Summer Program FGV/EMAp 2019

Introduction to Machine Learning with Python

Decision Trees and Random Forest

Prof. Luis Gustavo Nonato

University of São Paulo - São Carlos - SP

Classification and Regression Trees - CART

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The simplest model to be fitted in each sub-domain is a constant predictor, that is

$$f(\mathbf{x}) = \sum_{i=1}^{m} c_i I(\mathbf{x} \in R_i)$$

where m is the number of sub-domains, c_i is the constant predictor, and I is the indicator function, that is, $I(\mathbf{x} \in R_i) = 1$ if $\mathbf{x}$ lies on the sub-domain R_i and $I(\mathbf{x} \in R_i) = 0$ otherwise.

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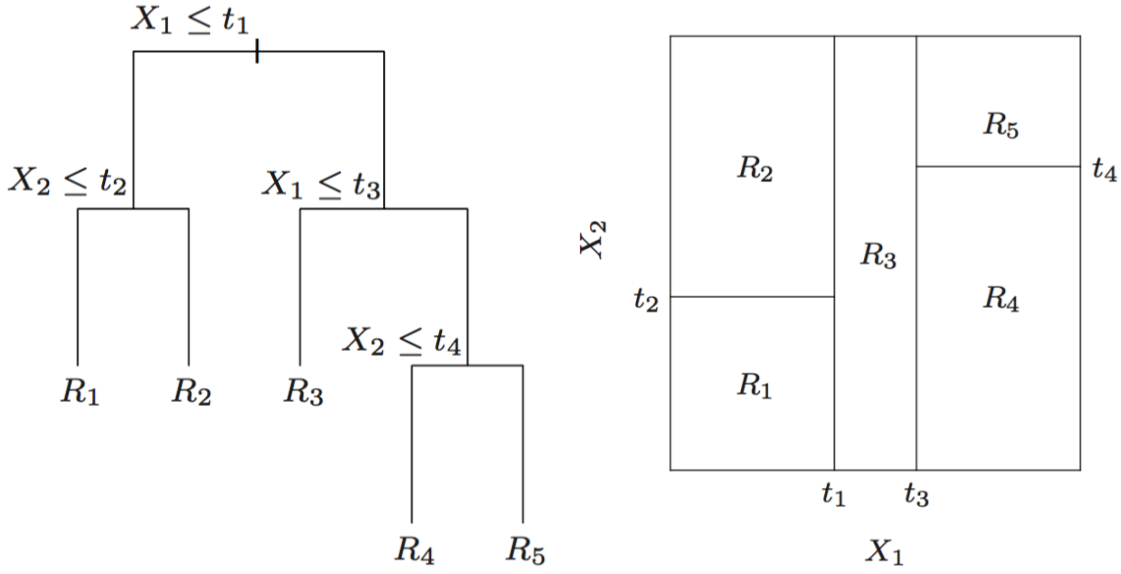

