STK2100 - Machine Learning and Statistical Methods for Prediction and Classification

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Generalised additive models and tree based methods

Covers Section 9.1 and 9.2

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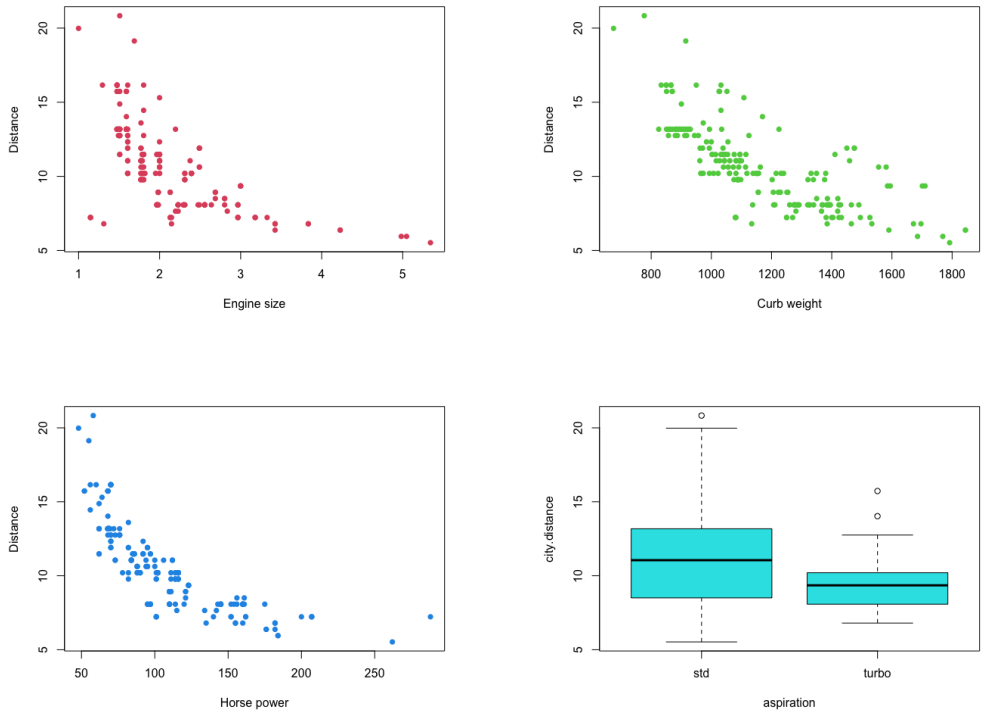
Example: Auto data

- Response: city distance covered (km/l) (`city.distance`)
- Explanatory variables:
  - engine size in l (`engine.size`)
  - curb weight in kg (`curb.weight`)
  - horse power (`HP`)
  - aspiration standard/turbo (`aspiration`)
- We want to predict the distance covered by fuel unit of a car based on properties of the car



Additive models

- Assume that we are in a regression setting with

$$Y = f(\mathbf{x}) + \varepsilon, \quad E[\varepsilon] = 0$$

- Quite often, we need more flexible relationships than linear ones to model $f(\mathbf{x})$
- So far, we used predefined basis functions to achieve nonlinearities, such as splines and kernel smoothers
- Now, we want to obtain more automatic, flexible statistical methods to model non-linear effects
- More specifically, we consider additive models

$$f(\mathbf{x}) = \alpha + \sum_{j=1}^{p} f_j(x_j)$$

- The $f_j(x_j)$s are typically assumed to be smooth and modelled with splines or kernel smoothers, but could also be linear terms or (global) polynomials in x_j

