Classification and Regression trees

(Recursive partitioning)

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Regression Trees

Non-parametric regression models

- **Non-parametric** (or semi-parametric) regression modelling keeps the usual specification:

$$y = g(x_1, \ldots, x_{p-1}, \epsilon)$$

  but relaxes the assumption of linearity, and replaces it with a much weaker assumption of a smooth g
- Pro's and con's
  - $\mapsto$ greater flexibility and potentially more accurate estimate of g
  - $\mapsto$ greater computation and often more difficult-to-interpret results: typically used for prediction, not interpretation
- Some examples of nonparametric regression models are:
  - $\mapsto$ Local Polynomial Regression
  - $\mapsto$ Kernel regression
  - $\mapsto$ Smoothing splines
  - $\mapsto$ (Generalized) Additive models
  - $\mapsto$ Decision (regression) trees

Step functions as approximators

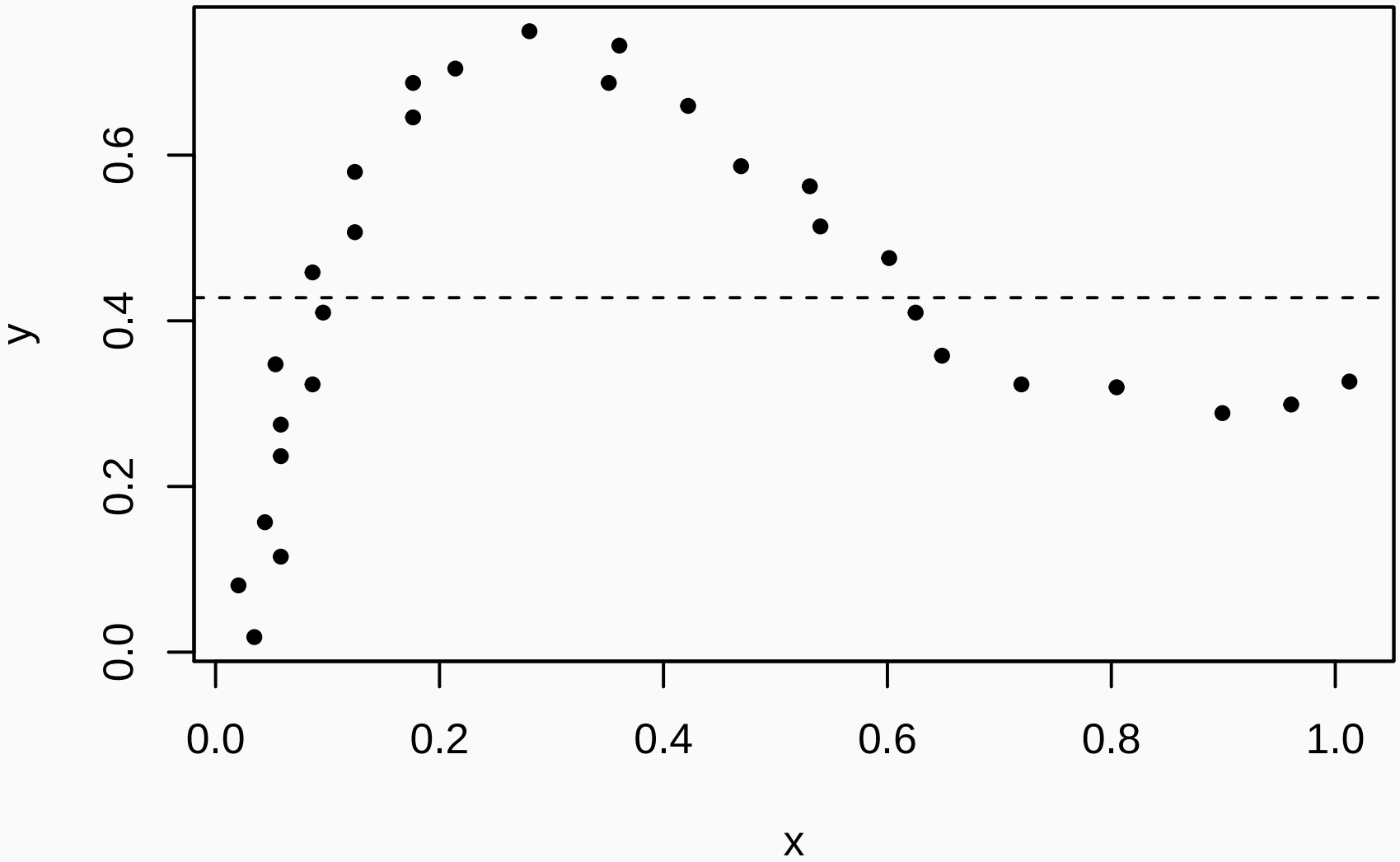
- A simple, yet effective, way to approximate a generic function $f(x)$ is to use a step function, that is, a piecewise constant function
- In such a case, there are various choices to be made:
  - where are the subdivision points to be placed?
  - which value of y must be assigned to each interval?
  - how many subdivisions of the x axis must be considered?
- The idea is to generalize the use of step functions to approximate (or predict) a response Y as function of some covariates.
- Note that Y could be of different nature: numeric, factor, count, ...

Step functions as a spline

- A step function actually is a spline of degree 0. Assume we want to fit such a function to a simple set of data.
- Subdivision points are now the knots and their position should be chosen to reflect changes of the function $f(x)$ (for instance more knots where the function is steeper)
- In a given interval the value of the constant can be chosen to be an average of the level of the function itself
- The choice of the number of subdivisions is critical: any increase in the number of steps increases the quality of the approximation, and therefore we are led to think of infinite subdivisions.
- However, this is counter to the requirement to use a approximate representation using few parameters and therefore to adopt a finite number of subdivisions.

