Decision trees

E. Scornet

Outline

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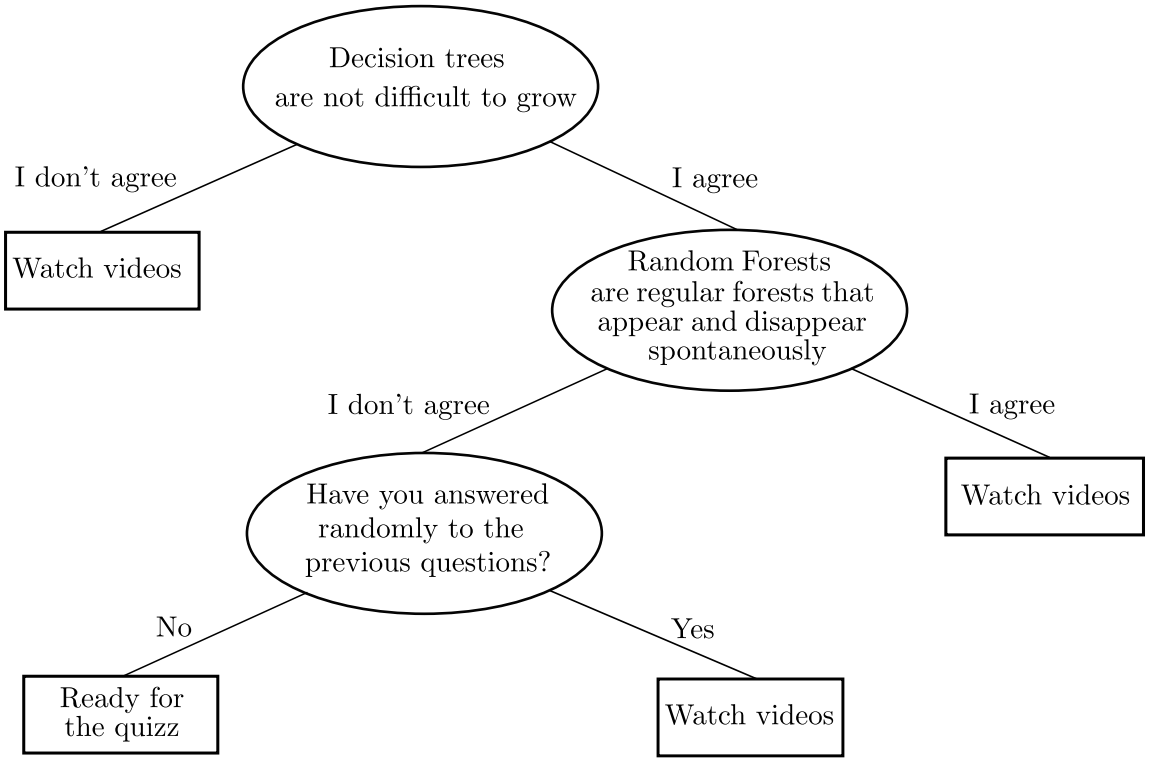
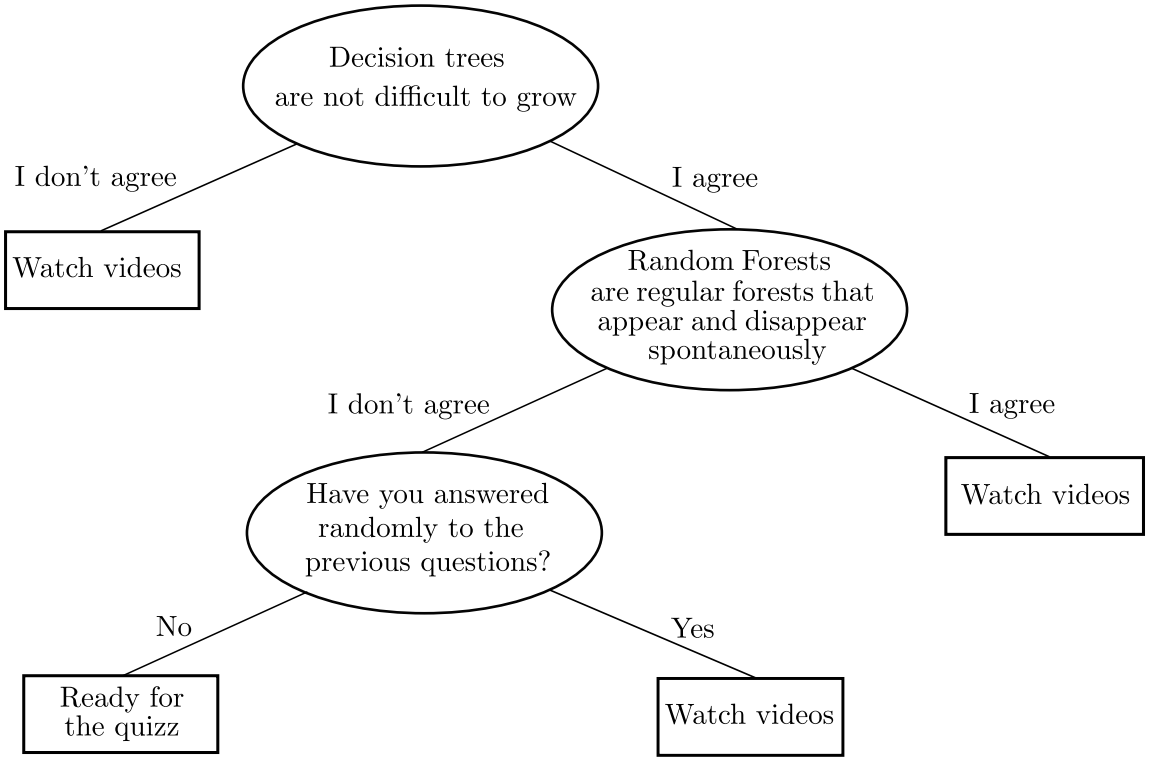


Decision trees

A first example - Should you (re)watch the videos on decision trees?



→ Such a tree comes from common sense or from domain experts.

Decision trees

Can we collect data to automatically create a decision tree, without domain experts?

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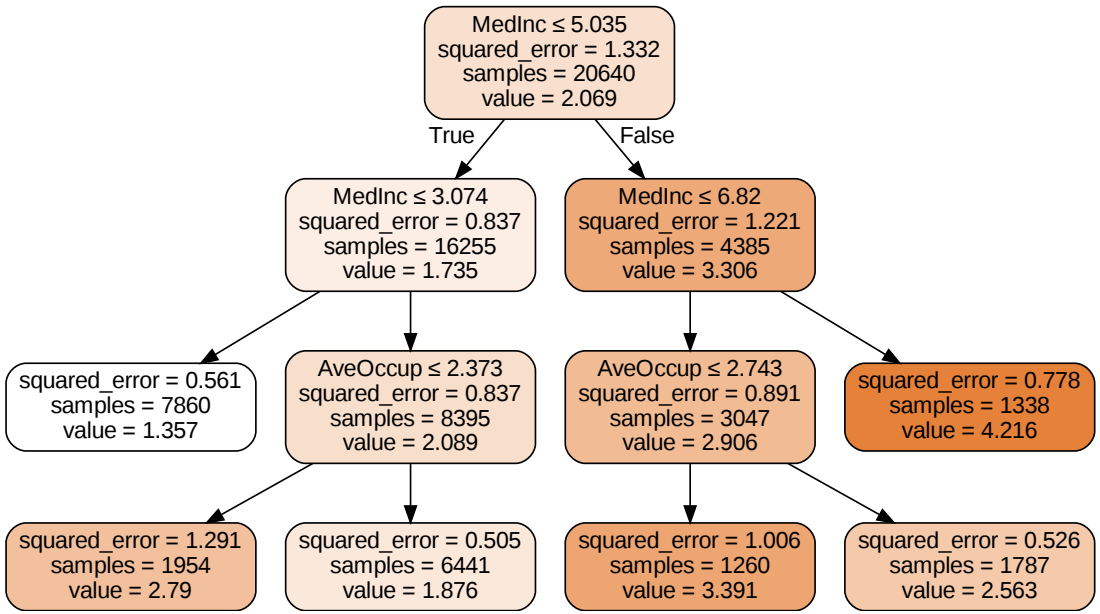
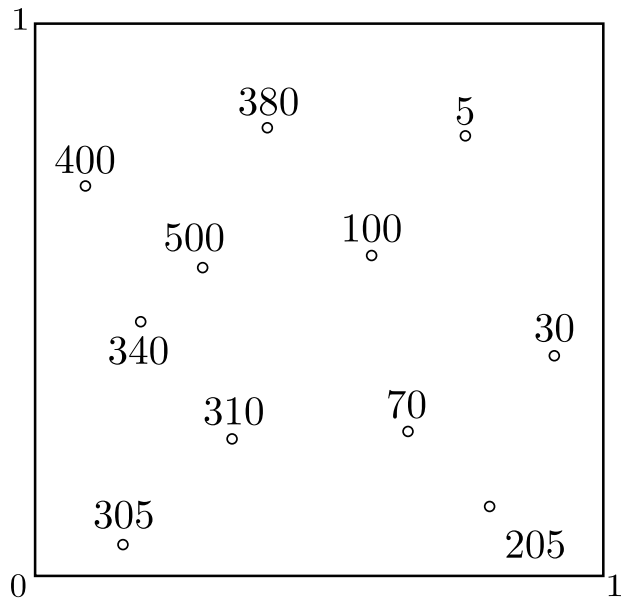


Figure: Output of a decision tree trained on a real-estate data set (1990 California housing data set).