Fitting criterion for additive models

- We assume the model $Y = \alpha + \sum_{j=1}^{p} f_j(X_j) + \varepsilon$, and have the observations $\{(\mathbf{x}_i, y_i), i = 1, ..., N\}$, where $\mathbf{x}_i \in \mathbb{R}^p$
- The criterion used to estimate the model is then the penalized sum of squares

$$\text{PRSS}(\alpha, f_1, f_2, ..., f_p) = \sum_{i=1}^{N} \left(y_i - \alpha - \sum_{j=1}^{p} f_j(x_{ij}) \right)^2 + \sum_{j=1}^{p} \lambda_j \int f_j''(t_j)^2 dt_j,$$

where $\lambda_j \geq 0$ are tuning parameters

Fitting criterion for additive models

- Based on results from Chapter 5, we know that each function f_j is a cubic spline with knots at each of the unique values of $x_{ij}, i = 1, ..., N$
- However the solution is not unique, and we need further constraints, more specifically

$$\sum_{i=1}^{N} f_j(x_{ij}) = 0, \quad j = 1, \ldots, p$$

- Then, it may be shown that $\hat{\alpha} = \frac{1}{N} \sum_{i=1}^{N} y_i = \bar{y}$
- The fact that we have procedures for fitting one f_j is used to construct a fitting algorithm called the Backfitting algorithm

The Backfitting algorithm for additive models

Backfitting algorithm for additive models

Initialise $\hat{\alpha} = \bar{y}$, $\hat{f}_j = 0, j = 1, ..., p$
while Convergence not reached **do**
  for $j = 1, ..., p$ **do**
    for $i = 1, ..., N$ **do**
      $r_i \leftarrow y_i - \hat{\alpha} - \sum_{k \neq j} \hat{f}_k(x_{ik})$
    end for
    Fit $\hat{f}_j = S_j(\{(r_i, x_{ij}\})$
    $\hat{f}_j \leftarrow \hat{f}_j - \frac{1}{N} \sum_{i=1}^{N} \hat{f}_j(x_{ij})$
  end for
end while

- The criterion for convergence is typically that the functions stabilise
- The algorithm can accomodate for different smoothing operators S_j, including local polynomial regression, kernel smoothers or even polynomial fits
- This makes it possible to include simple linear terms and allows for categorical covariates

Degrees of freedom

- For one-dimensional splines, we know that the prediction may be written as $\hat{\mathbf{y}} = \mathbf{S}\mathbf{y}$, so that the degrees of freedom are given by $tr(\mathbf{S})$
- In additive models, each f_j can be represented by a matrix $\mathbf{S}_j$
- Hence the degrees of freedom of f_j is given by $tr(\mathbf{S}_j) - 1$, where the -1 stems from the constraint $\sum_{i=1}^{N} f_j(x_{ij}) = 0$
- Note that this is a linear model with non-linear basis functions f_j
- Hence, "standard" testing procedures can be used to test the significance of the non-linear terms of the f_js
- The linear term of f_j has 1 degree of freedom
- This means that the non-linear part has $tr(\mathbf{S}_j) - 2$ degrees of freedom

Example: Auto data

See R code

Generalised additive models (GAM)

- Define $\mu(\mathbf{x}) = \mathrm{E}(Y|\mathbf{X} = \mathbf{x})$
- Further, assume that g is a strictly increasing, differentiable function
- Then, the generalised additive model (GAM) with link function g is given by

$$g\left(\mu(\mathbf{x})\right) = \alpha + \sum_{j=1}^{p} f_j(x_j)$$

- Common link functions are
  - the identity link $g(\mu) = \mu$, which gives the additive model
  - the logit link $g(\mu) = \mathit{logit}(\mu) = \log\left(\frac{\mu}{1-\mu}\right)$, as in the additive logistic regression model
  - the log link $g(\mu) = \log(\mu)$, used in log-additive models for Poisson count data or for Gamma regression

Additive logistic regression model

- Assume that $Y \in \{0, 1\}$
- Now $\mu(\mathbf{x}) = \mathrm{E}(Y|\mathbf{X} = \mathbf{x}) = \Pr(Y = 1|\mathbf{x})$
- The ordinary logistic regression model is given by

$$\mu(\mathbf{x}) = \Pr(Y = 1|\mathbf{x}) = \frac{\exp(\alpha + \sum_{j=1}^{p} \beta_j x_j)}{1 + \exp(\alpha + \sum_{j=1}^{p} \beta_j x_j)}$$

  or equivalently

$$\log\left(\frac{\mu(\mathbf{x})}{1 - \mu(\mathbf{x})}\right) = \alpha + \sum_{j=1}^{p} \beta_j x_j$$

