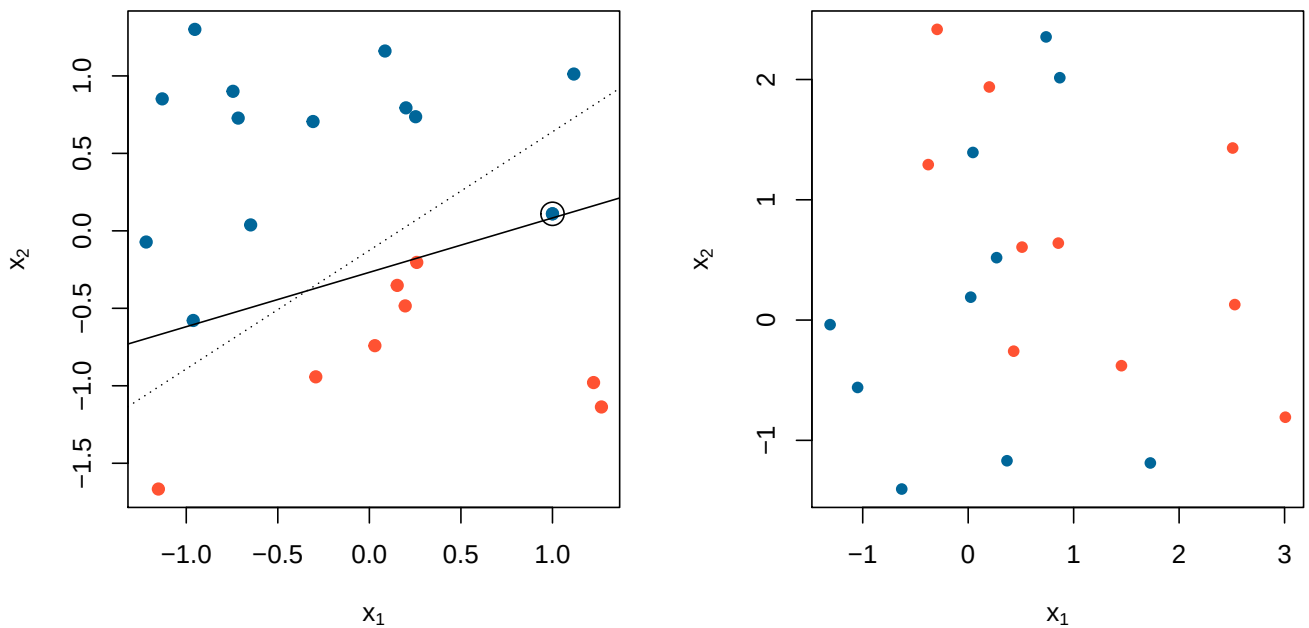


$$\max_{\beta,\beta_0,\|\beta\|=1} M, \text{ subject to } y_i(x_i^T\beta + \beta_0) \geq M, i = 1, \ldots, N$$

Noisy or non-separable data

The maximal margin classifier has issues in case of:

- Noisy data with outliers leading to poor solution (left panel - just added one data point to the previous example).
- Data non-separable by linear boundary (right panel).



Support vector classifier

The *support vector classifier* provides a solution by maximising a *soft* margin (regularization).

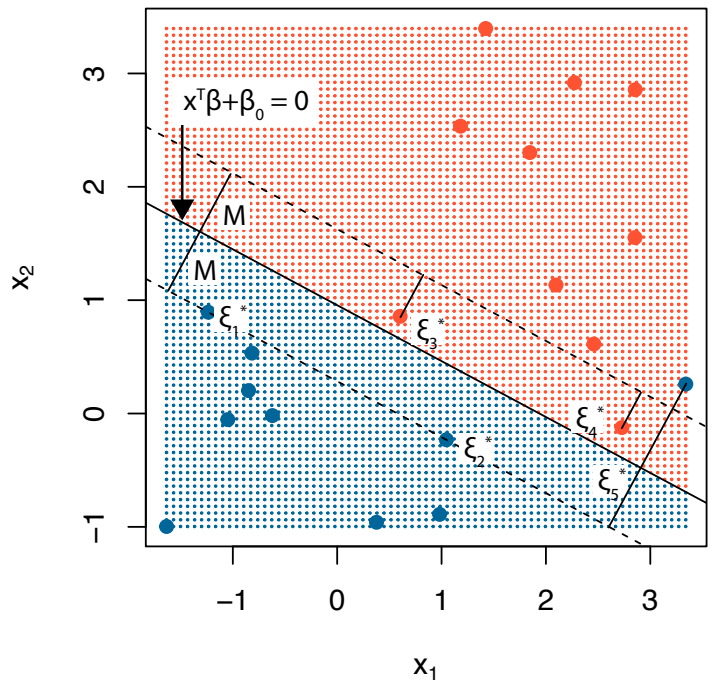
For this we can modify the optimization problem allowing some slack.

$$\max_{\beta,\beta_0,\|\beta\|=1} M, \text{ subject to } y_i(x_i^T\beta + \beta_0) \geq M(1-\xi_i), i = 1, \ldots, N$$

where $\xi_i \geq 0$ and $\sum_{i=1}^{N} \xi_i \leq C$. C is a constant that defines the budget we allow for the total amount of slack.