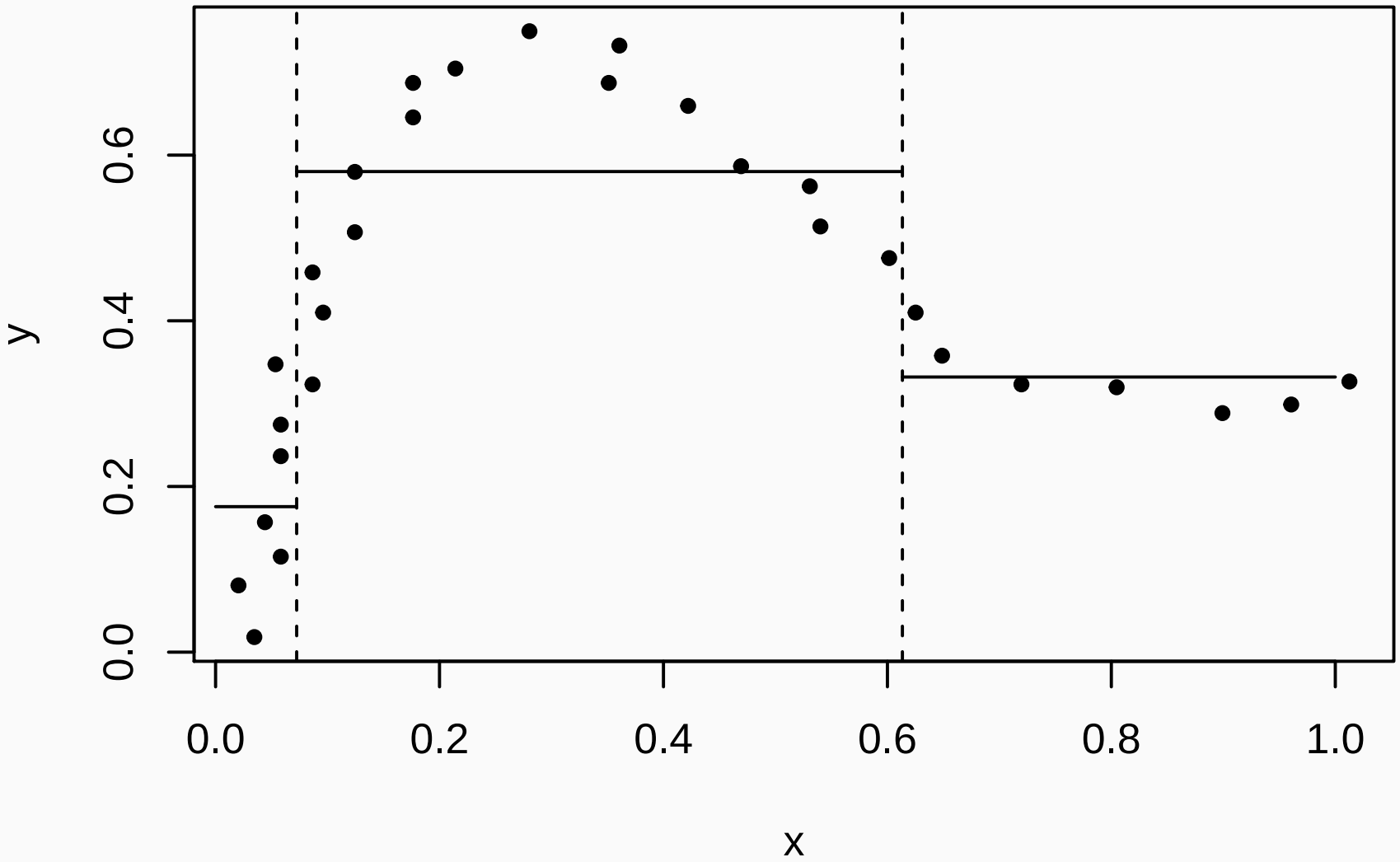
An introductory examples

- If y is quantitative a global approximation of y could be its mean. Or we can use a (regression) function $g(\cdot)$



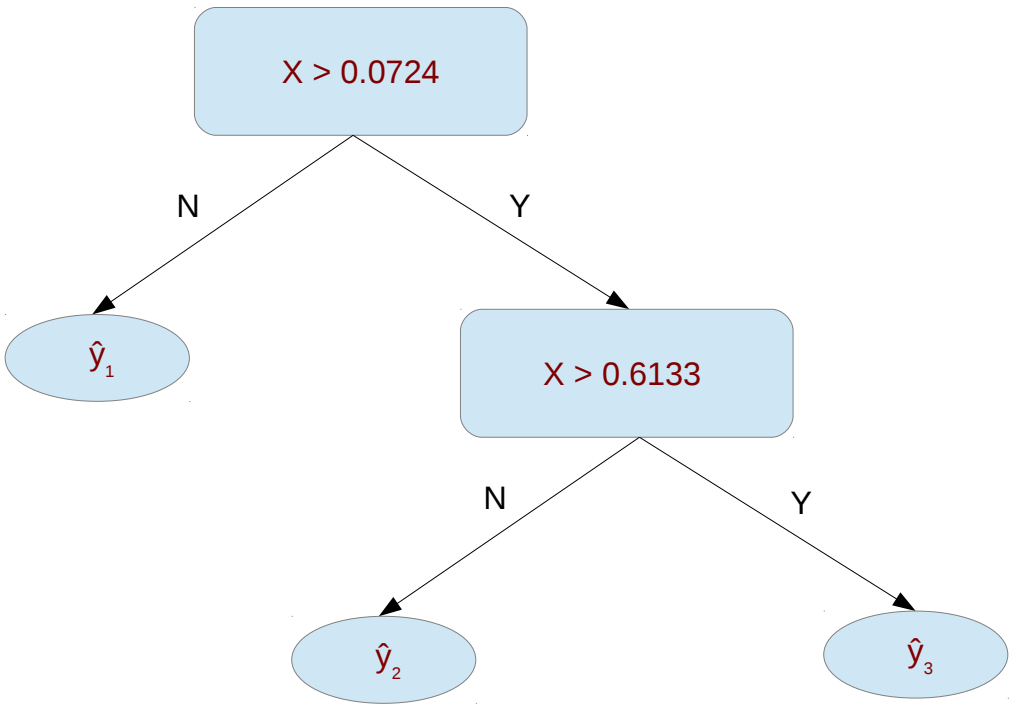
An introductory examples

- Now consider a subdivison on X and approximate y with its local mean $\hat{y}_i$ in the i-th interval and g is a piecewise constant function