- The additive logistic regression is given by

$$\log\left(\frac{\mu(\mathbf{x})}{1 - \mu(\mathbf{x})}\right) = \alpha + \sum_{j=1}^{p} f_j(x_j)$$

- It can also be generalised to several classes, i.e. $Y \in \{1, \ldots, K\}$

Fitting additive logistic regression models

- Additive logistic regression models can be fitted with a backfitting algorithm within a Newton-Raphson procedure, given below
- This procedure requires that the f_js accept observation weights, which is the case for most smoothing procedures

Fitting additive logistic regression models

Local scoring algorithm for additive logistic regression models

Initialise $\hat{\alpha} = \log(\bar{y}/(1-\bar{y}))$, $\hat{f}_j = 0, j = 1, ..., p$
for $i = 1, \ldots, N$ **do**
    Define $\hat{\eta}_i = \hat{\alpha} + \sum_{j=1}^{p} \hat{f}_j(x_{ij})$ and $\hat{p}_i = \exp(\hat{\eta}_i)/(1+\exp(\hat{\eta}_i))$
end for
while Convergence not reached **do**
    for $i = 1, \ldots, N$ **do**
        Construct the weights $w_i = \hat{p}_i(1-\hat{p}_i)$
        Construct the working target variable $z_i = \hat{\eta}_i + \frac{y_i - \hat{p}_i}{w_i}$
    end for
    Fit an additive model to the z_is with weights w_i, using a weighted backfitting algorithm, to get new estimates $\hat{\alpha}$, $\hat{f}_j$, $j = 1, \ldots, p$
end while

Example: E-mail spam data

- Response: indicator of whether the e-mail is spam True/False (`y`)
- Explanatory variables: there are 57 covariates, which are 57 of the most commonly occurring words and punctuation marks in the e-mails (`x1`,...`x57`)
- We want to predict whether an e-mail is spam or not based on the frequencies of the 57 commonly used words and punctuation marks

	`george`	`you`	`your`	`hp`	`free`	`hpl`	`!`	`our`
`spam`	0.00	2.26	1.38	0.02	0.52	0.01	0.51	0.51
`email`	1.27	1.27	0.44	0.90	0.07	0.43	0.11	0.18

See R code

Regression trees

- Another way of modelling non-linear effects and potentially complex interactions in $f(\mathbf{x})$ is through classificaion and regression trees (CART)
- We will consider regression trees first
- The model is then constructed by dividing the covariate space into separate regions R_m, $m = 1, \ldots, M$, and modelling the repsonse with a constant c_m inside each region
- More specifically, the model is given by

$$f(\mathbf{x}) = \sum_{m=1}^{M} c_m I(\mathbf{x} \in R_m)$$

Regression tree in two dimensions

Let us start with an example with a response Y and two numerical covariates x_1 and x_2

The procedure is as follows

- Binary splits are performed in one dimension at a time
- Regions are defined by sequential splits of existing regions by thresholding w.r.t. one of the covariates
- The response in each region is modelled with the average value of the y_is corresponding to $\mathbf{x}_i$s that fall into that region