Support vector classifier

The *support vector classifier* provides a solution by maximising a *soft* margin.



$$\max_{\beta,\beta_0,\|\beta\|=1} M, \text{ subject to } y_i(x_i^T\beta + \beta_0) \geq M(1-\xi_i), i = 1, \ldots, N$$

Slack variables

The slack variables $\xi = (\xi_1, \xi_2, \ldots, \xi_N)$ tell us how much each point is allowed to be on the wrong side of its margin (relative amount).

- $\xi = 0$ when the ith observation is on the correct side of the margin
- $\xi > 0$ when the ith observation is on the wrong side of the margin
- $\xi > 1$ when the ith observation is on the wrong side of the hyperplane

Regularization

The constant C (slack budget) is tunable and can be seen as a regularization parameter.

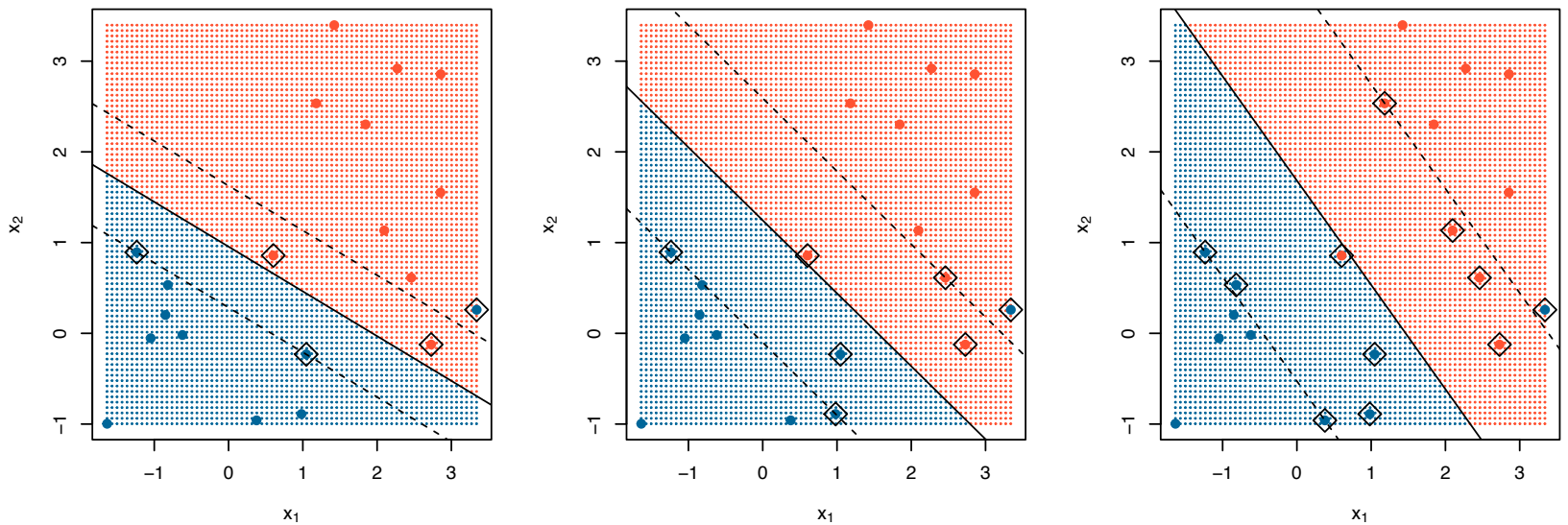
- $C = 0$ no budget for violation of the margin (maximum margin classifier)
- increasing C allows more slack allowed (wider margins)

Therefore C controls the bias-variance trade-off:

- small $C \rightarrow$ narrow margins $\rightarrow$ high fit to the data $\rightarrow$ low bias, high variance
- large $C \rightarrow$ wide margins $\rightarrow$ more violation allowed $\rightarrow$ high bias, low variance