Construction of Decision trees - regression



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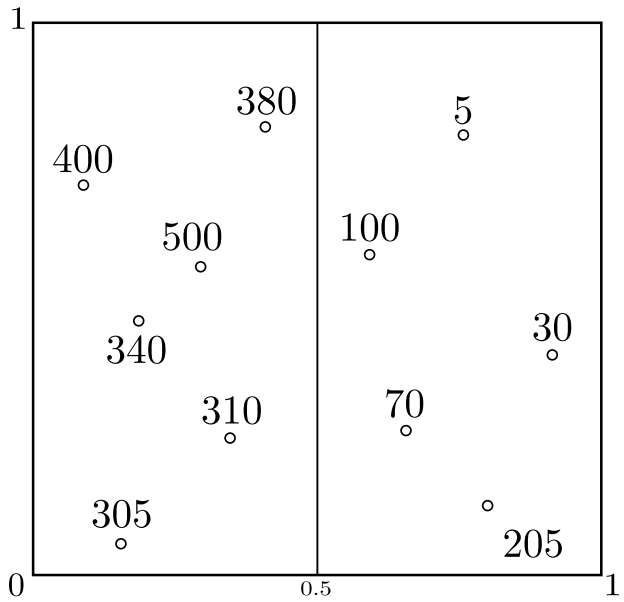

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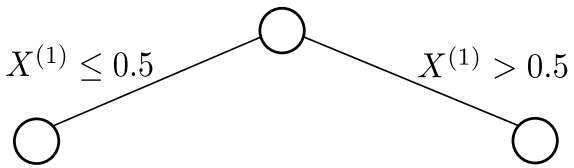

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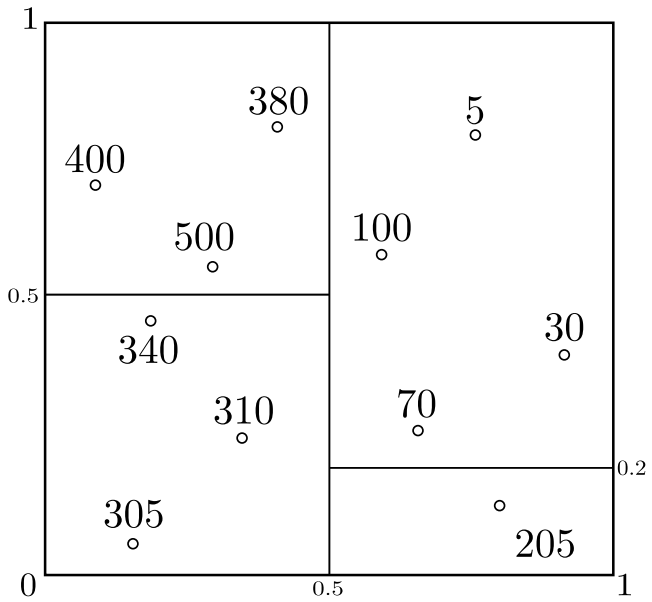

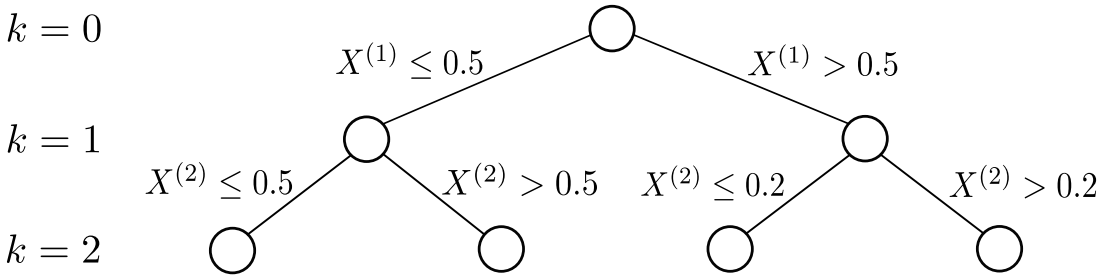

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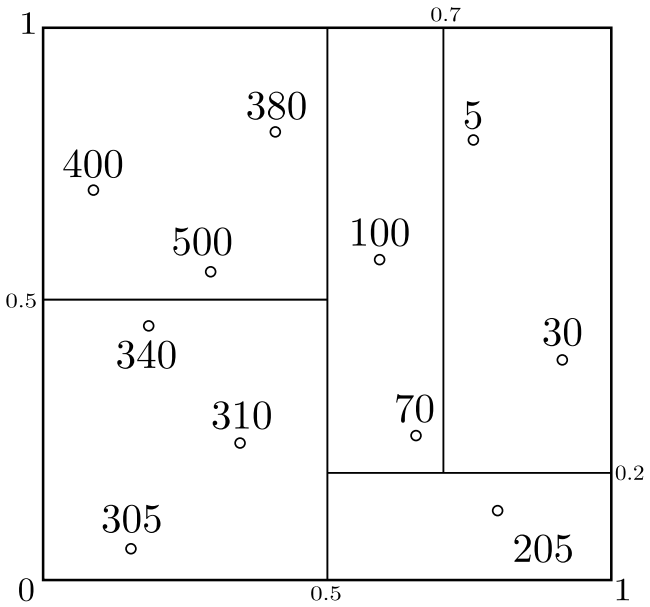

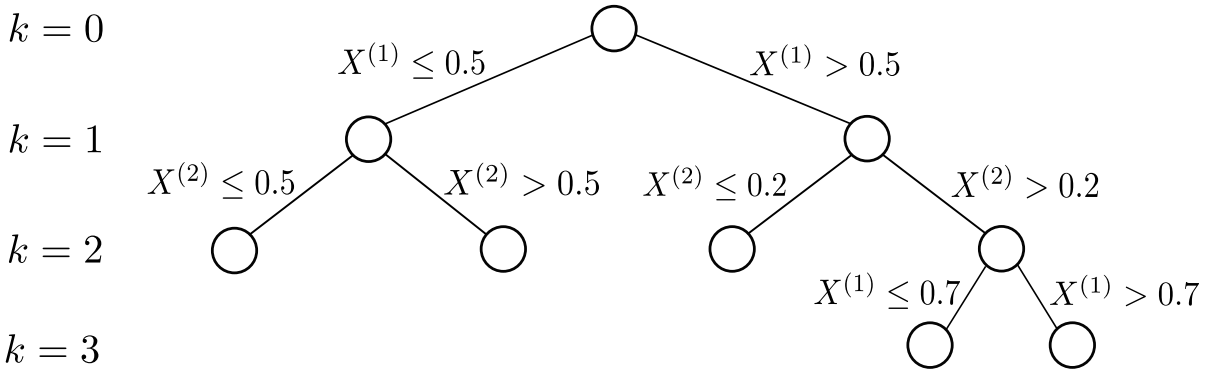

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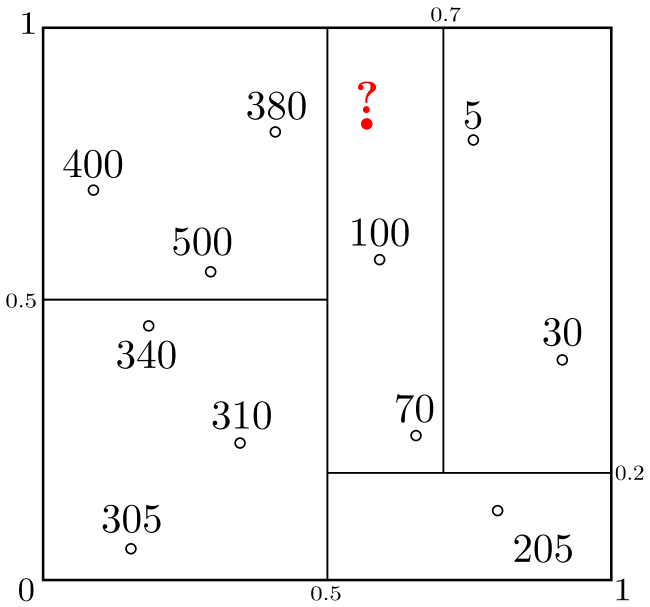

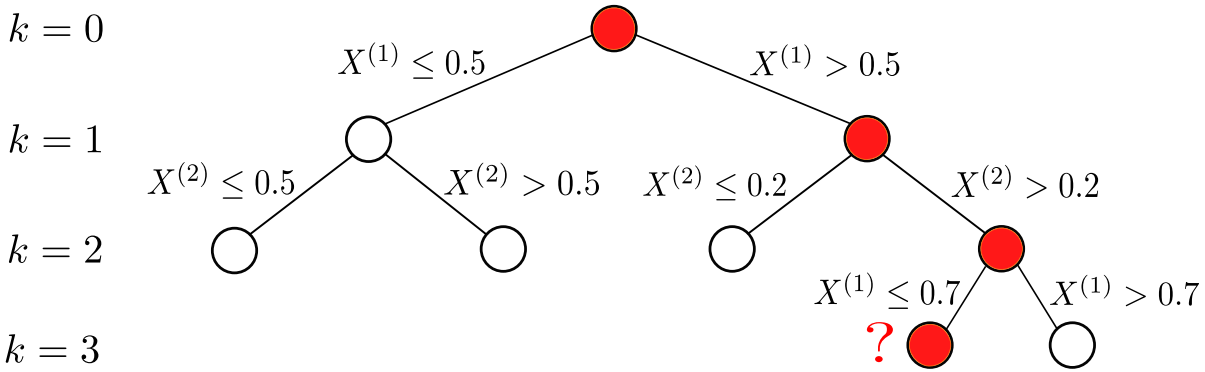

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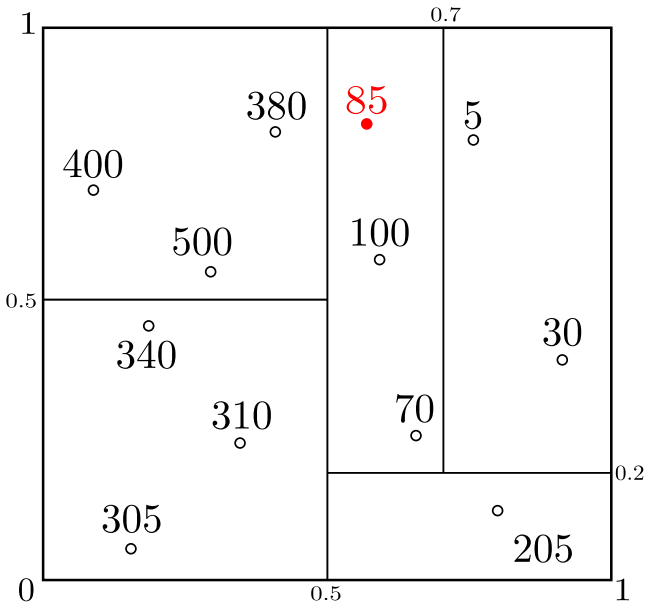

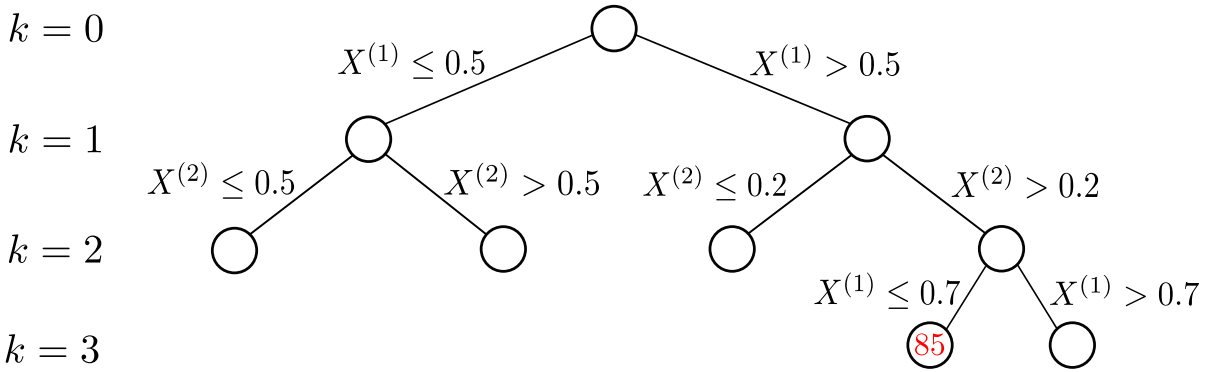

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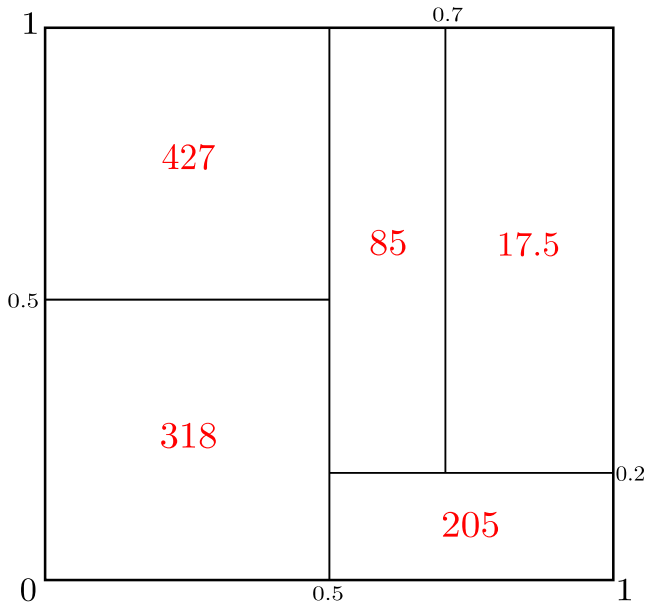