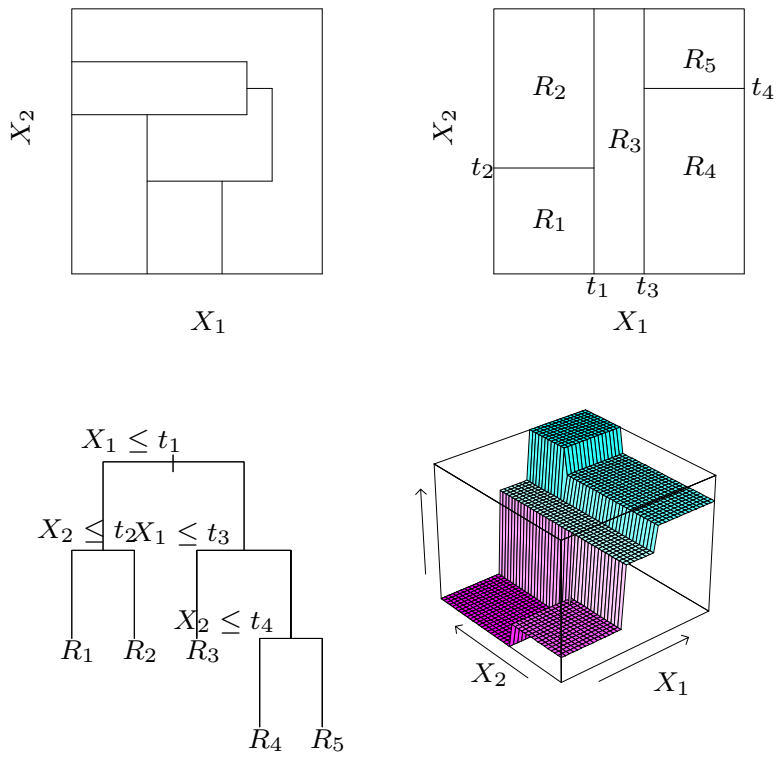
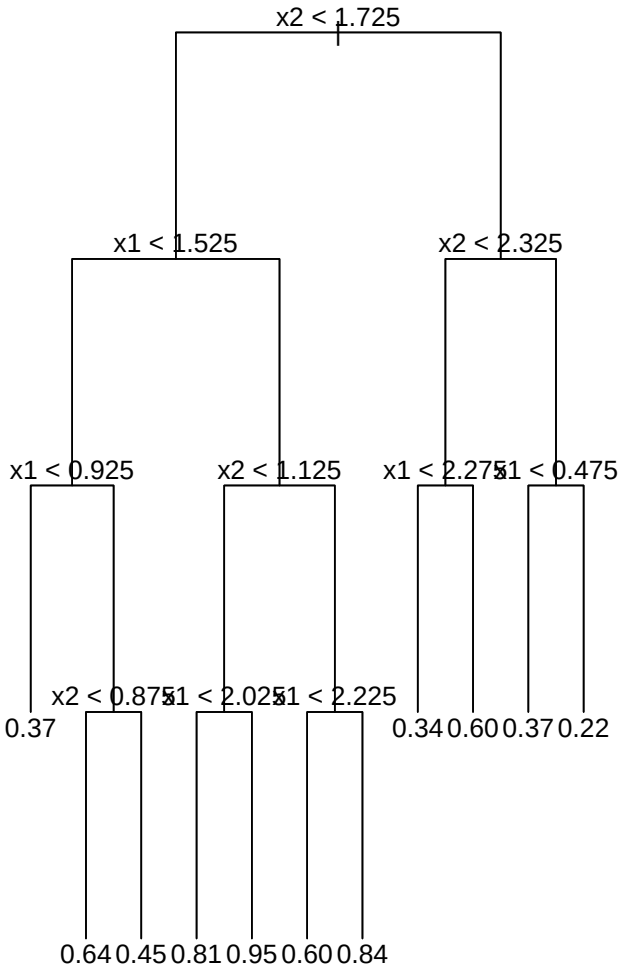
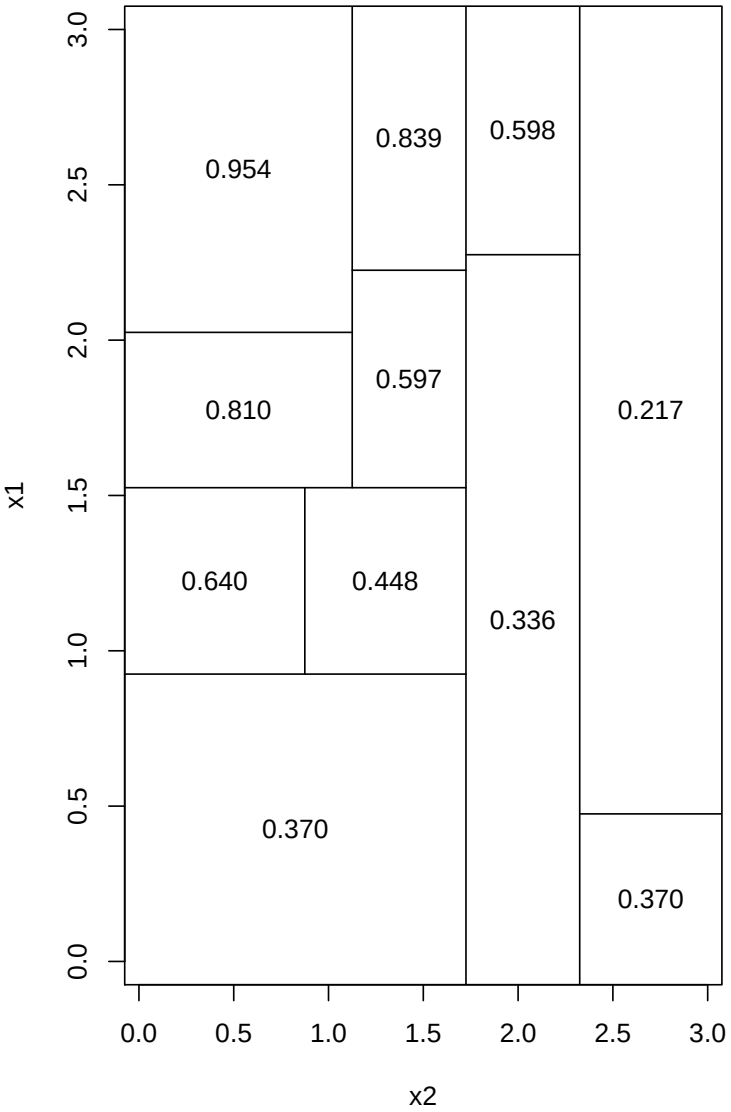