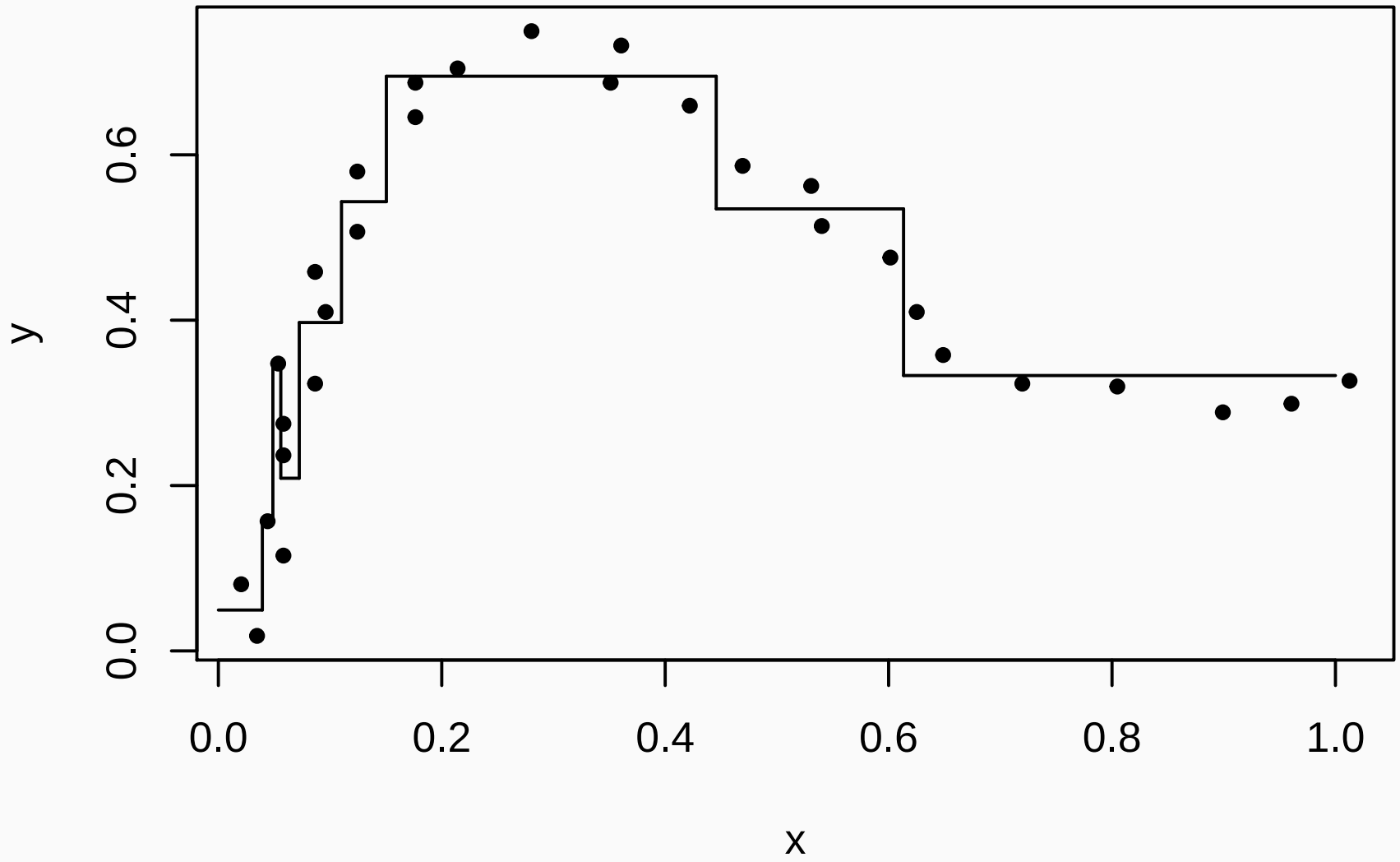
The tree

Note that the value $\hat{y}_i$ of the function g can be also described by the following tree



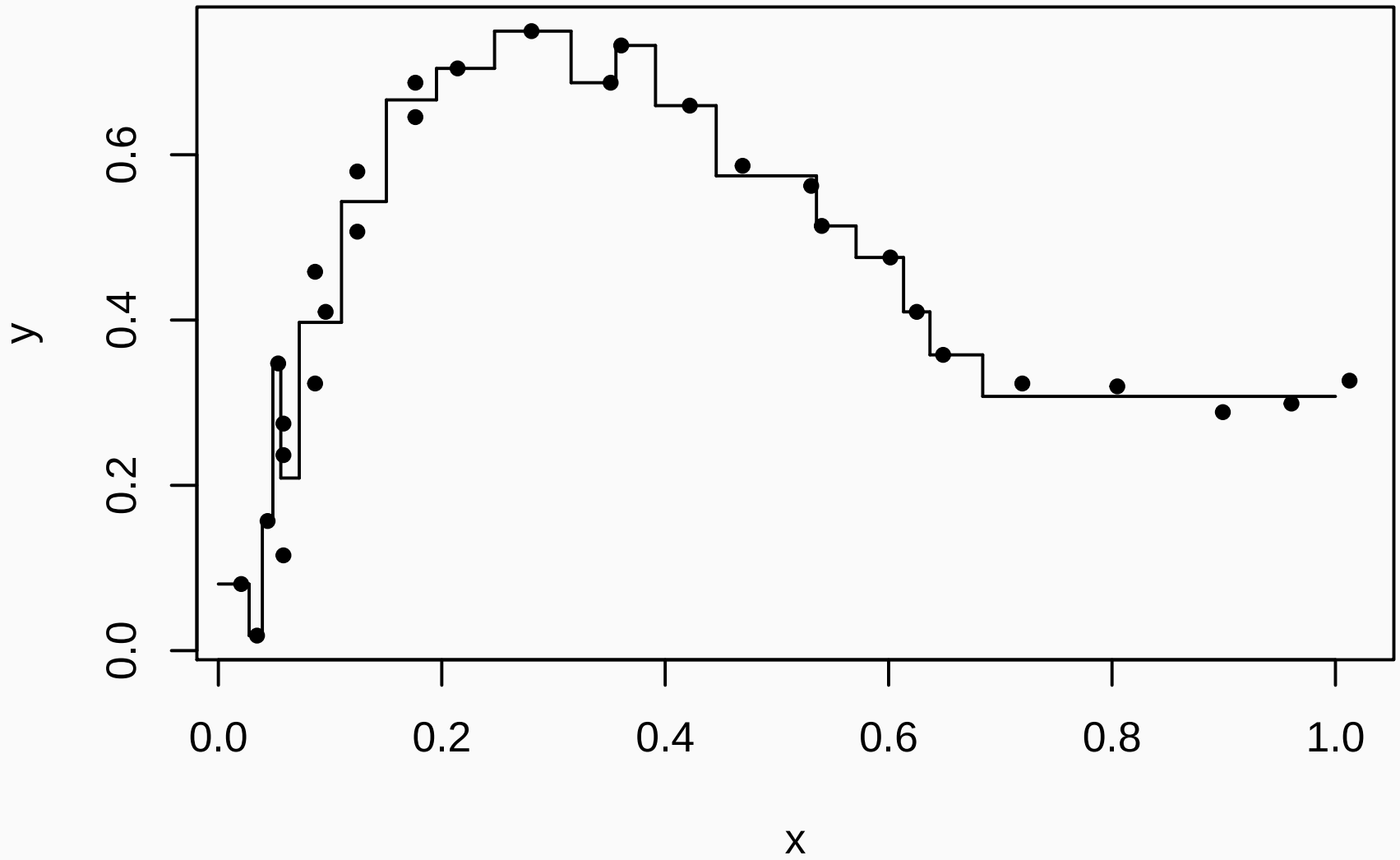
An introductory examples

- As the number of intervals increase, we could achieve a very accurate description of the data