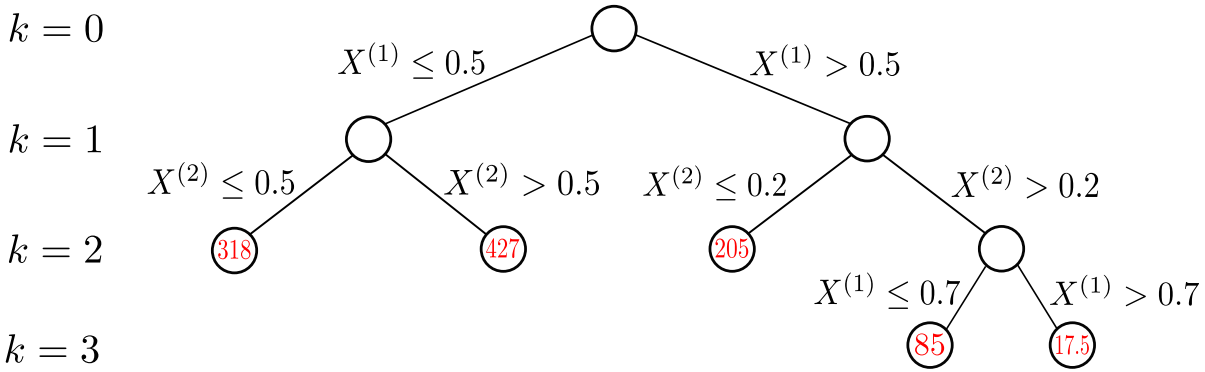

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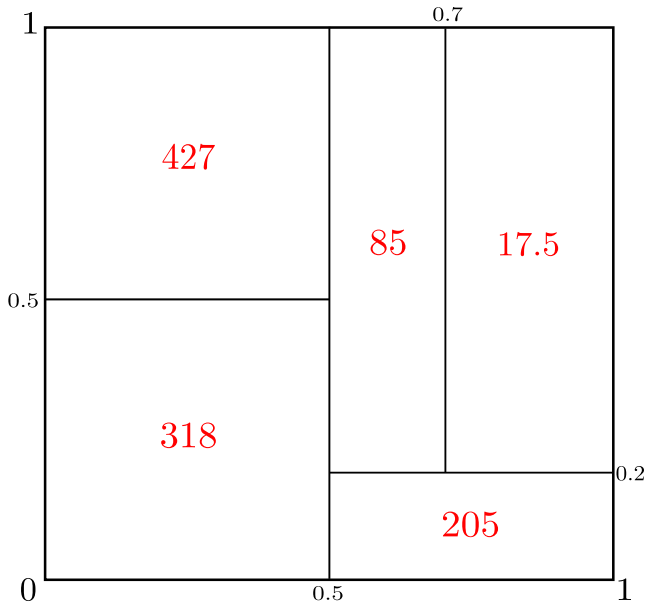
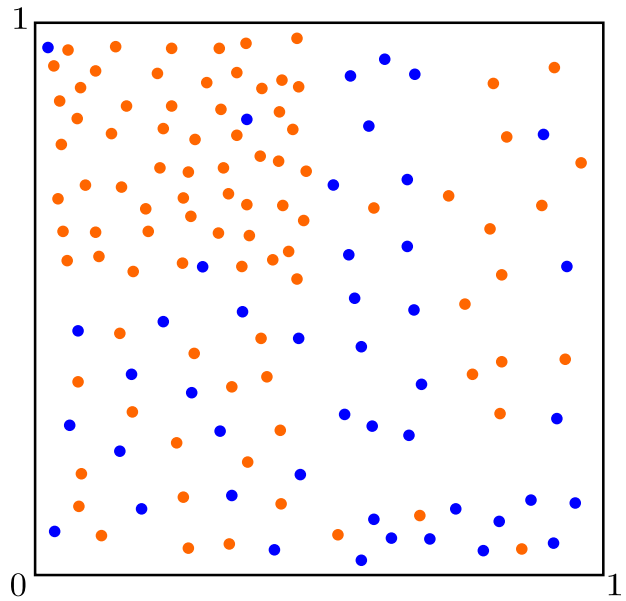


Decision tree building

- Requires a splitting rule
- Requires a stopping rule
- Requires a prediction rule
  $\rightarrow$ Average per leaf

Construction of Decision trees - classification



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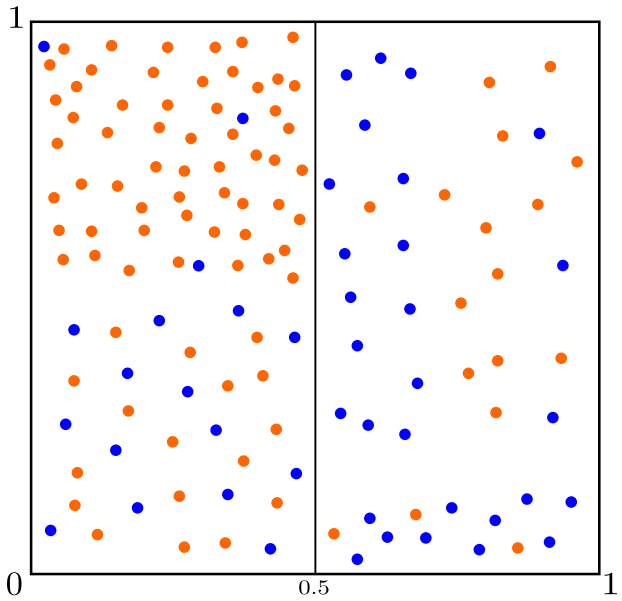

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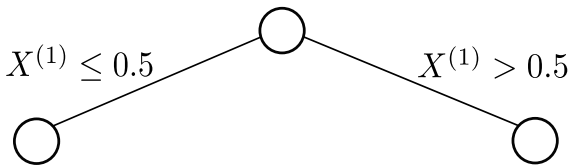

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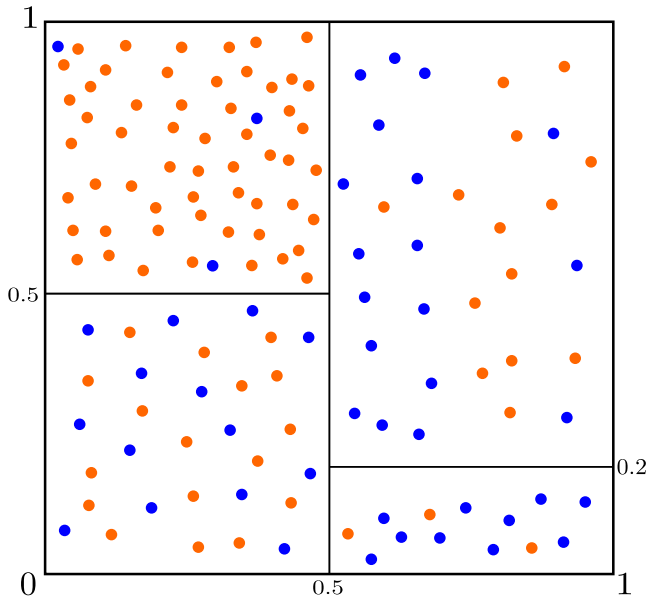

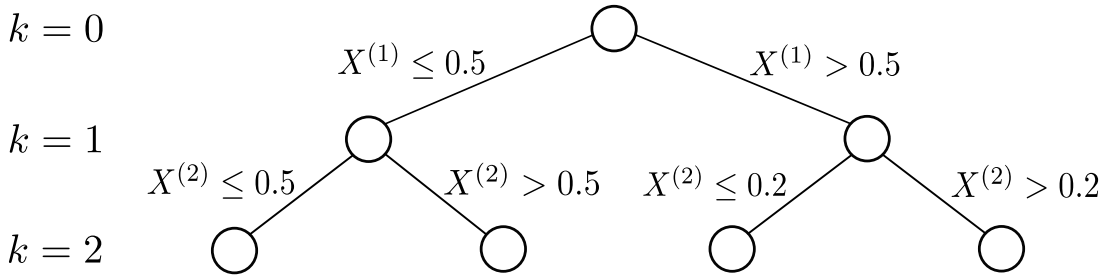

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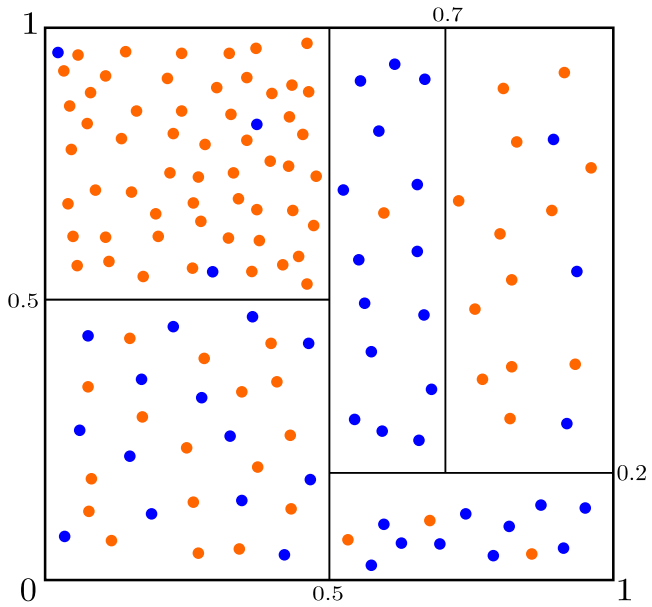