Example

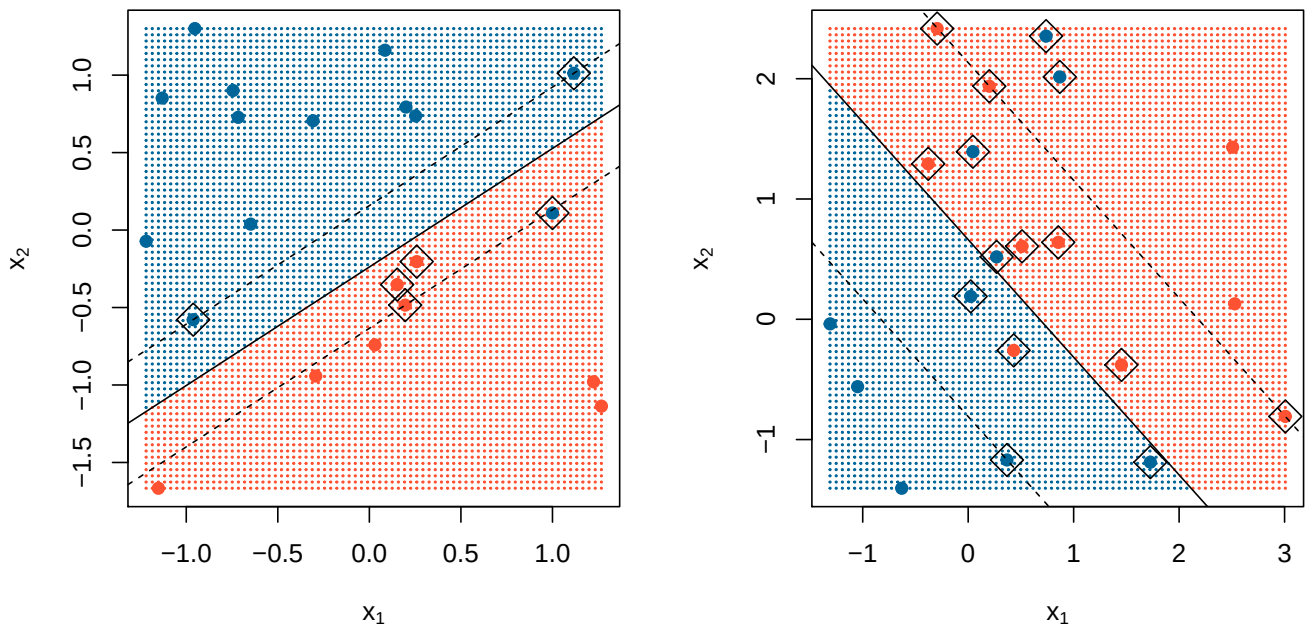
Example of support vector classifier for increasing values of C.



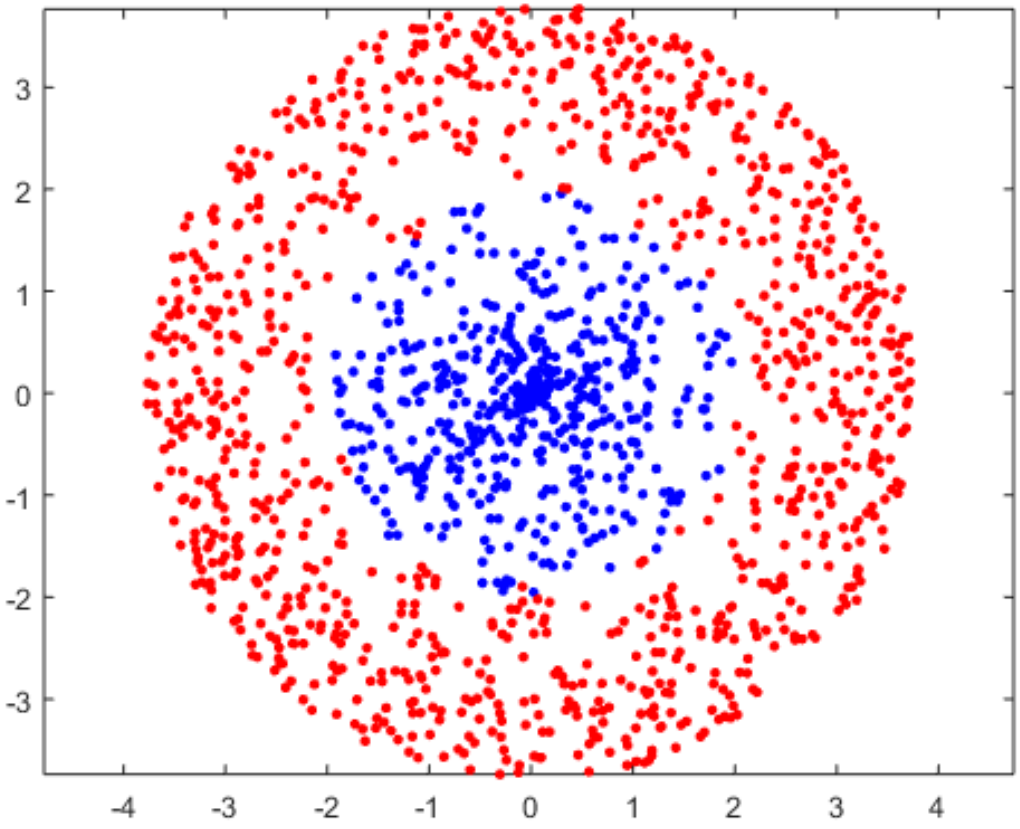
The *support points* (marked with diamonds), i.e. those with $\xi_i \neq 0$, are the only ones that determine the orientation of the margin.