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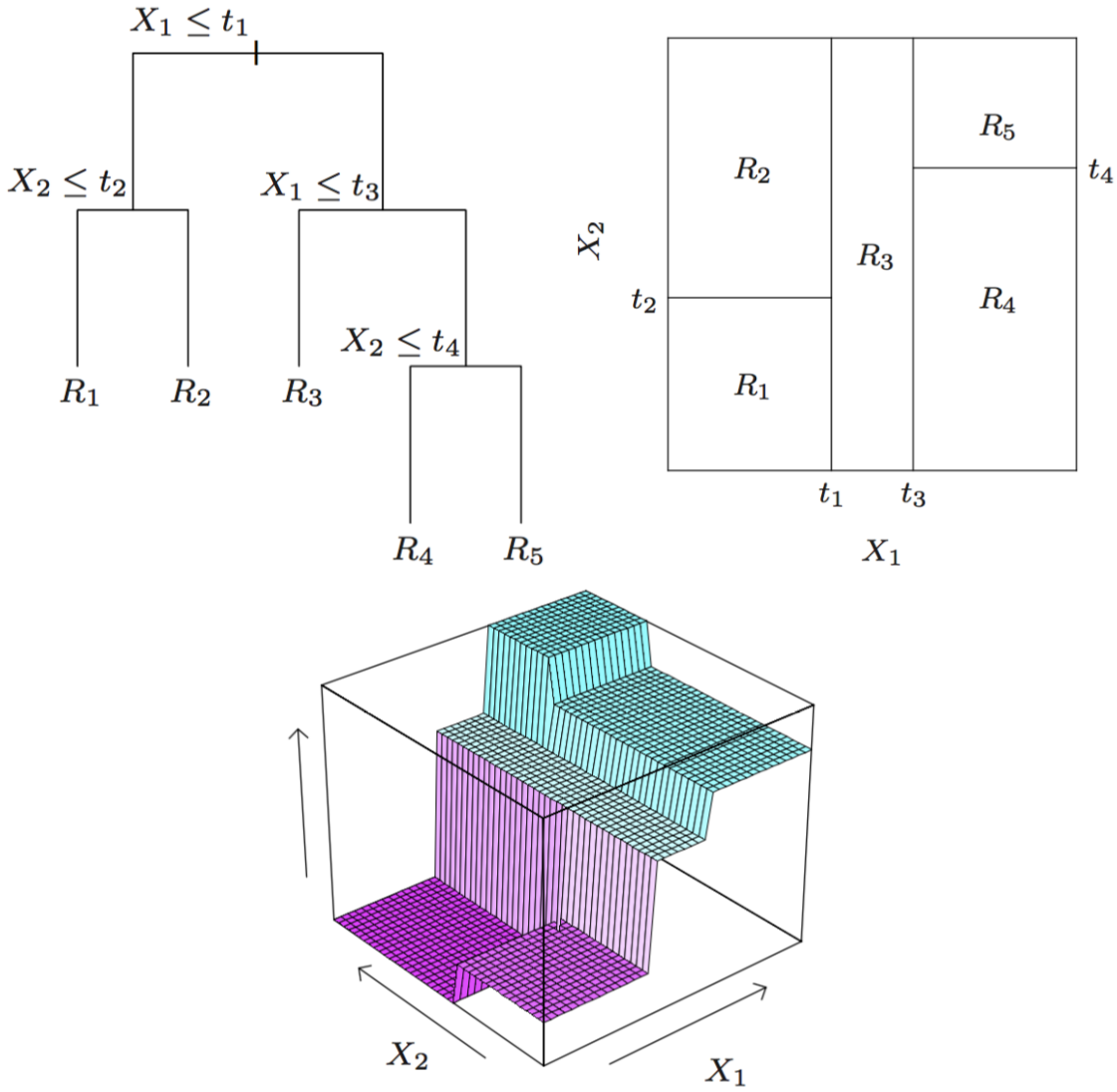

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- Which attribute to split in each step.
- How to find the splitting value.

Finding the Predictor

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It is easy to see that the minimizer is given by:

$$c_j = \texttt{ave}(y_i | \mathbf{x}_i \in R_j)$$

(regression trees)

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The pair (j,s) minimizing (1) is chosen as the optimal one for R.