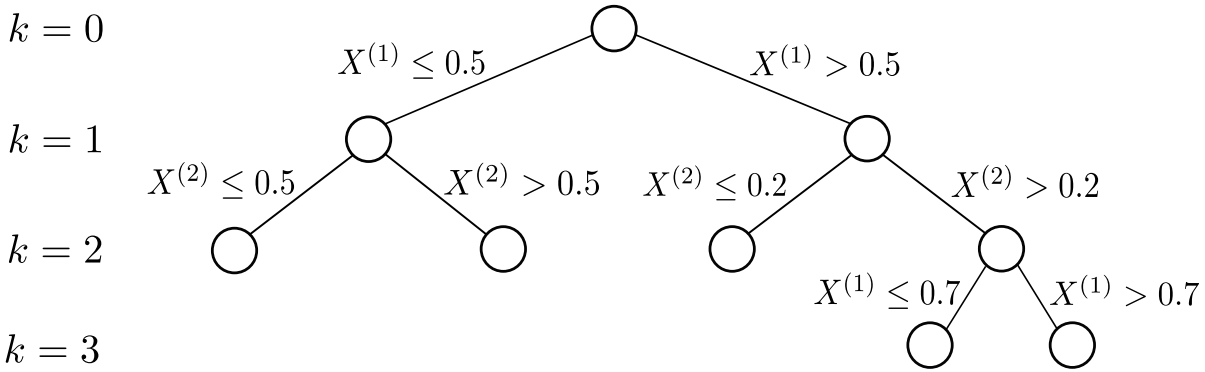

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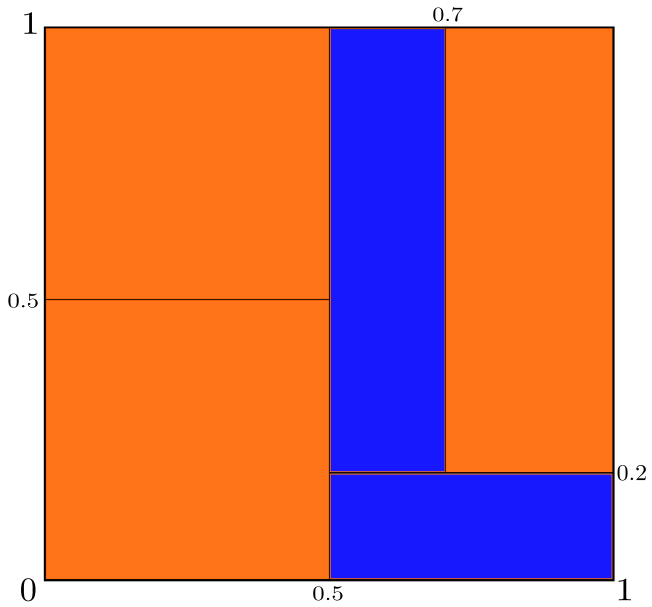

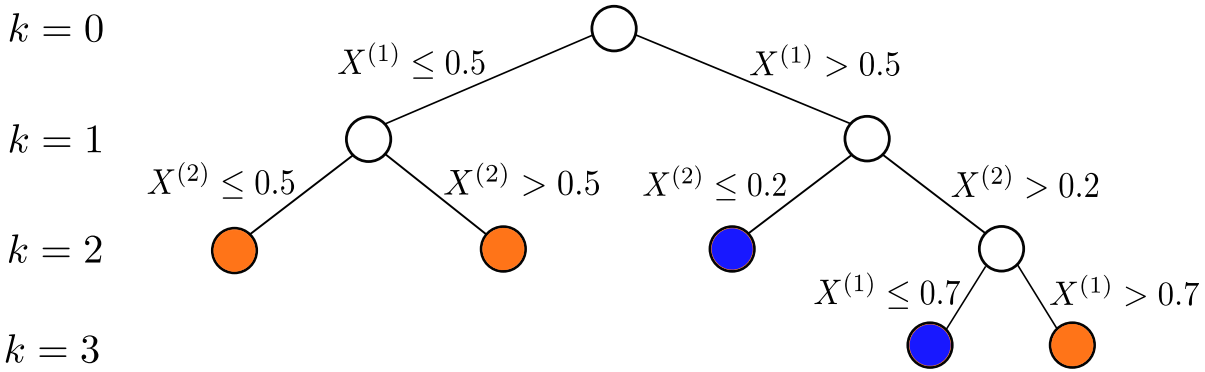

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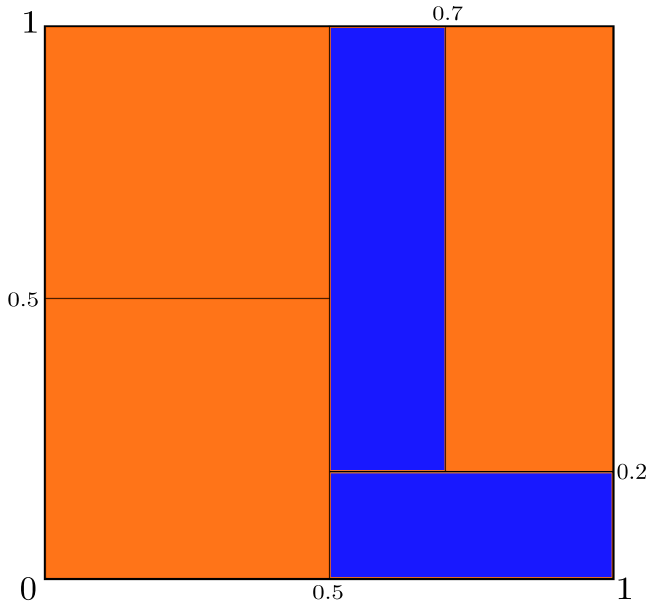

Decision tree building

- Requires a splitting rule
- Requires a stopping rule
- Requires a prediction rule
  $\rightarrow$ Majority vote per leaf

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Splitting criterion

Finding the best split in a cell A requires an impurity criterion Imp. Based on this criterion, one can define the impurity reduction associated to a split (j, s) as

$$\begin{aligned} &\Delta Imp(j, s; A) \\ =&Imp(A) - p_L Imp(A_L) - p_R Imp(A_R), \end{aligned} \tag{1}$$

where p_L (resp. p_R) is the fraction of observations in A that fall into A_L (resp. A_R).

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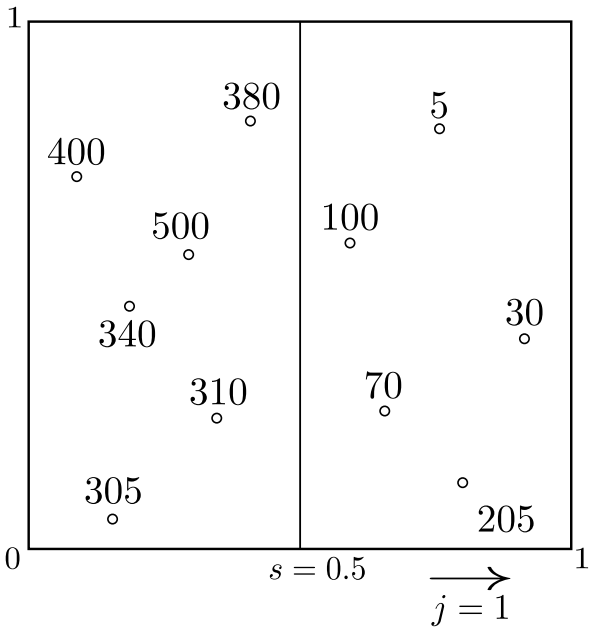

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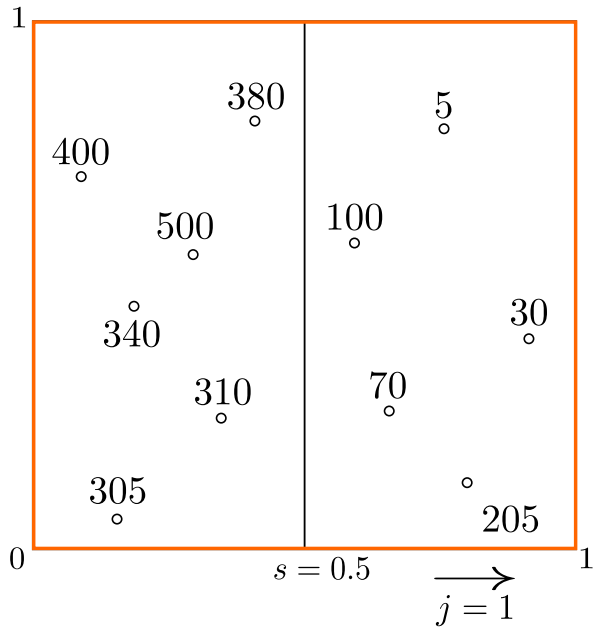

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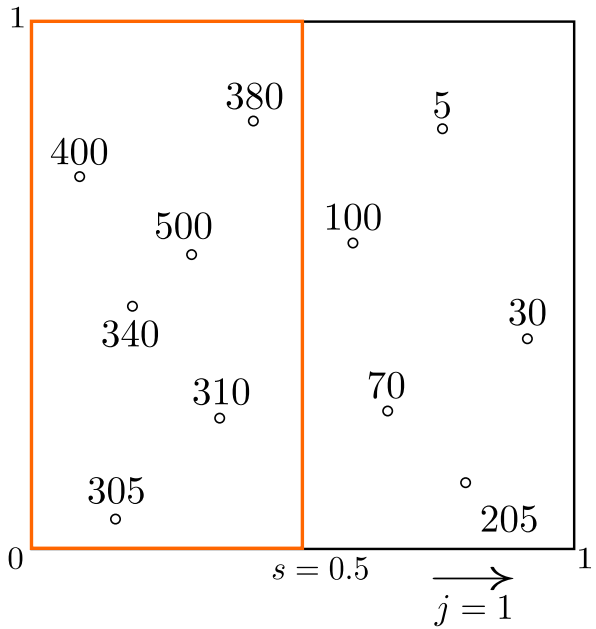

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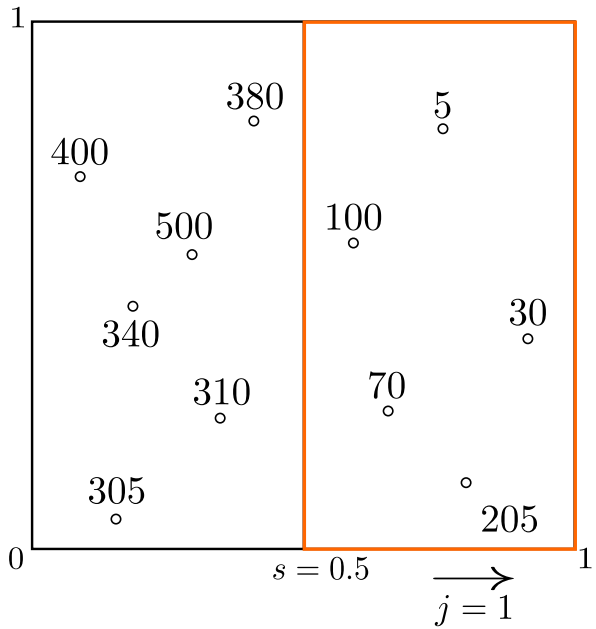

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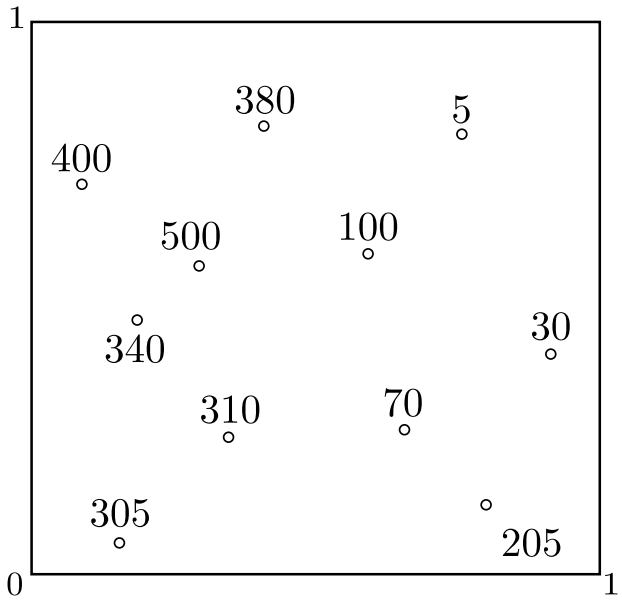
The best split $(j^\star, s^\star)$ is then chosen as

$$(j^\star, s^\star) \in \underset{j,s}{\operatorname{argmax}}\, \Delta Imp(j, s; A). \tag{2}$$

An instance of $Imp(A)$ in regression: the empirical variance of the Y_is in A.