An introductory examples

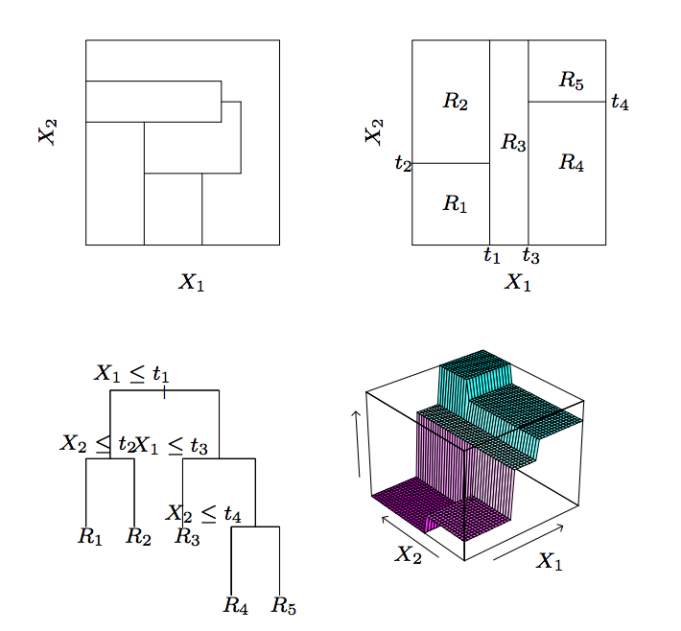
- As the number of intervals increase, we could achieve a very accurate description of the data (leading to overfitting)



Tree approximation

- Let's now consider a regression problem with continuous response Y and two covariates X_1 and X_2. We want to estimate the generic regression curve $E(Y) = f(x_1, x_2)$.
- The idea is again to partition the space spanned by the covariates and to model Y with a different constant in each element of the partition
- we restrict attention to recursive binary partitions.
    - First split the space into two regions, and model the response by the mean of Y in each region.
    - variable and split-point are chosen in order to achieve the best fit.
    - one or both of these regions are split into two more regions,
    - the process is continued, until some stopping rule is applied.

A simple example of tree partitioning for two covariates



In the top right panel first split at $X_1 = t_1$. Then the region $X_1 \leq t_1$ is split at $X_2 = t_2$ and the region $X_1 > t_1$ is split at $X_1 = t_3$. Finally, the region $X_1 > t_3$ is split at $X_2 = t_4$.
The result of such a recursive buinary splitting is a partition into the five regions $R_1, R_2, \ldots, R_5$ shown in the figure.

-The corresponding regression model predicts Y with a constant c_m in region R_m, that is,
$\hat{f}(X_1, X_2) = \sum_{m=1}^{5} c_m I\{(X_1, X_2) \in R_m\}$
- The sets R_m are rectangles, in the 2-dimensional space, with their edges parallel to the coordinate axes) and $c_1, \ldots, c_5$ are constants. Note that the top left panel represents a partition that cannot be obtained by recursive binary splitting

A regression tree

- More generally:
  - we want estimate a regression curve $f(x_1, x_2, \ldots, x_p)$ underlying the data by $\hat{f}(x_1, x_2, \ldots, x_p) = \sum_{m=1}^{M} c_m I\{(x_1, x_2, \ldots, x_p) \in R_m\}$ where $I(x_1, x_2, \ldots, x_p \in R_m)$ is the indicator function of the set R_m (R_m are rectangles, in the p-dimensional sense, with their edges parallel to the coordinate axes) and $c_1, \ldots, c_M$ are constants.
  - Given an objective function such as the Deviance

$$D = \sum_{i=1}^{n} (y_i - \hat{f}(x_{1i}, x_{2i}, \ldots, x_{pi}))^2$$

  - the goal is to define a partition of the space of the covariates that minimizes D

Building the Regression tree

- this minimization, even if we fix the number of the elements of the partition, involves very complex computation
- a sub-optimal approach is considered using a step-by-step optimization: we construct a sequence of gradually more refined approximations and to each of these we minimize the deviance relative to the passage from the current approximation to the previous one
- It is not ensured that we get the global maximum. This procedure is called greedy-algorithm
- This operation is represented by a series of binary splits
- Each internal node represents a value query on one of the variables – *e.g.* "Is $x_3 > 0.4$?". If the answer is 'Yes', go right, else go left.
- The terminal nodes are the decision nodes. Typically each terminal node is assigned a value, c_h, given by the arithmetic mean of the observed y_i having component x_{ji} falling in this node.

Growing the tree

- Trees are grown using a random subset of the available data (*the training data*), by recursive splitting
- A terminal node g is split into the left and right daughters (g_L and g_R) that increase the split criterion

$$D_g - D_{g_L} - D_{g_R}$$

  the most, where D is the deviance associated to a given node.
- To avoid the overfitting, a large tree T_0 is grown and then pruned backward
- Indeed a tree with n leaves is equivalent to a polynomial regression of degree $n - 1$
- detection of the variable X_j that achieve the best split at each node and which is the split point can be done very quickly and hence by scanning through all of the inputs
- Deviance can be adapted for dealing with a response that is a count or a duration

Pruning the tree

- Pruning criterion: cost of a subtree $T \in T_0$, is defined by

$$C_\alpha(J) = \sum_{j=1}^{J} D_j + \alpha_j$$

- Here the sum is over the terminal nodes of T, J is the number of terminal nodes in T and α is a cost-complexity parameter
- The choice of an optimal size is evaluated by cross-validation, or on a validation set.
- For each α the best subtree T_α is found via weakest link pruning
- Larger α gives smaller trees
- A best value $\hat{\alpha}$ is estimated via cross-validation (or on a validation set)
- Final chosen tree is $T_{\hat{\alpha}}$
- New observations are classified by passing their x down to a terminal node of the tree, and then using the relative c_h .