Noisy and non-separable data

The support vector classifier allows to have a good classifier in both the examples of noisy and non-separable data that we have seen earlier, where the maximal margin classifier was not working properly.



Non-linearly separable classes



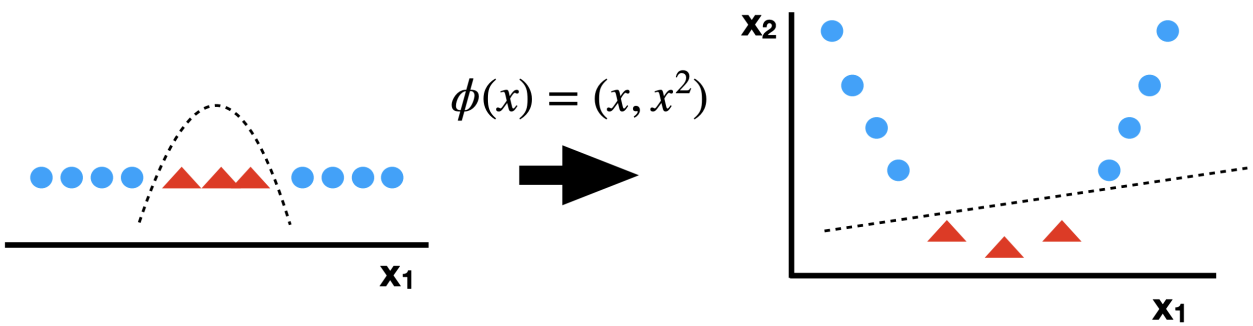
Classification with non-linear decision boundaries

Extension of the Support vector classifier to handle **non-linear class boundaries**. Idea: use of quadratic, cubic, and even higher-order polynomial functions of the predictors. Example:

$$X_1, X_2 \quad \rightarrow \quad X_1, X_1^2, X_2, X_2^2, X_1 X_2$$

$$f(x) = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \beta_3 X_2 + \beta_4 X 2 X_2^2 + \beta_5 X_1 X_2$$

Example with one dimension:



Support vector machines

Problems:

- Infeasible for high p
- Which polynomial order?

Support vector machines (SVM): extension of the support vector classifier which enlarges the feature space by using **kernels**.

The kernel approach is an efficient computational methodology to enlarge the feature space.

Support Vector Machines

Inner product definition: $\langle a, b \rangle = \sum_{i=1}^{p} a_i b_i$, where a,b are vectors

The solution to the support vector classifier problem involves only the inner products of the observations. The inner product of two observations x_i, x_i' is given by

$$\langle x_i, x_i' \rangle = \sum_{j=1}^{p} x_{ij} x_{i'j}$$

Then, the linear support vector classifier can be represented as:

$$f(x) = \beta_0 + \sum_{i=1}^{N} \hat{\alpha}_i \langle x, x_i \rangle$$

where there are N parameters $\hat{\alpha}_i$, one per training observation.

Support Vector Machines

$\hat{\alpha}_i$ is nonzero only for the support vectors.

So if S is the collection of indices of these support points, we can rewrite f(x) which involves far fewer terms than before:

$$f(x) = \beta_0 + \sum_{i \in S} \hat{\alpha}_i \langle x, x_i \rangle,$$

Abstraction of the inner product:

$$K(x_i, x_i'),$$

where we refer to K as *kernel*. A *kernel* is a function that quantifies the similarity of two observations.

Support Vector Machines

Linear kernel: $K(x_i, x_i') = \sum_{j=1}^{p} x_{ij} x_{i'j}$
Polynomial kernel of degree d: $K(x_i, x_i') = (1 + \sum_{j=1}^{p} x_{ij} x_{i'j})^d$
Radial kernel: $K(x_i, x_i') = exp(-\gamma \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2)$

What is the advantage of using a kernel rather than simply enlarging the feature space using functions of the original features?

- Computational advantage: we don't work in the enlarged feature space.
- Automatically computes inner product for high dimensional space of features.
- Avoid overfitting by automatically squashing down most dimensions.

Extension to multi-class

So far, binary classification, in other words, two-class setting.

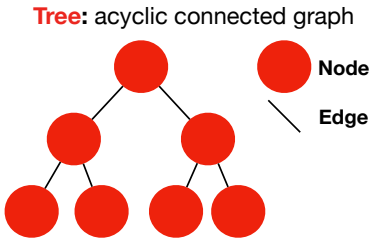
SVMs: concept of separating hyperplanes does not lend itself to more than two classes.