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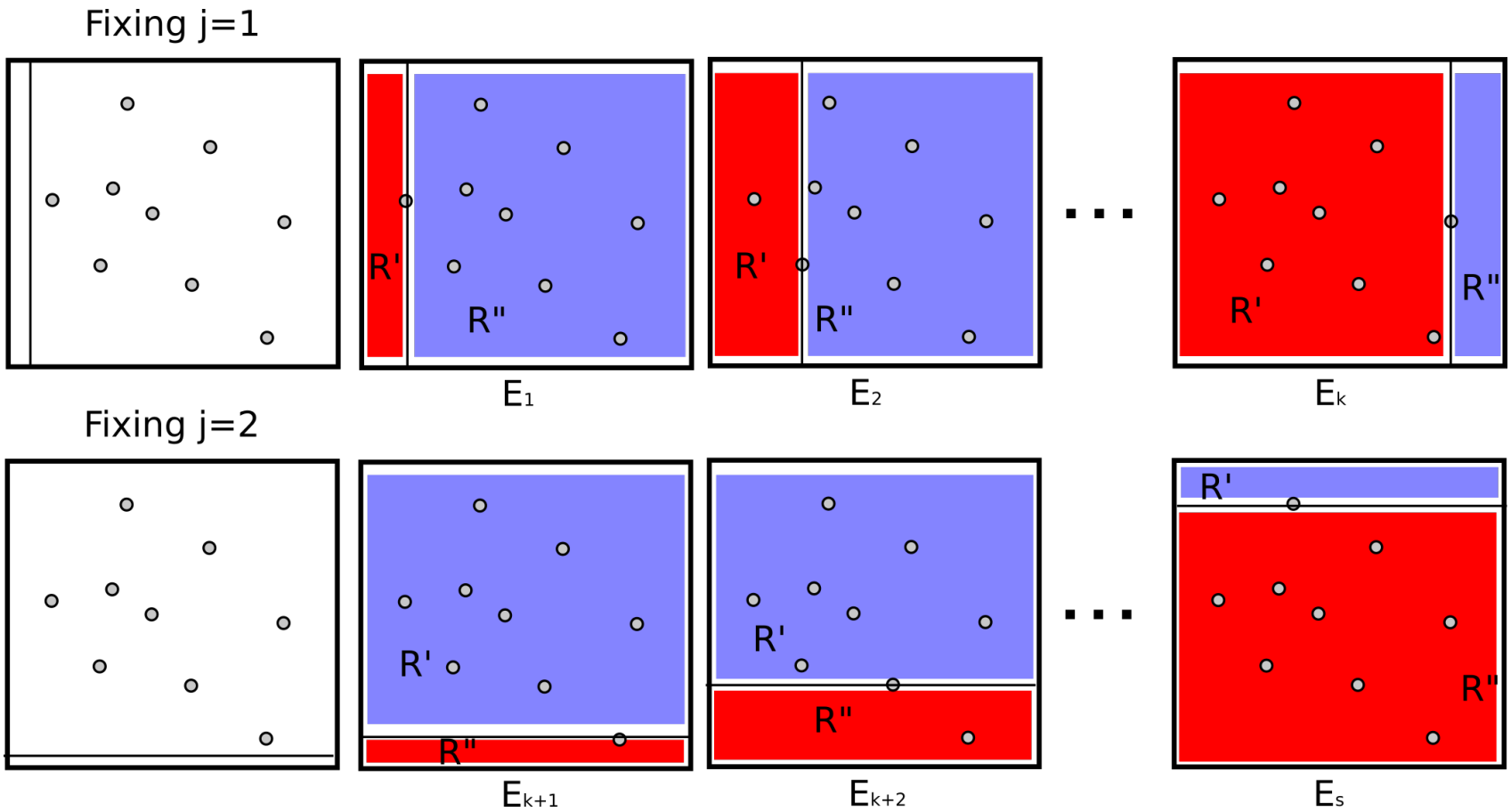
$$E_i = \Big(\sum_{\mathbf{x}_i \in R'(j,s)} (y_i - c')^2 + \sum_{\mathbf{x}_i \in R''(j,s)} (y_i - c'')^2 \Big)$$



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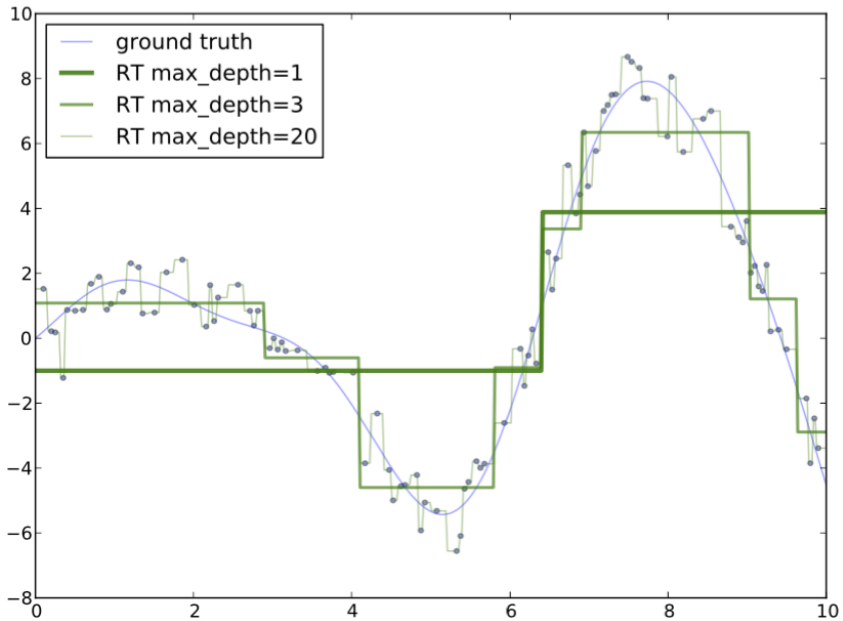