Finding the best split - an example



- Consider splits at the middle of two consecutive observations
- For each split, compute the decrease in impurity between the parent node and the two resulting nodes.

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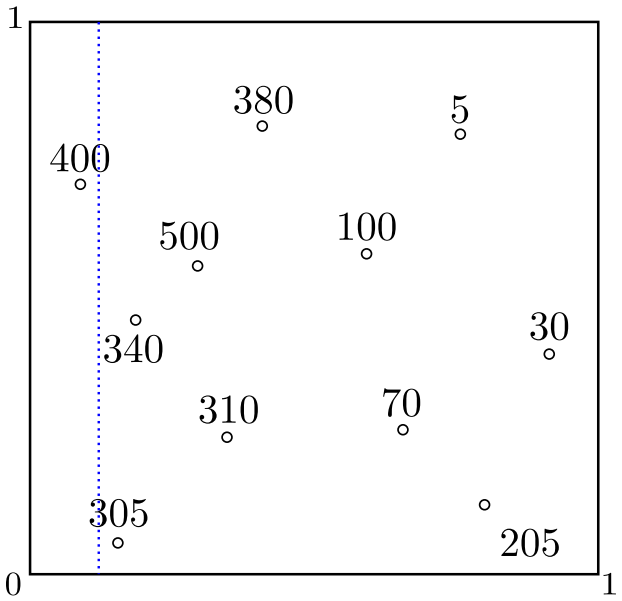

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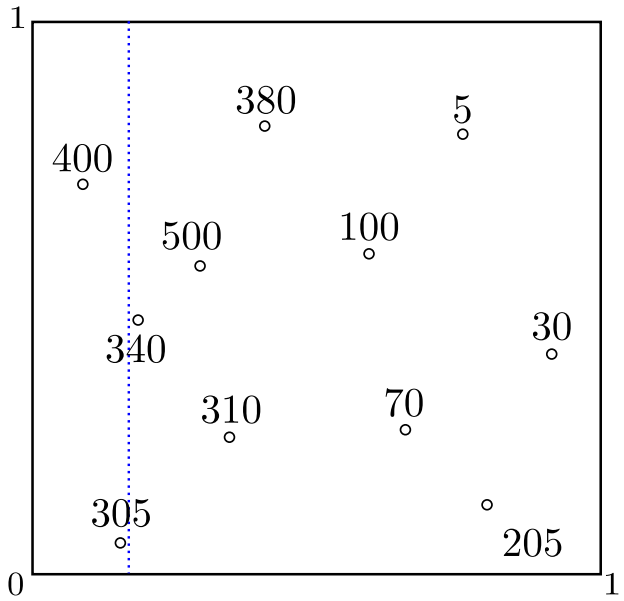

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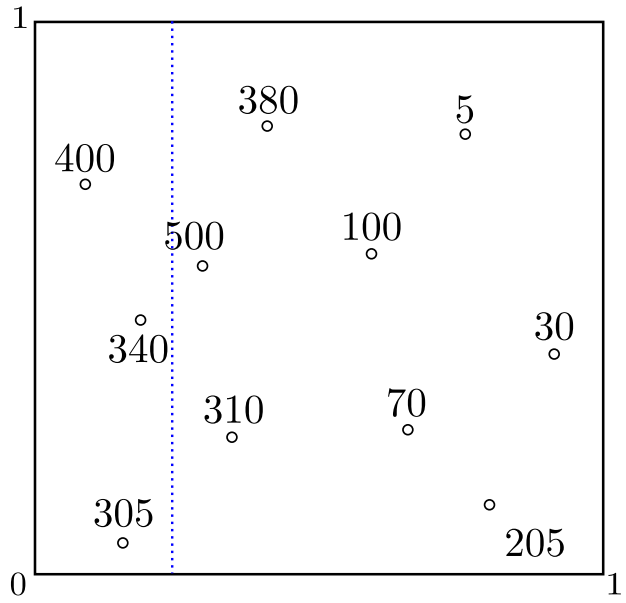

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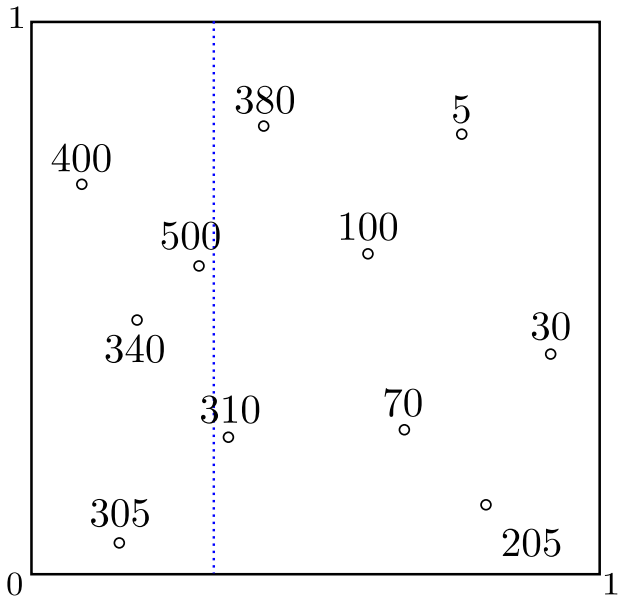

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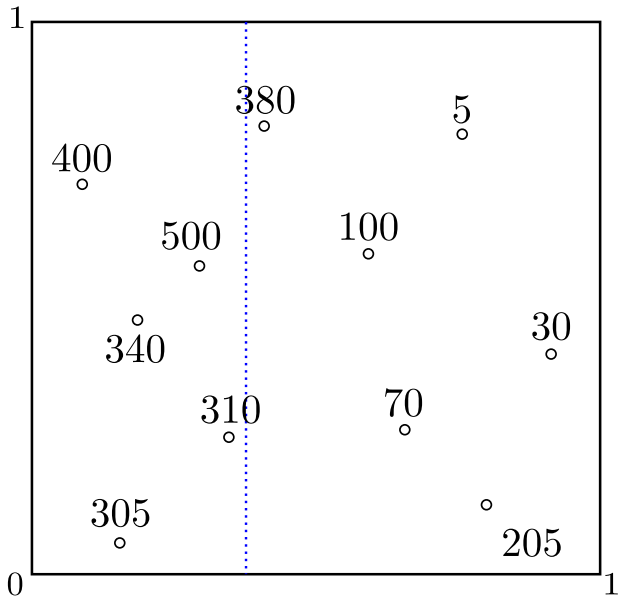

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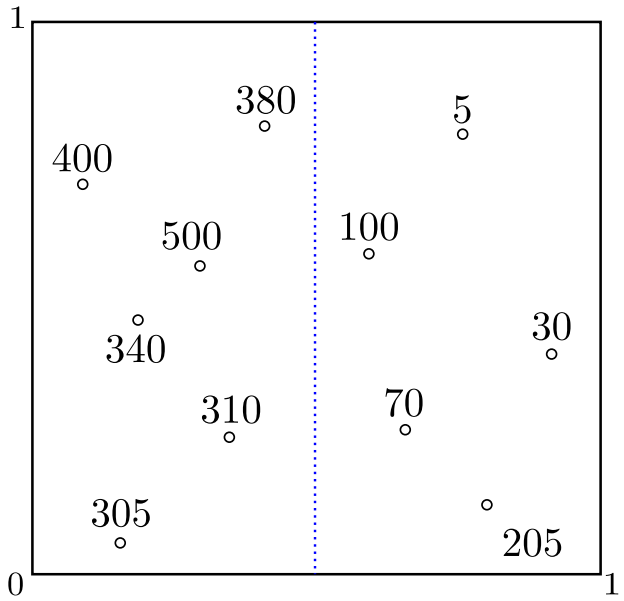

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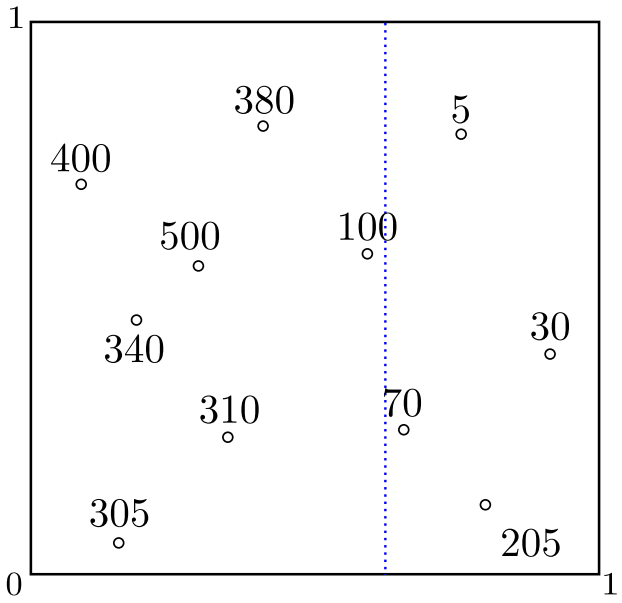

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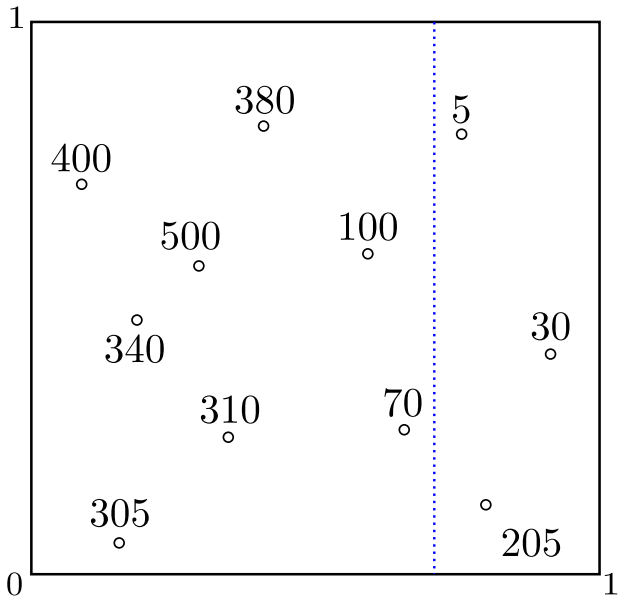