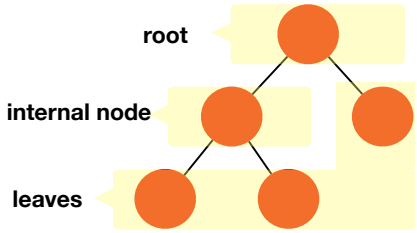
Two approaches for extending SVMs to K$>$2 classes classification:

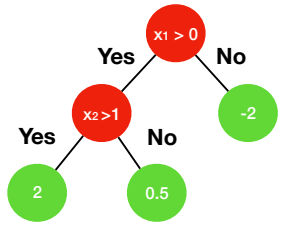
- One-Versus-One Classification: $\binom{K}{2}$ SVMs comparing pair of classes. We assign the test observation to the class most frequently selected in these pairwise classification.
- One-Versus-All Classification: K SVMs, each time comparing one of the K classes to the remaining K-1 classes. We assign the test observation to the class (SVM in this case) with the best discrimination rule.

Tree-based methods

- Can be used for *regression* or *classification*
- Partition the feature space into a set of rectangles (consecutive binary partitions)
- This can be summarised into a tree: decision-trees



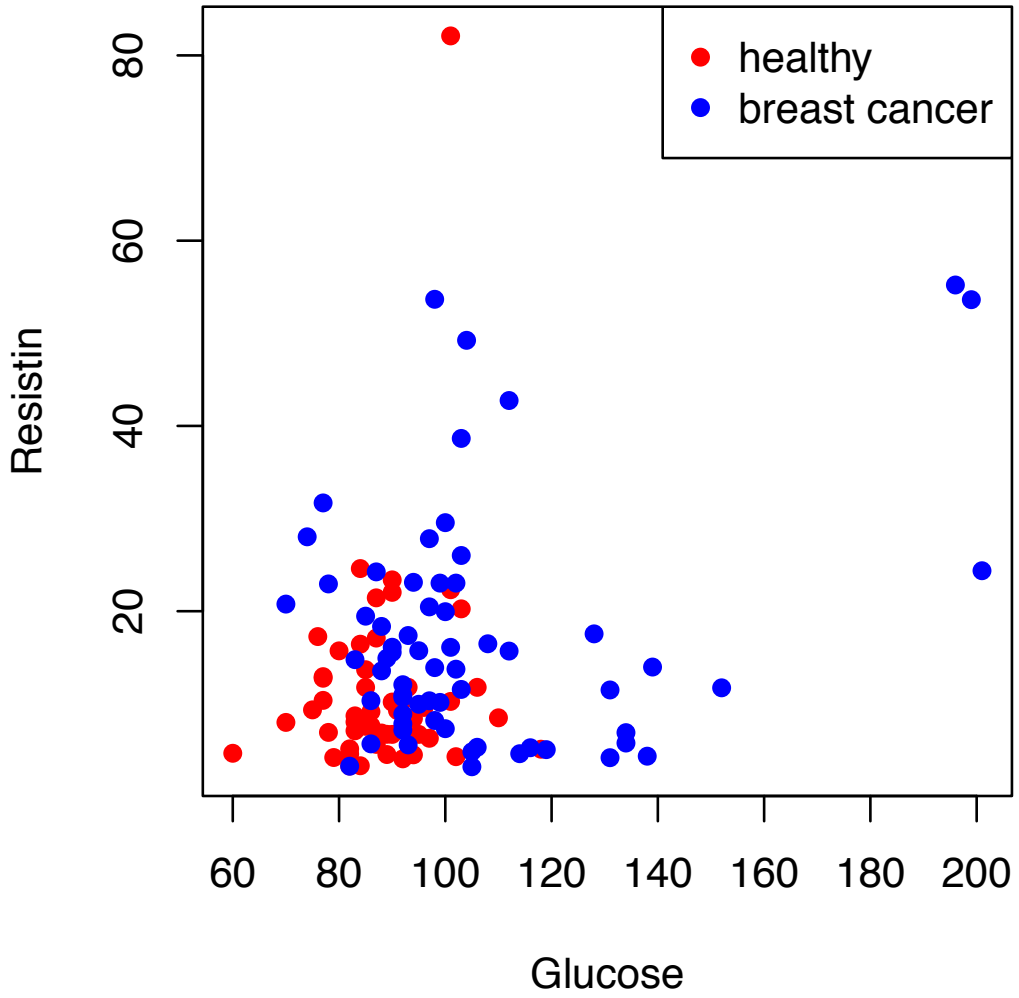




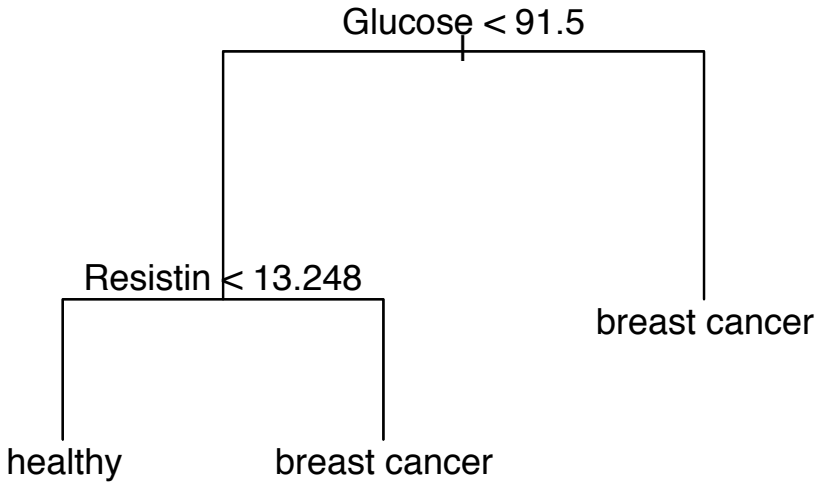
Decision tree: binary tree, graphical representation of a function.
Root & internal nodes: splitting condition
Leaves: predictions