Illustration of a tree structure





Fitting regression trees

- Fitting a regression tree consists in finding the splits that define the regions R_m, and estimating the constants c_m, $m = 1, \ldots, M$
- The objective function that is used in the fitting is

$$
\begin{aligned}
\text{RSS} &= \sum_{i=1}^{N} (y_i - f(\mathbf{x}_i))^2 \\
&= \sum_{i=1}^{N} \left(y_i - \sum_{m=1}^{M} c_m I(\mathbf{x}_i \in R_m) \right)^2 \\
&= \sum_{m=1}^{M} \sum_{\{i:\mathbf{x}_i \in R_m\}} (y_i - c_m)^2
\end{aligned}
$$

- Searching through all possible combinations of splits is computationally impossible
- Instead, a greedy search is performed

Fitting regression trees

- For all covariates x_j, $j = 1, \ldots, p$, and all possible split points, i.e. unique values of x_j, define the two regions

$$R_1(j, s) = I(x_j \leq s) \quad \text{and} \quad R_2(j, s) = I(x_j > s)$$

and with $N_m = \sum_{i=1}^{N} I(\mathbf{x}_i \in R_m)$, $m = 1, 2$, let

$$\hat{c}_1 = \frac{1}{N_1} \sum_{\{i:\mathbf{x}_i \in R_1\}} y_i \quad \text{and} \quad \hat{c}_2 = \frac{1}{N_2} \sum_{\{i:\mathbf{x}_i \in R_2\}} y_i$$

- Choose the pair (j, s) that minimises

$$\sum_{\{i:\mathbf{x}_i \in R_1\}} (y_i - \hat{c}_1)^2 + \sum_{\{i:\mathbf{x}_i \in R_2\}} (y_i - \hat{c}_2)^2$$