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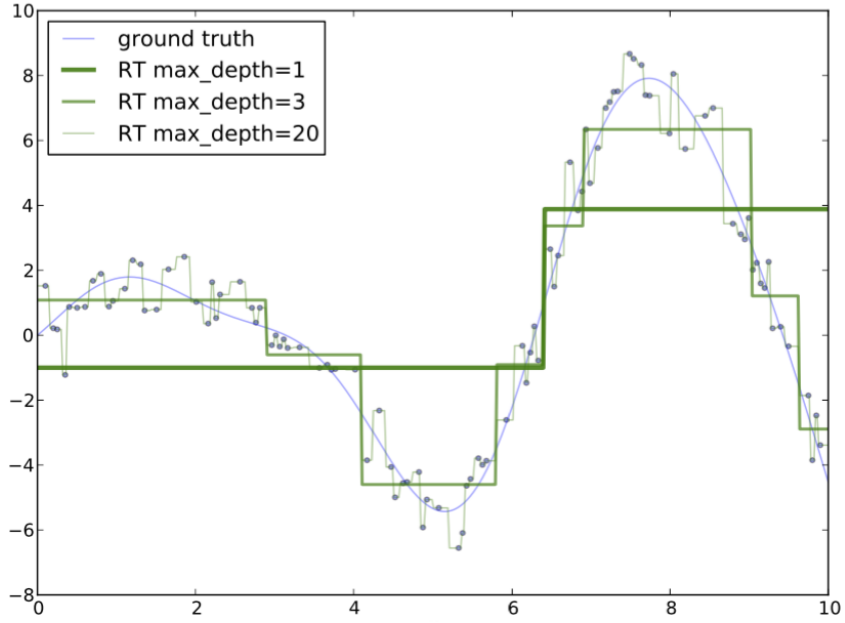

A common procedure is to grow the tree until a maximum node size (say 5) is reached in each sub-domain and then prune the tree using a *cost-complexity pruning*.

Classification Tree

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Supposing k classes, the classification of a point $\mathbf{x} \in R_j$ is given by majority voting, that is,

$$k(j) = \arg\max_k p_{jk} = \arg\max_k \frac{1}{n_j} \sum_{\mathbf{x}_i \in R_j} I(y_i = k)$$

where p_{jk} is the proportion of class k in the region R_j.

Bagging, Random Forest, and Boosting

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- A number B of bootstrap datasets are generated;
- The model is fitted in each dataset and the behaviour examined over the B replications.

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This reasoning applies to any regression or classification procedure, not only for trees.

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The *Bagging* procedure:

1. Compute B bootstrapped training sets $b_1, \ldots, b_B$
2. Train a model f^i (grow the tree) in each b_i
3. Given a new input $\mathbf{x}$
   - Regression:
     Predicts $\hat{f}(\mathbf{x}) = \frac{1}{B} \sum_{i=1}^{B} f^{b_i}(\mathbf{x})$
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- This avoid the use of cross-validation.

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- Therefore, predictions from distinct trees tend to be highly correlated
- The effect of bagging in correlated variables is not so good (does not substantially reduce variance)