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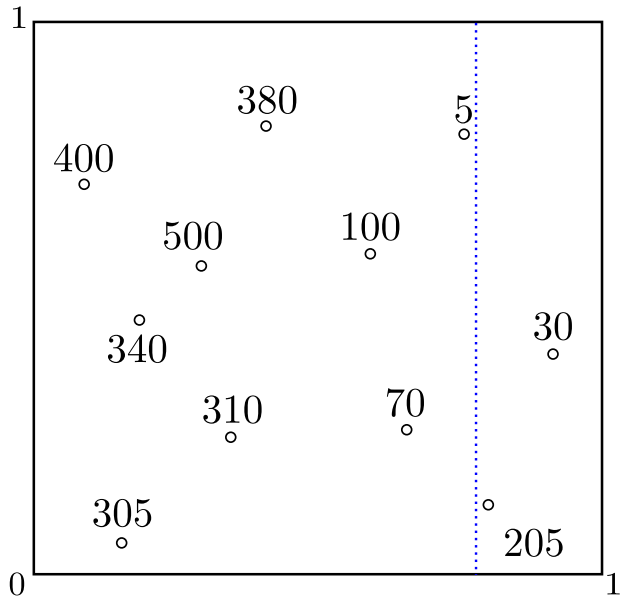

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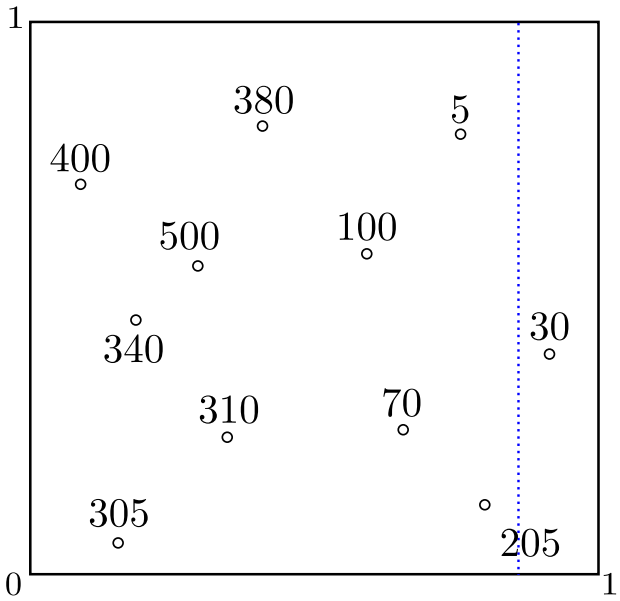

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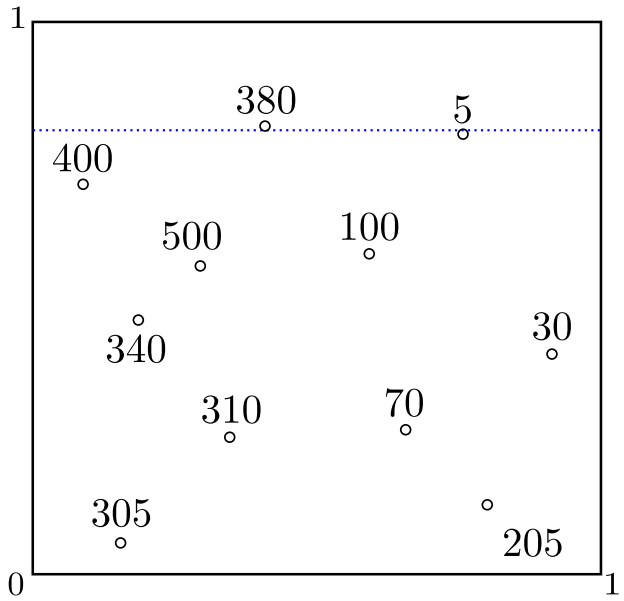

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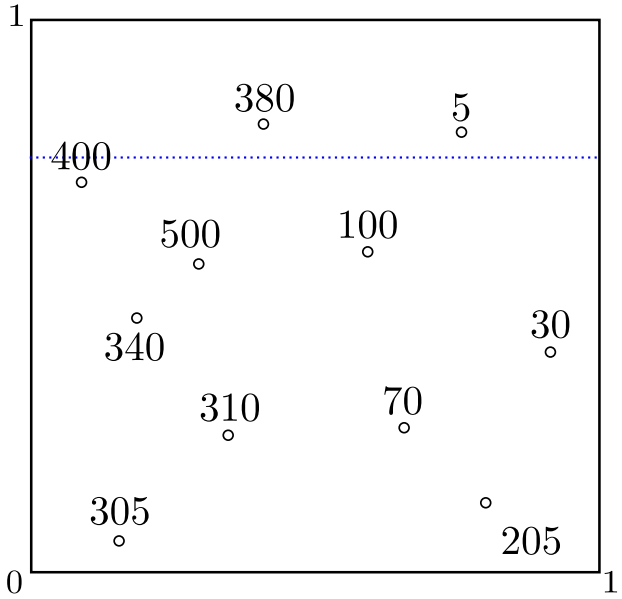

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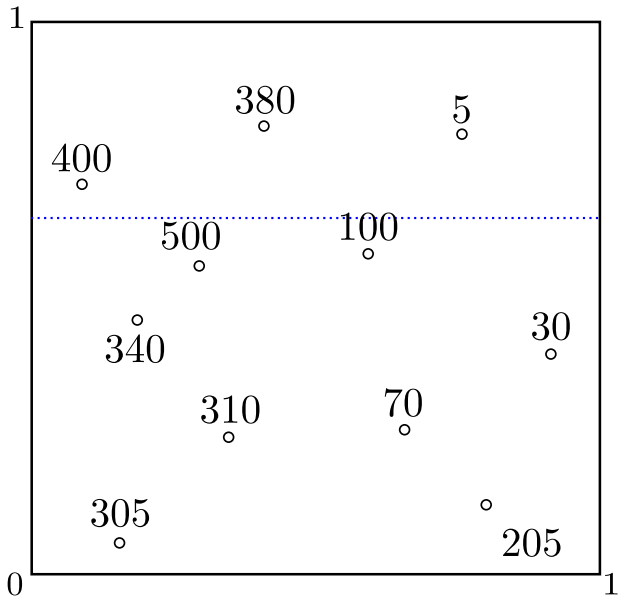

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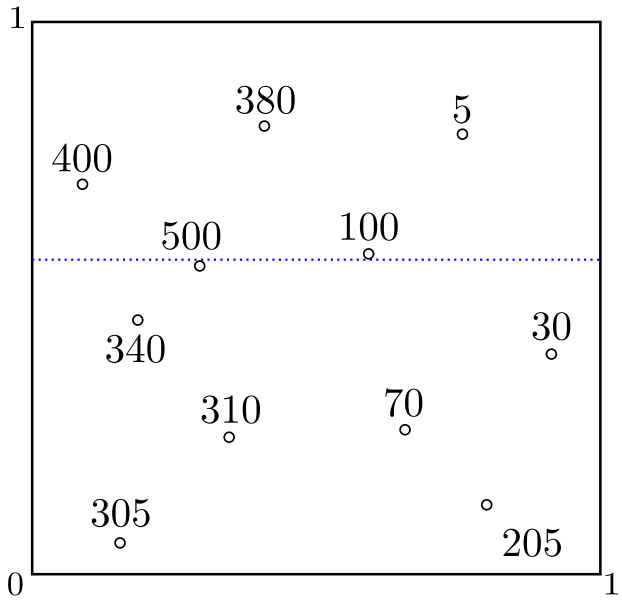

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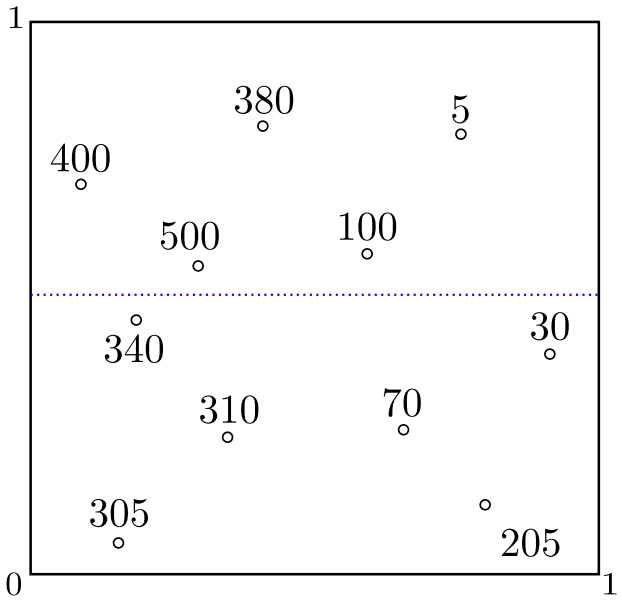

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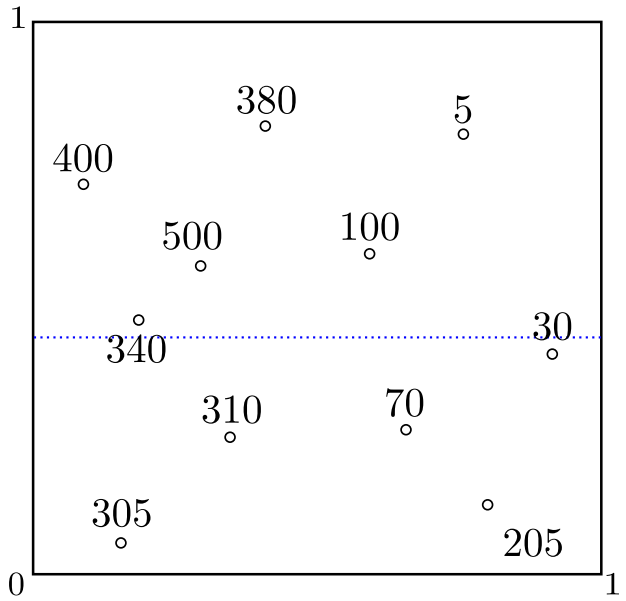

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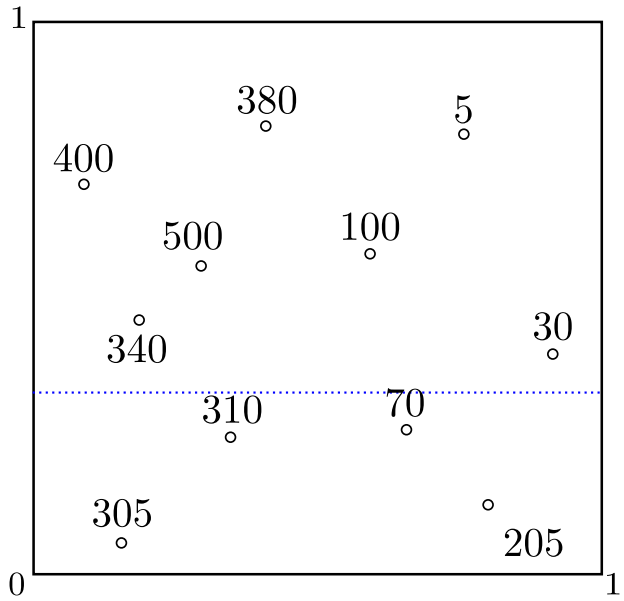