- Next, we partition the data into the two regions R_1 and R_2, and repeat the splitting process
- This is continued until there are $M = N$ regions, or a pre-specified minimum node size has been reached

Pruning of regression trees

- The fitting procedure results in a large tree, that is likely to overfit the data
- A possible strategy is to stop the growing of the tree earlier
- However, it is more advantageous to first grow a large tree, and then prune it
- Let T_0 be the large tree that has been grown, and let $T \subset T_0$ be a sub-tree, obtained by pruning, i.e. collapsing some of the internal nodes of T_0
- Introduce the penalty or cost-complexity

$$C_\alpha(T) = \sum_{m=1}^{|T|} N_m Q_m(T) + \alpha |T|, \quad \alpha \geq 0$$

where $N_m = \sum_{i=1}^{N} I(\mathbf{x}_i \in R_m)$ and $Q_m(T)$ is the node impurity given by

$$Q_m(T) = \frac{1}{N_m} \sum_{\{i:\mathbf{x}_i \in R_m\}} (y_i - \hat{c}_m)^2$$

Pruning of regression trees

- The idea is, for each α, to find the sub-tree $T_\alpha \subseteq T_0$ that minimises $C_\alpha(T)$
- It may be shown, that for each α, there is a unique T_α, so that when we increase α, we can find optimal trees by a sequence of pruning operations on the current tree
- To optimise $C_\alpha(T)$, we sequentially remove the leaf which minimises $C_\alpha(T)$, i.e. the leaf which makes the smallest increase in $\sum_{m=1}^{M} N_m Q_m(T)$
- The tuning parameter α must be chosen, for instance using cross-validation

Example: Auto data

See R code

Classification trees

- Assume now that $Y \in \{0, 1, ..., K-1\}$
- Following ideas from regression trees, classification trees model the response with a constant probability $p_{m,k}$ of class k, for $k = 1, \ldots, K$, in each region R_m, i.e.

$$p_k(\mathbf{x}) = \sum_{m=1}^{M} p_{m,k} I(\mathbf{x} \in R_m)$$

- The classification is then obtained as

$$\widehat{Y} = \arg\max_k p_k(\mathbf{x})$$

Fitting classification trees

- Given the regions R_m, the $p_{m,k}$s are estimated by

$$\hat{p}_{m,k} = \frac{1}{N_m} \sum_{\{i:\mathbf{x}_i \in R_m\}} I(y_i = k)$$

- The regions R_m are found in the same way as for regression trees, based on a fitness criterion of the type $\sum_{m=1}^{|T|} N_m Q_m(T)$, with a suitable node impurity $Q_m(T)$

Fitting classification trees

- Impurity measures that are used for classification are
  - the deviance, also called the cross-entropy D:

$$Q_m(T) = -\sum_{k=1}^{K} \hat{p}_{mk} \log(\hat{p}_{mk}), \text{ with } D = -2l(\hat{p}_{11}, \ldots, \hat{p}_{K|T|}) = \sum_{m=1}^{|T|} N_m Q_m(T)$$

  - the misclassification error, with $\hat{p}_{mk(m)} = \max_k \hat{p}_{mk}$:

$$Q_m(T) = \frac{1}{N_m} \sum_{\{i:\mathbf{x}_i \in R_m\}} I(y_i \neq \hat{y}_i) = 1 - \hat{p}_{mk(m)}$$

  - the Gini index:

$$Q_m(T) = \sum_{k \neq k'} \hat{p}_{mk} \hat{p}_{mk'} = \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk})$$

- After a large tree has been grown, pruning can be performed as for regression trees, using the same impurity mesure as for growing the tree

Tree methods - properties

- Advantages of tree methods:
  - Logical simplicity and ease of "communication"
  - Simple, compact mathematical formulation
  - Speed of computation
  - Can easily deal with categorical covariates
- Disadvantages of tree methods:
  - Instable results
  - Difficult to capture additive structure
  - Difficult to do statistical inference
  - Lack of smoothness

Example: E-mail spam data

See R code