An example

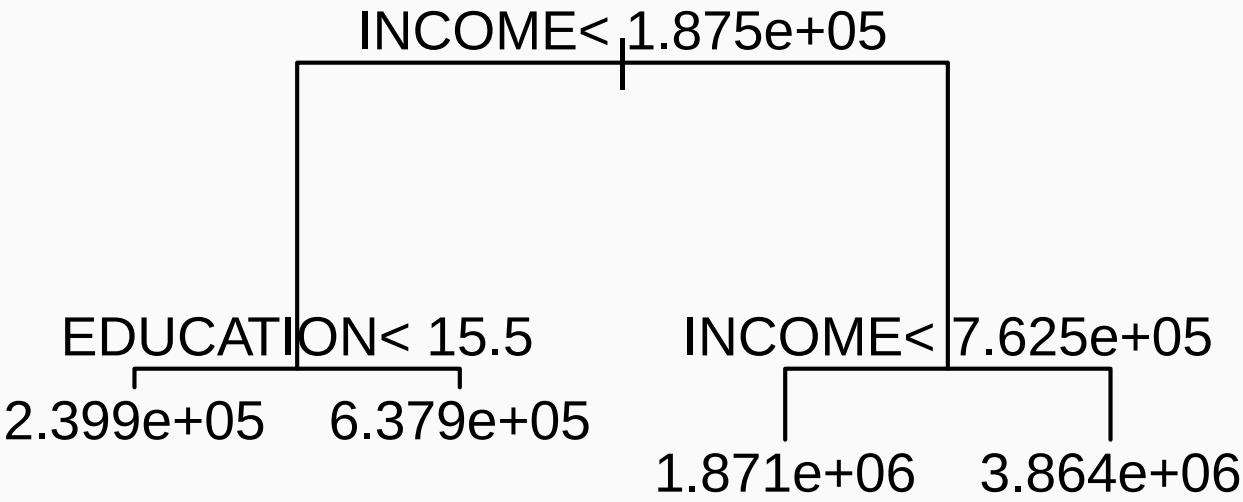
The variable FACE refer to the amount of life insurance bought by the head of a household. We want to predict it by using "INCOME", number of household members, AGE, Education, etc. For illustration, a tree with maximum depth=2 is considered. Package `rpart` is used.

```
TL <- read.csv("TL.csv", header=TRUE, sep=",", row.names=1)
library(rpart)
attach(TL)
```

```
m2 <- rpart(FACE~INCOME+MARSTAT+NUMHH+EDUCATION+AGE,
            control=rpart.control(maxdepth=2))
m2
```

```
## n= 275
##
## node), split, n, deviance, yval
##       * denotes terminal node
##
## 1) root 275 7.681561e+14  747581.5
##   2) INCOME< 187500 227 2.629158e+14  413511.5
##     4) EDUCATION< 15.5 128 1.075360e+14  239930.5 *
##     5) EDUCATION>=15.5 99 1.465367e+14  637939.4 *
##   3) INCOME>=187500 48 3.600986e+14 2327454.0
##     6) INCOME< 762500 37 1.905974e+14 1870751.0 *
##     7) INCOME>=762500 11 1.358255e+14 3863636.0 *
```

The tree


INCOME< 1.875e+05
EDUCATION< 15.5
INCOME< 7.625e+05
2.399e+05
6.379e+05
1.871e+06
3.864e+06

Regression trees: Advantages

- Logical simplicity and ease of ‘communication’ (particularly those with a non-quantitative background)
- The step function has a simple, compact mathematical formulation in terms of information to be stored
- Speed of computation and can take advantage of parallel calculation
- Can handle huge datasets
- Can handle mixed predictors: quantitative and factors
- Easy ignore redundant variables and automatically detects interactions among variables
- Handle missing data elegantly
- Small trees are easy to interpret

Regression trees: Disadvantages

- Instability of results: very sensitive to the insertion/changes in the sample
- Difficulty in upgrading: if more data arrive, they cannot be added to the already constructed tree; it is necessary to start again from the beginning.
- Difficulty of approximating some mathematically simple functions, particularly if they are steep,
- Statistical inference: formal procedures of statistical inference such as hypothesis testing, confidence intervals, and others are not available.
- (over?) emphasizes interactions
- large trees are hard to interpret
- prediction surface is not smooth

Dealing with missing data

- It is quite common to have observations with missing values for one or more input features. The usual approach in statistics is to impute (fill-in) the missing values in some way.
- However, the first issue in dealing with missing data is whether the missing data introduce a sample selection that can bias results of analyses.
- It is important consider if missing data arise by a
  - Missing Completely at Random (MCAR) mechanism *(no bias)*
  - Missing at Random (MAR) mechanism *(possible bias if the dependence on missingness on some observed covariates are not recognized)*
  - Missing Not at Random (MNAR) mechanism *(huge problems, likely to have non negligible bias)*
- For the first, and possibly, the second case, in regression trees two approaches can be used when predictors have missing values:
  - if it is categorical, add a specific category for missing values
  - if it is continuous, use surrogate predictors to be used when observation is missing on the primary predictor.

Classification Trees

Classification Trees

- If the target (response) variable is a categorical variable taking values $1, 2, \ldots, K$, the only changes needed in the tree algorithm pertain to the criteria for splitting nodes and possibly pruning the tree.
- In these cases the tree will be used for predicting the categorical response and this is labeled as a **classification problem**. And the tree is then a **Classification tree**.
- Also in this case a tree is a hierarchical structure formed by:
    - root: the predictor space
    - nodes:
        1. internal: test an explanatory variable (and splits the predictor space)
        2. terminal (leaf): assign a label class
    - branches: corresponds to values of the explanatory variables
- A tree is constructed by repeated splits of the predictor space (root) into subregions (nodes). Each terminal region is associated with a prediction and their union form a partition of the predictor space.