Example

Coimbra Breast Cancer dataset
(Patricio, M., et al, BMC Cancer, 2018)



Example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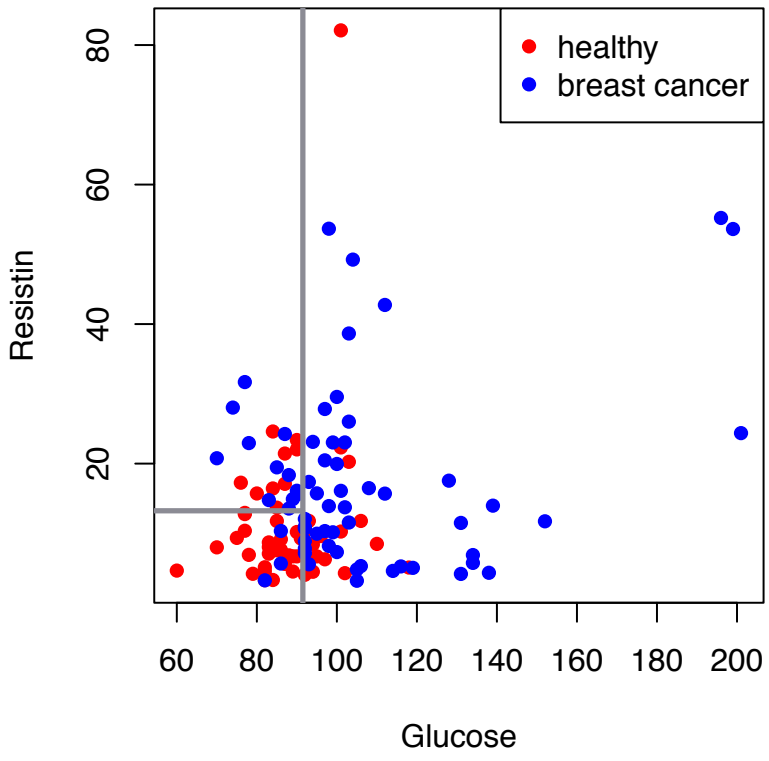
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How to build a decision-tree

To grow a decision-tree we need a set of training data with N observations consisting in p inputs and a response $(x_1, y_1) \dots (x_N, y_N)$, where each $x_i = (x_{i1}, x_{i2}, \dots, x_{ip})^T$ is a vector of feature measurements for the ith case.

The algorithm should build the decision tree that:

- divides the predictor space in M non-overlapping regions R_m with $m = 1, ..., M$ (M number of leaves). For each observation that falls in the same region R_m we make the same prediction.
- this partition should minimise the RSS (for regression) or the misclassification (for classification).

How to build a decision-tree

It is infeasible to evaluate every possible partition of the feature space.