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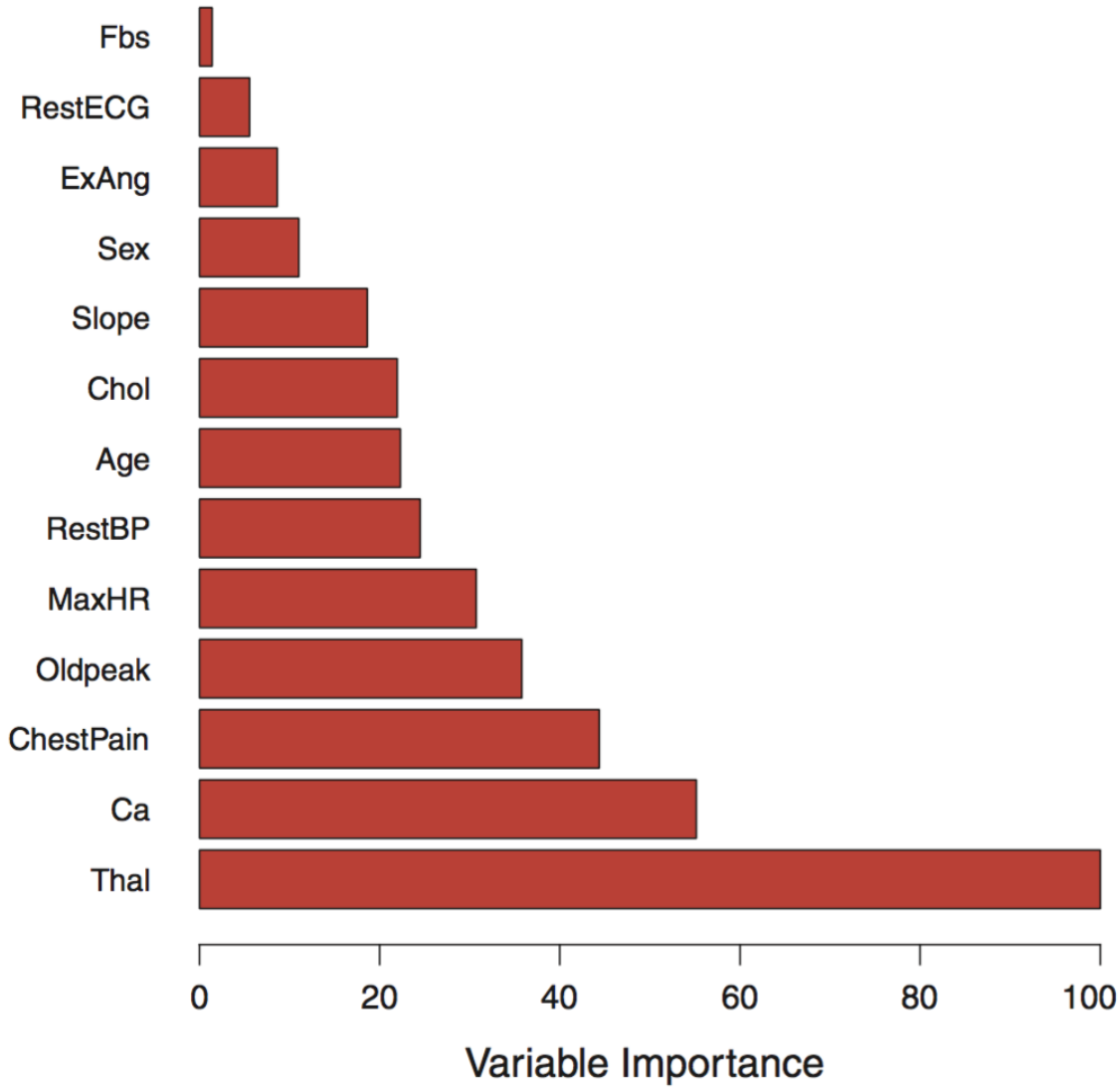

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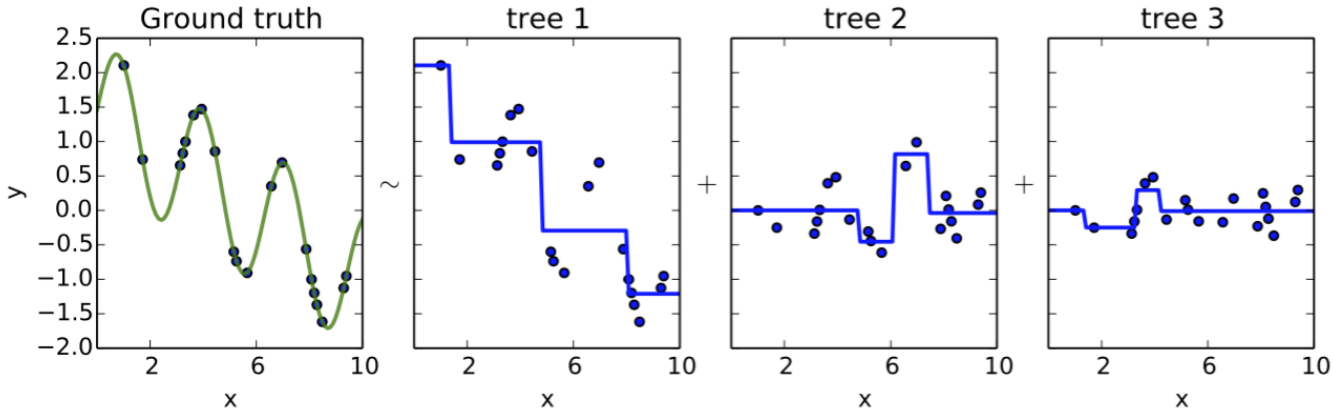

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The idea is to weight training samples according to their relevance to reduce prediction error.

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Boosted trees tend to present good results in practice.