Growing a classification tree

The following elements are needed

- A set of splits
- A goodness of split criterion
- A stop-splitting rule
- A rule for assigning every terminal node to a class
- Each split depends on the value of a single predictor x_j and depends on the nature of x_j:
  - qualitative, with values in $\mathcal{L} = \{l_1, \ldots, l_K\}$: a split is any question as "is $x_j \in S_{\mathcal{L}}$?" with $S_{\mathcal{L}}$ a subset of $\mathcal{L}$;
  - quantitative, with range (a, b): a split is any question as "is $x_j \leq s$?" with $a \leq s < b$
- Examples
  - "Is the age of the subject not greater than 60?"
  - "Is the weather cloudy or rainy?"
- At each step of the tree growing procedure, the best split is identified for each predictor and, among these, the best of the best is selected.

The goodness of split criterion

- The objective of classification tree construction is to finally obtain nodes that are as **pure** as possible, i.e., the split should send towards each branch observations of the same class
- It makes sense to consider good a split when it leads to a high **reduction of impurity** of the node (a high increase of the prediction/classification accuracy).
- Consider a node t for a two class classification problem, the two calsses of y have frequency $p(t)$ and $1 - p(t)$. A natural **impurity measure** of a node t is, the so called Misclassification error:

$$i(t) = 1 - max(p(t), (1 - p(t))$$

- If the node is equipped with a split sending a proportion of p_L and p_R to the left and, respectively right, the gained reduction of impurity is:

$$\Delta i(t) = i(t) - p_L i(t_L) - p_R i(t_R)$$

- The best split is the split which maximizes the reduction of impurity
- Other measures of impurity could be used (Gini or Entropy based)

Impurity measures

More generally, for a given node m that defines a region R_M with N_M observations, $\hat{p}_{mk}$ is the observed proportion of cases in class k. The observation at the node will be classified in class $k(m)$ that is the class for which $\hat{p}_{mk}$ is larger. The following impurity measures can be defined:

- Misclassification error:

$$\frac{1}{N_M} \sum_{i \in R_m} I(y_i \neq k(m)) = 1 - \hat{p}_{mk(m)}$$

- Gini index (heterogeneity index):

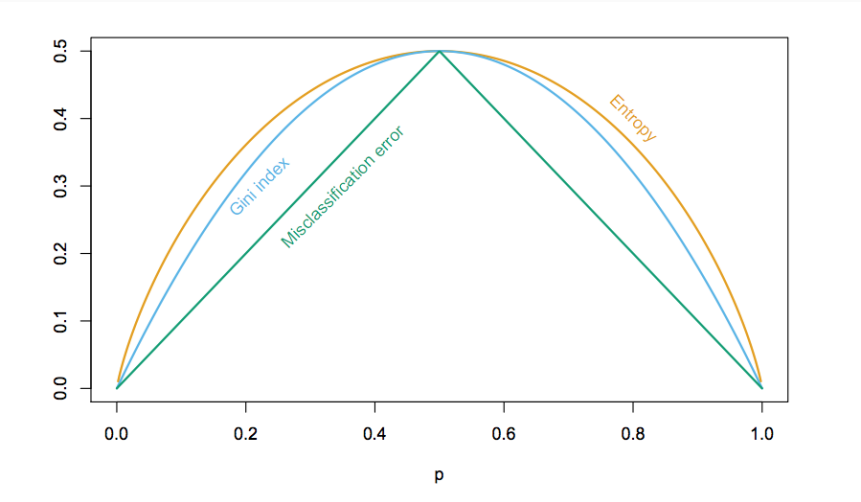
$$G = \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk})$$

- Entropy:

$$H = -\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}$$

Measures of impurity in two class problems

- for $K = 2$, with p the observed proportion in the second class, these three measures are respectively:
  - $1 - \max(p, 1-p)$
  - $2p(1-p) = 2(p - p^2)$
  - $-p\log p - (1-p)\log(1-p)$



Avoiding overfitting

- If the overall accuracy is too low we may always make the tree growing further
- The flexibility of the trees would in principle allow for building a perfect classification rule
- A tree that perfectly fits the sample data probably overfits the data: useless for predicting new data, not used for training the tree!
- A useful practice is to evaluate the accuracy of the estimated tree on a test set (out-of-sample).
- Often for Regression and Classification trees the available data are randomly subdivided into three sets:
    - the training set (to grow the tree)
    - the validation set (to prune it)
    - the test set (to evaluate it)
- Evaluation of the quality of the three can be achieved with usual tools for evaluating the prediction (classification) quality: Mean squared prediction errors, confusion matrices, ROC curves (see the R package 'caret)