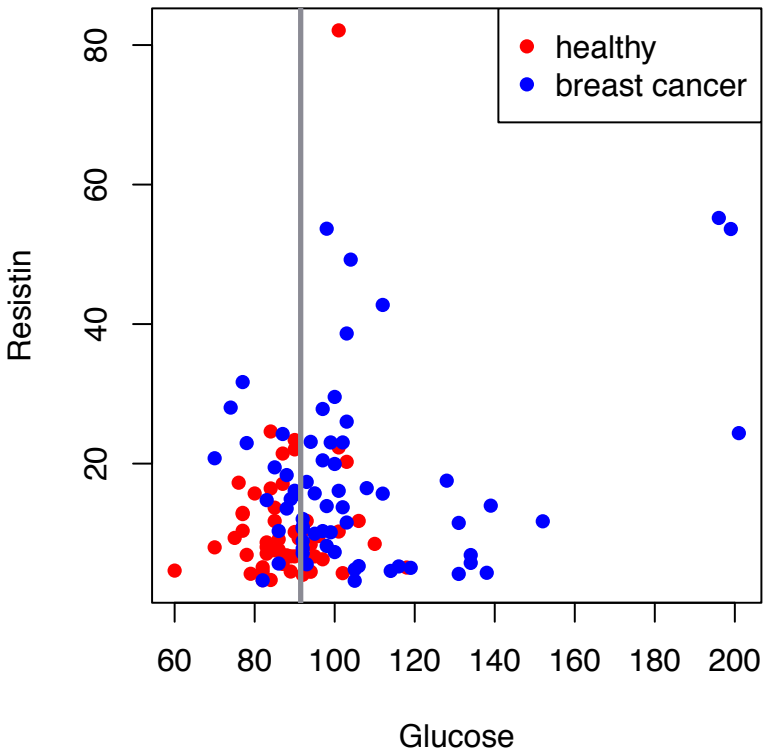
We adopt an approach that is:

- *top-down*: starts from the top of the tree and proceeds with subsequent splits.
- *greedy*: it looks at the optimal splitting at that specific step of the tree, without looking ahead.

How to build a decision-tree

- We start from the top of the tree and we select the variable X_j and the splitting point s to define the pair of half-planes $R_1(j, s) = \{X | X_j \leq s\}$ and $R_2(j, s) = \{X | X_j > s\}$ that leads to the greatest reduction of the cost function.
- This will generate two nodes, for each of the node we repeat the procedure but looking only at the data in that half-plane.
- This continue until we reach a termination criterion (e.g. no region with more than 5 observations).

Example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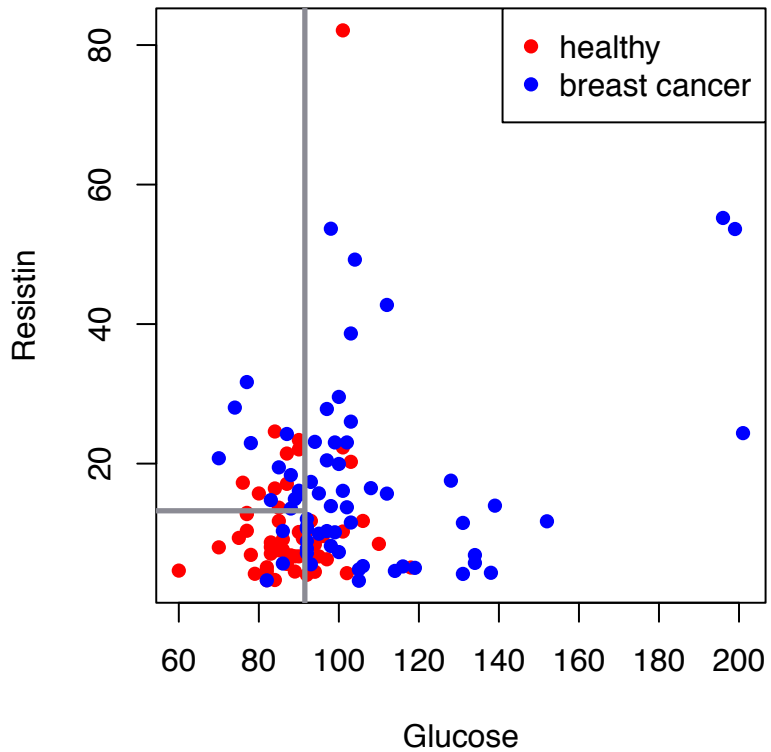
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Cost functions

Let N_m be the number of observations falling in region R_m.
For **regression**:

$$\frac{1}{N_m} \sum_{x_i \in R_m} (y_i - \hat{c}_m)^2 \quad \text{, where} \quad \hat{c}_m = \frac{1}{N_m} \sum_{x_i \in R_m} y_i$$

For **classification**:

$$\hat{p}_{mk} = \frac{1}{N_m} \sum_{x_i \in R_m} I(y_i = k)$$

is the proportion of training observations in region m that are from class k. Different measures of node impurity include:

- **Misclassification error**: $1 - \max_k \hat{p}_{mk}$
- **Gini index**: $\sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk})$
- **Cross-entropy or deviance** $-\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}$

Predictions using a decision-tree

What value will each leaf predict?

- For **regression**: the average of the training observations falling in the region R_m of the leaf m.
- For **classification**: the most occurring class in the region R_m of the leaf m.