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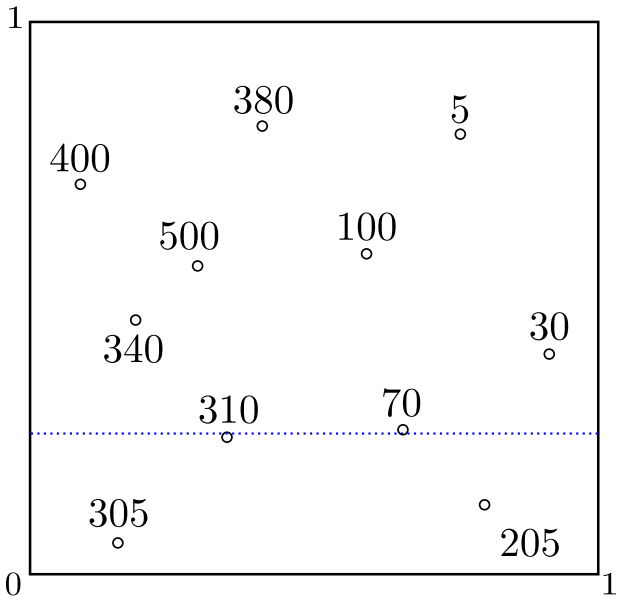

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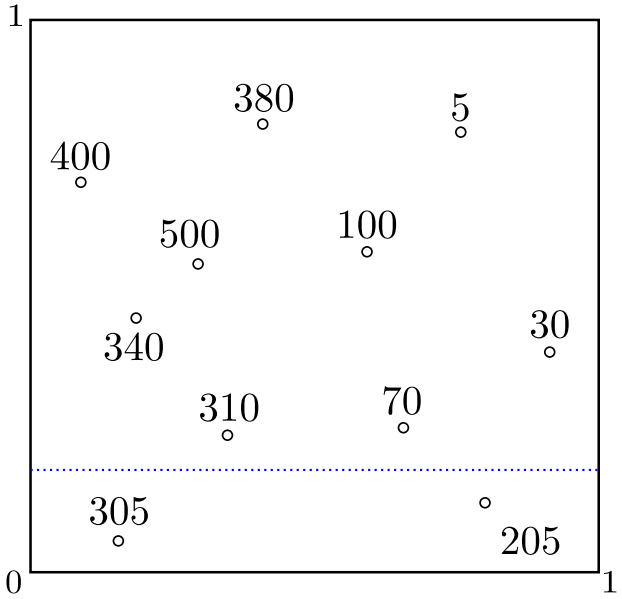

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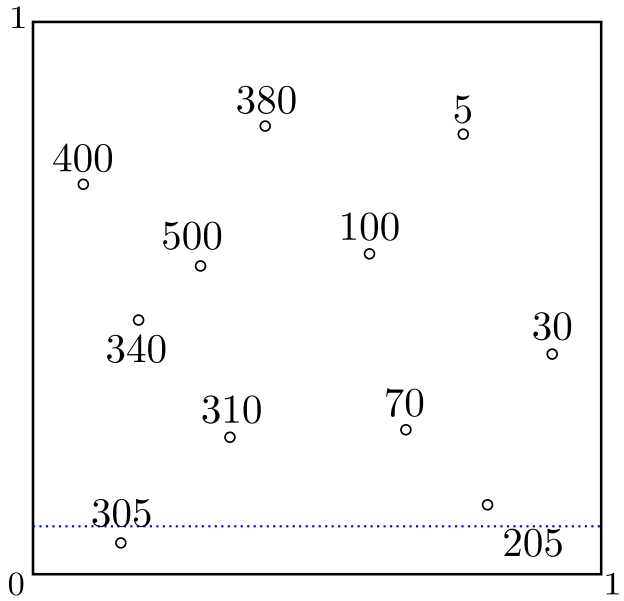

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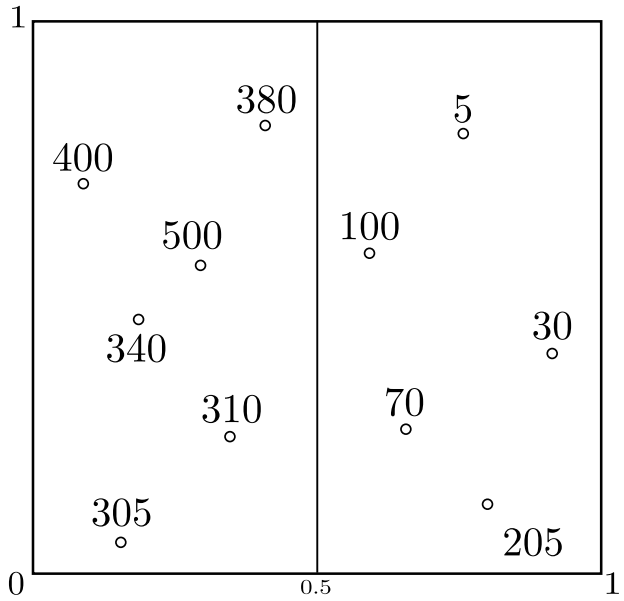

- Consider splits at the middle of two consecutive observations
- For each split, compute the decrease in impurity between the parent node and the two resulting nodes.
- Select the split maximizing the decrease in impurity

Impurity criteria

For **regression**, letting $N_n(A)$ the number of observations in the cell A and $\bar{Y}_A$ the mean of the Y_is in A:

- Variance

$$Imp_V(A) = \frac{1}{N_n(A)} \sum_{i, X_i \in A} (Y_i - \bar{Y}_A)^2, \tag{3}$$

- Mean absolute deviation around the median

$$\begin{aligned} &Imp_{L_1}(A) \\ =&\frac{1}{N_n(A)} \sum_{i, X_i \in A} |Y_i - \mathrm{Med}(Y_i : X_i \in A)|. \end{aligned} \tag{4}$$

Impurity criteria

For **classification**, letting $p_{k,n}(A)$ the proportion of observations in A such that $Y = k$:

- Misclassification error rate

$$Imp_{err}(A) = 1 - \max_{1 \leq k \leq K} p_{k,n}(A) \quad (3)$$

- Gini

$$Imp_G(A) = \sum_{k=1}^{K} p_{k,n}(A)(1 - p_{k,n}(A)). \quad (4)$$

- Entropy

$$Imp_H(A) = -\sum_{k=1}^{K} p_{k,n}(A) \log_2(p_{k,n}(A)). \quad (5)$$

Splitting criterion and risk of the method

Consider the variance as impurity measure:

$$Imp(A) = \frac{1}{N_n(A)} \sum_{i, X_i \in A} (Y_i - \bar{Y}_A)^2. \qquad (6)$$

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For any split (j, s) in any cell A resulting in cells A_L and A_R, the impurity reduction takes the form

$$\begin{aligned} &\Delta Imp(j, s; A) \\ =&Imp(A) - p_L Imp(A_L) - p_R Imp(A_R) \\ =&\frac{1}{N_n(A)} \sum_{i, X_i \in A} (Y_i - \bar{Y}_A)^2 \\ &- \frac{1}{N_n(A)} \sum_{i, X_i \in A} (Y_i - \bar{Y}_{A_L} \mathbb{1}_{X_i \in A_L} - \bar{Y}_{A_R} \mathbb{1}_{X_i \in A_R})^2. \end{aligned} \tag{7}$$

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This corresponds to the square loss of a predictor, which is piecewise constant on A_L and A_R, whose values equal the mean of Y_i's in each cell.

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Optimal partition. Finding the tree partition with the minimal quadratic risk on the training set.

- Statistically sound
- Computationally infeasible

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Greedy partition. At each step, finding the split with the minimal quadratic risk on the training set.

- Not the best predictive performances
- Computationally cheap

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Classification

- The entropy impurity is related to the cross-entropy loss
- The Gini impurity is not related to any loss, as it does not correspond to a majority vote but rather a random one
- The misclassification error rate is related to $0-1$ loss, which should not be used, as detailed hereafter.

Classification - which impurity to use?

We can choose between

- Misclassification rate

$$Imp_{err}(A) = 1 - \max_{1 \leq k \leq K} p_{k,n}(A) \qquad (6)$$

- Gini

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Classification - which impurity to use?

In a binary classification setting, impurities can be rewritten as

- Misclassification rate

$$Imp_{err}(A) = 1 - \max_{k \in \{0,1\}} p_{k,n}(A) \tag{6}$$

- Gini

$$Imp_G(A) = 2p_{0,n}(A)(1 - p_{0,n}(A)) \tag{7}$$

- Entropy

$$\begin{aligned} Imp_H(A) = &- p_{0,n}(A) \log_2(p_{0,n}(A)) \\ &- (1 - p_{0,n}(A)) \log_2(1 - p_{0,n}(A)) \end{aligned} \tag{8}$$

Classification - which impurity to use?

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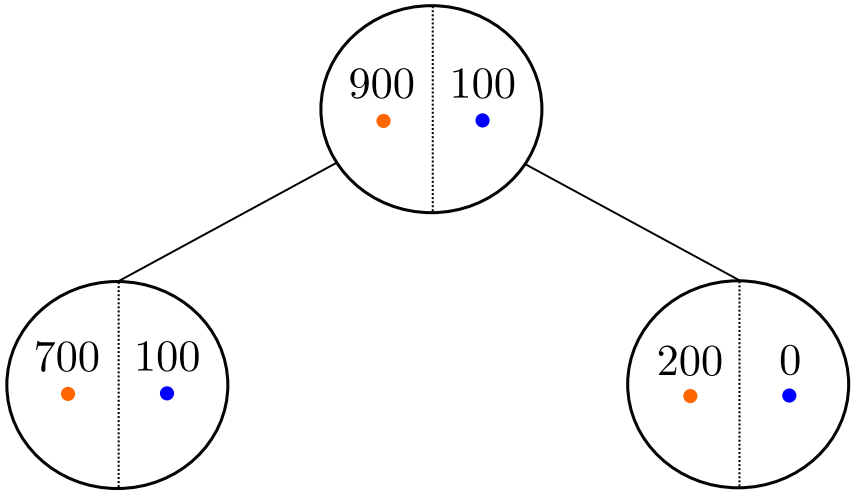