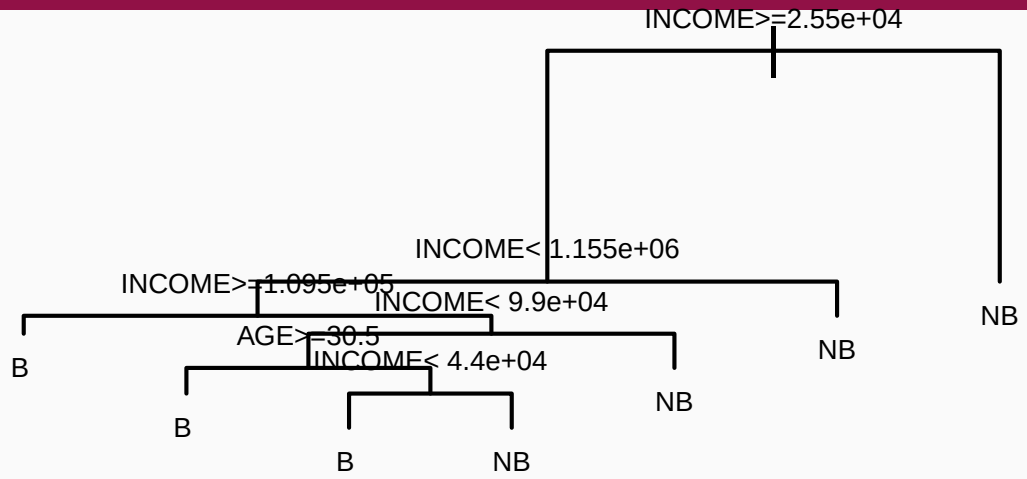
An example of two class tree

We want to predict now if a life insurance policy is bougth using the same covariates

```
TL <- read.csv("TLbin.csv", header=TRUE, sep=",", row.names=1);
attach(TL); set.seed(4321); ind.train <- sample(1:500,300) ;
TL.train <- TL[ind.train,]; TL.test <- TL[-ind.train,]
tree <- rpart(FACEPOS~., data=TL.train); tree
```

```
## n= 300
##
## node), split, n, loss, yval, (yprob)
##       * denotes terminal node
##
##  1) root 300 136 B (0.5466667 0.4533333)
##    2) INCOME>=25500 235  90 B (0.6170213 0.3829787)
##      4) INCOME< 1155000 227  84 B (0.6299559 0.3700441)
##        8) INCOME>=109500 72  19 B (0.7361111 0.2638889) *
##        9) INCOME< 109500 155  65 B (0.5806452 0.4193548)
##         18) INCOME< 99000 145  58 B (0.6000000 0.4000000)
##           36) AGE>=30.5 122  45 B (0.6311475 0.3688525) *
##           37) AGE< 30.5 23  10 NB (0.4347826 0.5652174)
##             74) INCOME< 44000 14   5 B (0.6428571 0.3571429) *
##             75) INCOME>=44000 9   1 NB (0.1111111 0.8888889) *
##         19) INCOME>=99000 10   3 NB (0.3000000 0.7000000) *
##      5) INCOME>=1155000 8   2 NB (0.2500000 0.7500000) *
##    3) INCOME< 25500 65  19 NB (0.2923077 0.7076923) *
```

The tree




```
pred.test <-predict(tree, newdata=TL.test, type="class")
t <-table(TL.test$FACEPOS, pred.test)
t
```

```
##     pred.test
##       B NB
##   B  78 33
##   NB 49 40
```

```
sum(diag(t))/sum(t)
```

```
## [1] 0.59
```

MARS: Multivariate Adaptive Regression Splines

- MARS is an adaptive procedure for regression, and is well suited for high dimensional problems (i.e., a large number of inputs).
- It can be viewed as a generalization of stepwise linear regression or a modification of the CART. This latter approach for regression tree leads to smoother prediction surfaces
- A hybrid of MARS called PolyMARS specifically designed to handle classification problems has been also proposed
- MARS is a semi-parametric method that like CART uses a greedy algorithm and recursively adapt a curve to the regression surface
- At each step it is chosen a couple of basis functions recursively selecting the variable X that is most appropriate and the optimal position of the knot.

MARS

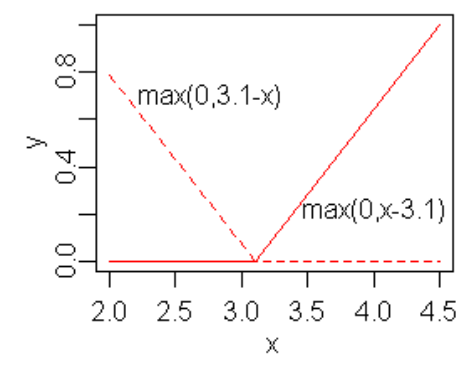
- MARS builds models of the form

$$\hat{f}(x) = \sum_{i=1}^{k} c_i B_i(x)$$

- The model is a weighted sum of basis functions $B_i(x)$. Each c_i is a constant coefficient.
- Each basis function $B_i(x)$ takes one of the following three forms:
  1. a constant
  2. a hinge function. A hinge function has the form $\max(0, x - const)$ or $\max(0, const - x)$.
     MARS automatically selects variables and values of those variables for knots of the hinge functions.
  3. a product of two or more hinge functions. These basis functions can model interaction between two or more variables.

MARS

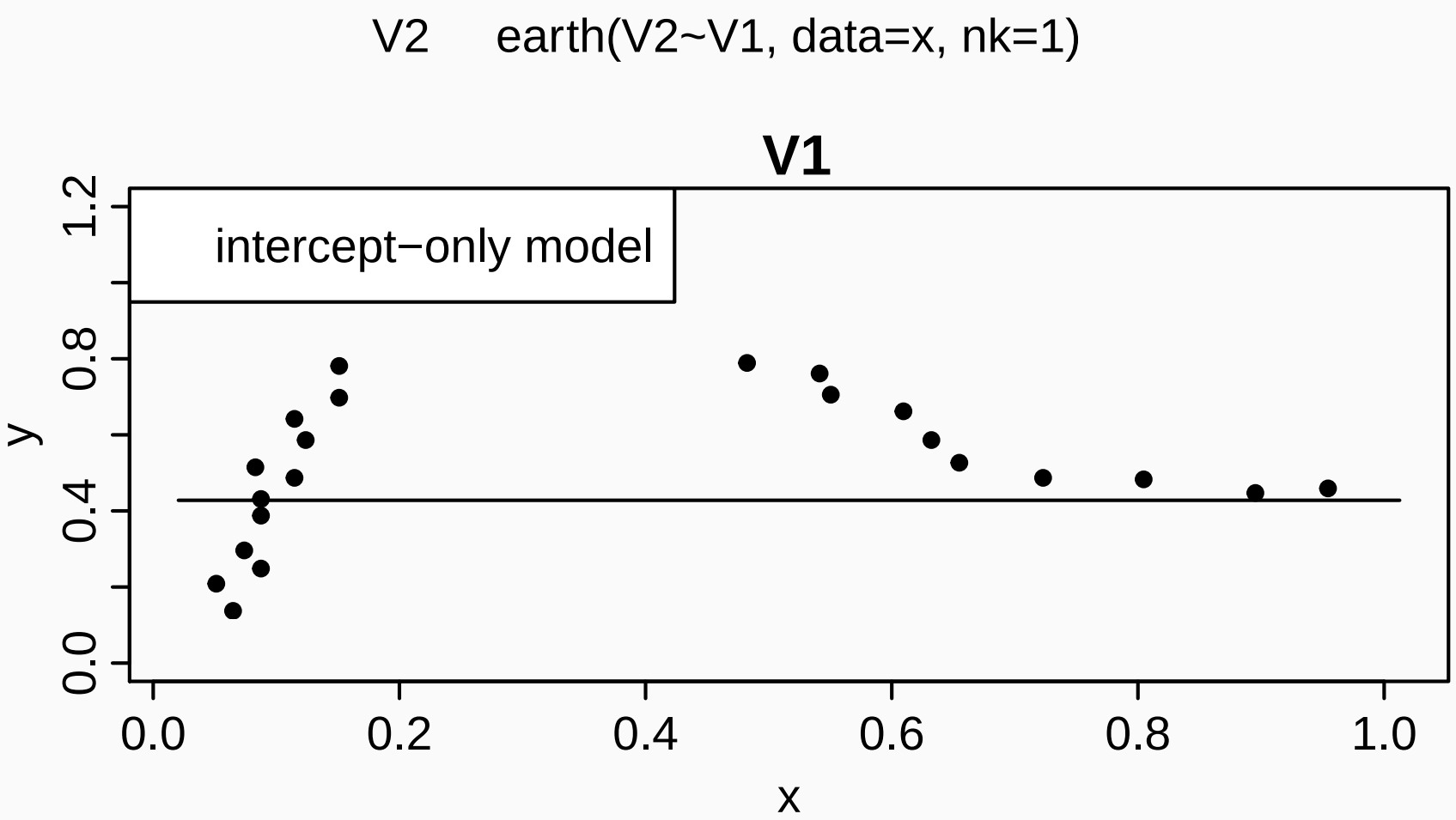
This is an example of a couple of Hinge functions