Pruning a tree

Idea: build a large tree T_0 and then prune it back to a subtree T. This is done defining a cost complexity criterion:

$$\sum_{m=1}^{|T|} \sum_{x_i \in R_m} (y_i - \hat{c}_m)^2 + \alpha |T|$$

where:

- $|T|$ is the number of leaves in a subtree T
- $\hat{c}_m = \frac{1}{N_m} \sum_{x_i \in R_m} y_i$
- α is a regularisation parameter (tuned with cross-validation)

Pros and cons

- Tree-based methods are simple and easily interpretable (appealing for clinical decision making process)
- They often suffer of low prediction accuracy
- Solutions: combine different trees to derive a consensus predictions (we will discuss *bagging*, *random forests*, *boosting*)
- Combining a large number of trees can improve predictions at the price of loosing a bit interpretability

Bagging (or bootstrap aggregation)

General concept: the average of N observations with variance σ^2 gives an observation with variance σ^2/N

Idea: Instead of pruning big trees, build multiple independent big trees and average their predictions.

How to build independent trees with only one dataset? With **bootstrap**.

How to do bagging

- Generate B different training datasets by bootstrapping (sampling with replacement).
- Build a decision-tree for each bootstrapped dataset (without pruning).
- Obtain the final predictions by averaging (regression) or majority vote (classification).

Bagging reduces the variance without increasing the bias.

Out of bag error estimation

How to estimate the test error of a bagged model?

Idea: on average, each bagged tree makes use of about 2/3 of the observations. We can use the remaining 1/3, called out-of-bag observations (OOB), to estimate prediction error.

For each observation i we consider all the trees in which the observation was OOB. This yields to about B/3 predictions for that observation that can be averaged.

Variable importance measure

Problem: we reduce variance but at the price of losing interpretability.

Idea: Obtain a measure of the importance of each predictor looking at the how much they decrease the cost function (RSS for regression, Gini index for classification) in average across the B trees.

Random forest

How can we improve performance over bagging? Performing random subselections of the features.

This decorrelates the trees and reduces variance.

Random forests:

- build a large number of decision-trees using bootstrapped training data (same as bagging)
- at each split select a subset of m features out of the p as possible split candidate. A typical choice of m is $m \simeq \sqrt{p}$.

Boosting

With **boosting** the trees are grown sequentially.

- Instead of building a lot of large trees, with boosting we sequentially build small trees (with d splits).
- Each tree fits a shrunken version of the residuals of the previous tree, compensating partially the bias of the previous tree. The shrinkage factor is called λ
- The higher B (i.e. the number of trees), the smaller the bias and the higher the variance

Choice of hyper-parameters:

- B: cross-validation
- λ: typically 0.01 or 0.001 (note: small λ will require large B)
- d: typically 1.

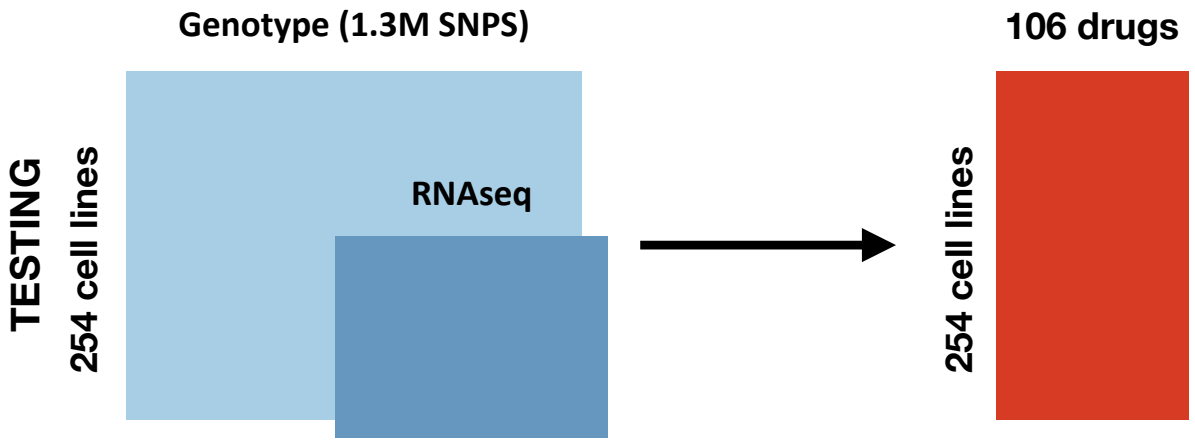
Summary

- Decision-trees are simple and interpretable but suffer from poor predictions.
- Combining multiple trees allows improving predictions at the price of loosing interpretability.
- Random forests and boosting are state-of-the-art models for supervised learning.

Case study: prediction of human population response

Open DREAM challenge (http://dreamchallenges.org/) with 213 participants.

- Subchallenge 1: predict cytotoxicity of new cell lines based on the genotype.
- Subchallenge 2: predict cytotoxicity of new compounds based on their chemical attributes.



Eduati et al., Nature Biotechnology, 2015

For both subchallenges the best performing methods were based on random forests.