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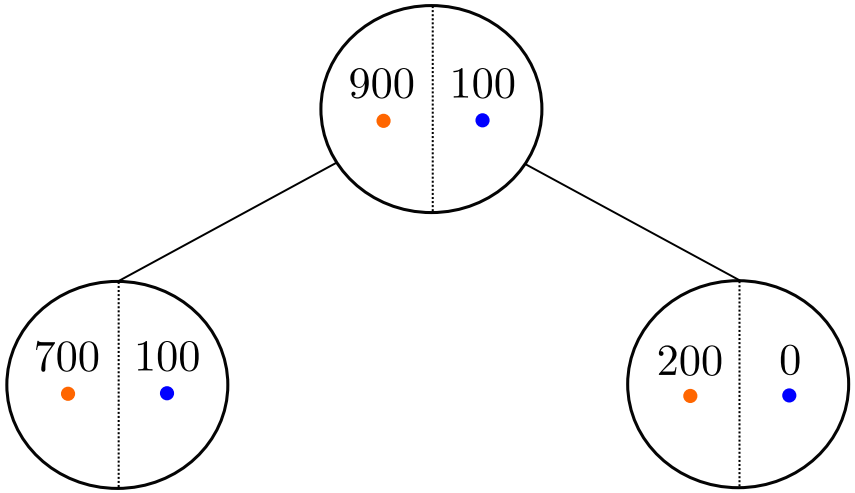

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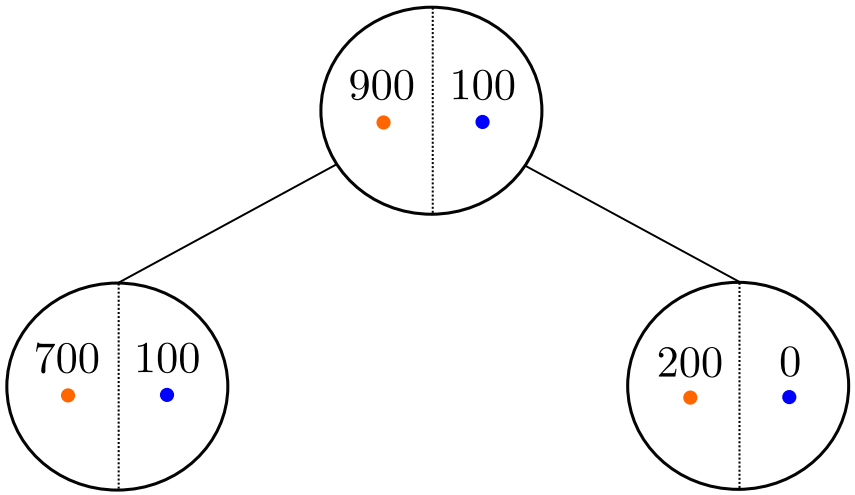

- Since $\Delta Imp_{err} = 0$, the split appears to be non-informative.
- But the right node is pure! The decrease in impurity for the two other criterion is

$$\Delta Imp_G(A) = 0.005$$
$$\text{and} \quad \Delta Imp_H(A) = 0.01. \qquad (6)$$

Classification - which impurity to use?

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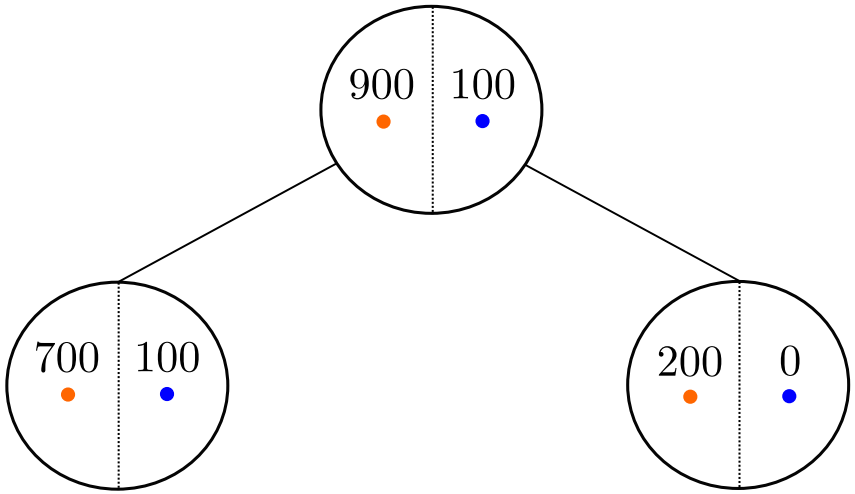

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This phenomenon results from the fact that the misclassification rate in the binary setting is not strictly concave, contrary to the Entrope/Gini criterion. More explanation here[a]

[a] https://tushaargvs.github.io/assets/teaching/dt-notes-2020.pdf

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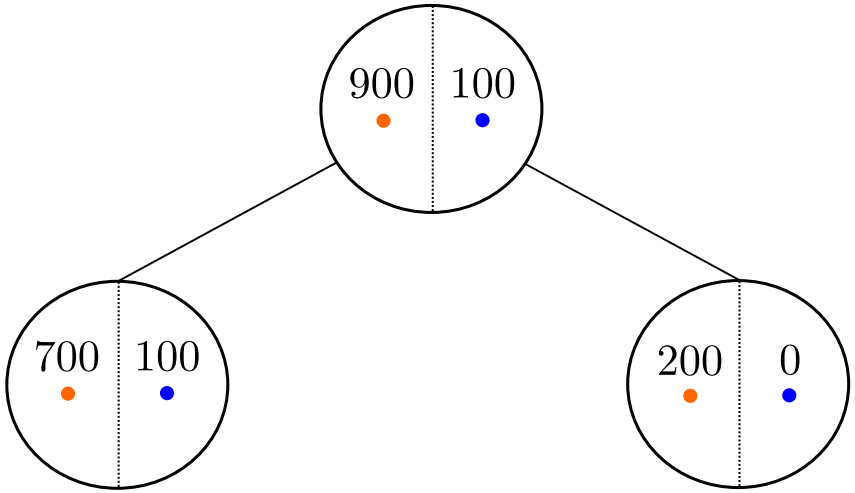

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Misclassification criterion is not precise enough to be used for building trees.

Outline

Decision tree

Now that we have defined a splitting rule, let us see the rest of the tree construction.

Decision tree building

- Splitting rule (Variance in regression, Gini or Entropy in classification)

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Prediction rule:

- Regression - Average of labels per leaf

$$\hat{t}_n(x) = \sum_{i=1}^{n} Y_i \frac{\mathbb{1}_{X_i \in A_n(x)}}{N_n(A_n(x))} \qquad (6)$$

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- Classification - Majority vote per leaf

$$\hat{t}_n(x) = \underset{k \in \{1,\dots,K\}}{\operatorname{argmax}} \sum_{i=1}^{n} \frac{\mathbb{1}_{Y_i = k} \mathbb{1}_{X_i \in A_n(x)}}{N_n(A_n(x))} \tag{7}$$

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- Splitting rule (Variance in regression, Gini or Entropy in classification)
- Stopping rule (by default, one observation per leaf)
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Outline

Handling different types of features

There exist three main types of features:

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- Ordinal (Glasgow score)
- Nominal (Medical treatments)

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Nominal features. For nominal feature, it makes no sense to consider such splits: there is no natural order on treatments.

Nominal features

A **nominal features** $X^{(j)}$ can take different discrete values that are not ordered. For example, $X^{(j)}$ can be the type of treatment, which is surgical, chemical, or nothing (three different modalities).

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Exhaustive search Letting $\mathcal{C}$ the set of all modalities of a variable, any split along this variable is of the form C versus C^c for any $C \subset \mathcal{C}$.

- All partitions of modalities in two groups is admissible
- Computationally costly / infeasible to evaluate all these splits for variables with high cardinality (number of modalities)

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Common practice - One-hot encoding Creating as many new (dummy) variables as modalities. In our example, our treatment variable would become

$(1, 0, 0)$ for surgical treatments, $(0, 1, 0)$ for chemical treatments,
$(0, 0, 1)$ for no treatment

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One-hot encoding is the most common encoding method.

A clever encoding: Target encoding

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- Choose an impurity (misclassification rate, entropy or Gini)
- Consider a nominal variable X_j that can take L modalities. Reorder it so that the empirical probabilities in a given cell A satisfy

$$\begin{aligned} &\mathbb{P}_n[Y=1|X_j=C_1, X\in A] \\ \leq &\mathbb{P}_n[Y=1|X_j=C_2, X\in A] \\ \leq &\ \dots \\ \leq &\mathbb{P}_n[Y=1|X_j=C_L, X\in A]. \end{aligned} \tag{6}$$

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- Then the best split (that maximizes the decrease in impurity) is of the form

$$X_j \in \{C_1, \dots, C_\ell\} \quad \text{vs} \quad X_j \in \{C_{\ell+1}, \dots, C_L\}. \tag{7}$$

This is a result from Fisher 1958

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Summary. Finding the optimal split by reordering and then evaluating $L-1$ splits instead of $2^{L-1}-1$ splits for exhaustive search (and L splits with suboptimal decision for one-hot encoding).

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Extension to regression. The same procedure holds in regression by considering the average values of Y for each modality (instead of the probabilities).

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- setting parameters to limit the depth of the tree (`min-samples-leaf`, `min-samples-split`, `max-depth`)
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$\rightarrow$ Stopping the tree construction when the splitting criterion is low is not a valid strategy.

Pruning strategies

Two types of pruning strategies exist:

- Reducing Error, consists in removing branches of the fully-grown tree, based on the error computed on an extra data set (validation set). Simple but implies that less data are used for the training of the tree (first step).
- Cost-complexity pruning (CART) is based on a penalization of the decision tree error via the number of leaves.

Pruning strategies

Cost-complexity pruning. Let T_0 be the trained fully-grown tree. We denote by $R(T)$ the risk of any tree T, defined as either the misclassification rate (1 - accuracy) or the weighted impurity of each one of its leaves:

$$R(T) = \sum_{A \in \text{Leaf}(T)} p_A Imp(A), \tag{8}$$

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As mentioned before, for a fully-grown tree T_0, $R(T_0) = 0$ and then does not give a good measure of predictive performances of T_0.

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For all $\alpha > 0$, we define the cost-complexity measure $R_\alpha(T)$ as

$$R_\alpha(T) = R(T) + \alpha|\text{Leaf}(T)|, \tag{9}$$

where $|\text{Leaf}(T)|$ is the number of leaves in T.

A cross-validation procedure can then be used to select the best value for α, therefore producing an shallower tree than T_0.

Outline

Final algorithm

Tree construction

- Input: a dataset, an impurity measure.
- At each node A, select the best split via
$$(j^\star, s^\star) \in \underset{j \in \{1,\dots,d\}, s \in \text{range}(X^{(j)})}{\text{argmax}} \Delta Imp(j, s; A).$$
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Tree prediction Tthe tree prediction at x_{new} is given by the average / majority vote among the training observations falling into the same leaf as x_{new}.

Pro/cons

Benefits

- Work in classification and regression
- Can handle categorical and continuous features
- Interpretable
- Invariant by monotonic transformation of the data
- Missing values
- Numerical complexity : $nd \log n$
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Drawbacks

- Non-robust to small changes in data
- Limited approximation capacity (thresholded nature)

[Fis58] Walter D Fisher. “On grouping for maximum homogeneity”. In: *Journal of the American statistical Association* 53.284 (1958), pp. 789–798.