- Although they might seem quite different, the MARS and CART strategies actually have strong similarities.
- Suppose we take the CART procedure and make the following changes:
  - Replace step functions by the piecewise linear basis functions $I(x - t > 0)$ and $I(x - t \leq 0)$.
  - When a model term is involved in a multiplication by a candidate term, it gets replaced by the interaction, and hence is not available for further interactions.
  - With these changes, the MARS forward procedure is the same as the CART tree-growing algorithm.

An example

```
mod1=earth(V2~V1,data=x,nk=1)
plotmo(mod1,xlab="x",ylab="y", ylim=c(0,1.2)); points(x,pch=20)
```



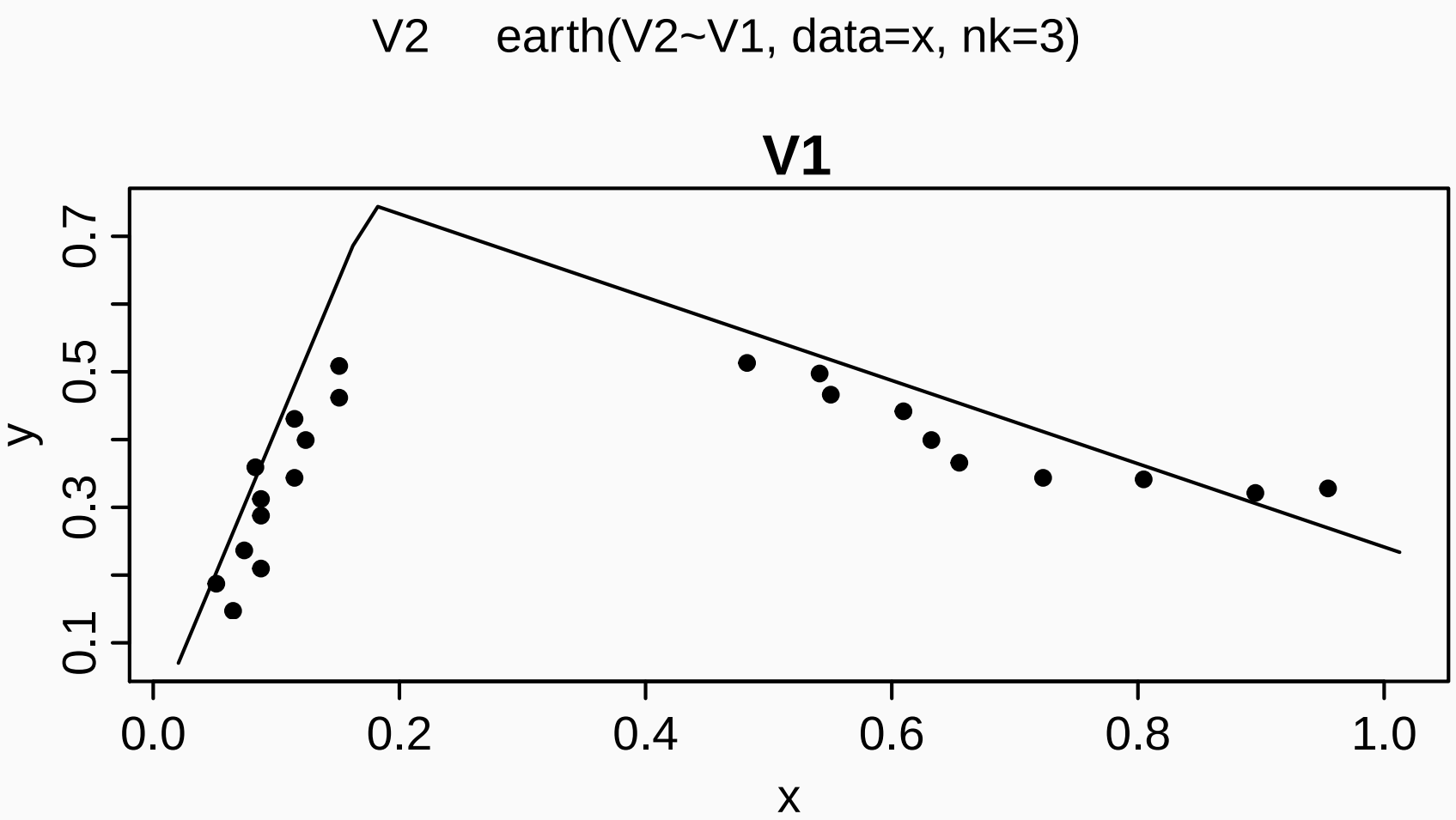
An example

```
summary(mod1)
```

```
## Call: earth(formula=V2~V1, data=x, nk=1)
##
##             coefficients
## (Intercept)    0.4279076
##
## Selected 1 of 1 terms, and 0 of 1 predictors
## Termination condition: Reached nk 1
## Importance: V1-unused
## Number of terms at each degree of interaction: 1 (intercept only model)
## GCV 0.04290529    RSS 1.202778    GRSq 0    RSq 0
```

An example

```
mod2=earth(V2~V1,data=x,nk=3)
plotmo(mod2,xlab="x",ylab="y"); points(x,pch=20)
```



An example

```
summary(mod2)
```

```
## Call: earth(formula=V2~V1, data=x, nk=3)
##
##                coefficients
## (Intercept)       0.7476095
## h(0.176378-V1)   -4.3458394
## h(V1-0.176378)   -0.6146156
##
## Selected 3 of 3 terms, and 1 of 1 predictors
## Termination condition: Reached nk 3
## Importance: V1
## Number of terms at each degree of interaction: 1 2 (additive model)
## GCV 0.00632364    RSS 0.1317425    GRSq 0.852614    RSq 0.8904682
```