Trees and Rules and Optimization

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Açıklanabilir Yapay Öğrenme - II

Outline

- Decision Trees (DTs)
  - CART
- Optimization Models
  - Optimal Classification Trees
  - State-of-the-art
- Rules and Rule Set Generation
  - Column Generation
  - Extensions
- Takeaways

Regression Trees

Distinct and nonoverlapping regions

$X_1, X_2, \ldots, X_p \longrightarrow R_1, R_2, \ldots, R_m$

Prediction: Mean of the response values for the training observations in R_m

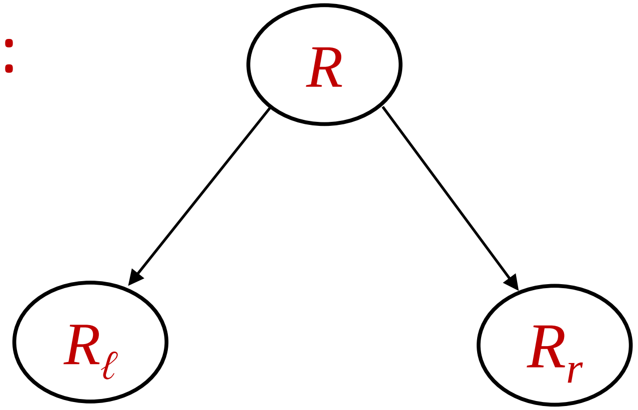
$$\hat{y}_m = \frac{1}{N_m} \sum_{\{x_i \in R_m\}} y_i$$

Goal: Finding the regions such that sum of squares is minimized

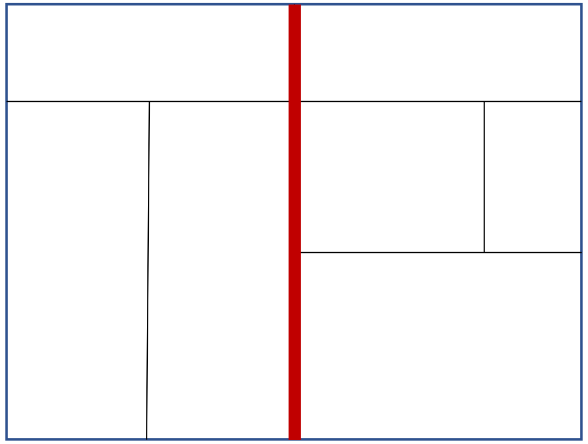
$$\sum_{j=1}^{m} \sum_{\{x_i \in R_j\}} (y_i - \hat{y}_j)^2$$

How to grow a Regression Tree?

Recursive Binary Splitting:



$$R_\ell(j,s) = \{X \mid X_j \le s\} \qquad R_r(j,s) = \{X \mid X_j > s\}$$



Find j and s minimizing the sum of squared error

$$\sum_{\{x_i \in R_\ell(j,s)\}} (y_i - \hat{y}_\ell)^2 + \sum_{\{x_i \in R_r(j,s)\}} (y_i - \hat{y}_r)^2$$

Until when?

Goal: Avoiding overfitting with a fully grown or large tree
(Selecting a subtree that leads to a lowest test error rate)

CART:
1) Grow a large tree until each leaf has a minimum sample size, e.g. 5.
2) Pruning large tree based on cost-complexity, $C_\alpha(T)$.

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

Pruning: Successively collapse the internal node that produces the smallest per-node increase in sum of squared errors.
- Use k-fold cross validation to tune α.

Classification Trees

Similar to a regression tree but uses different error measures based on *impurity* of a region.

Prediction: Majority voting of classes among the training observations in R_m

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

$$\hat{y}_m = \arg\max_k \hat{p}_{mk}$$

Error Measures

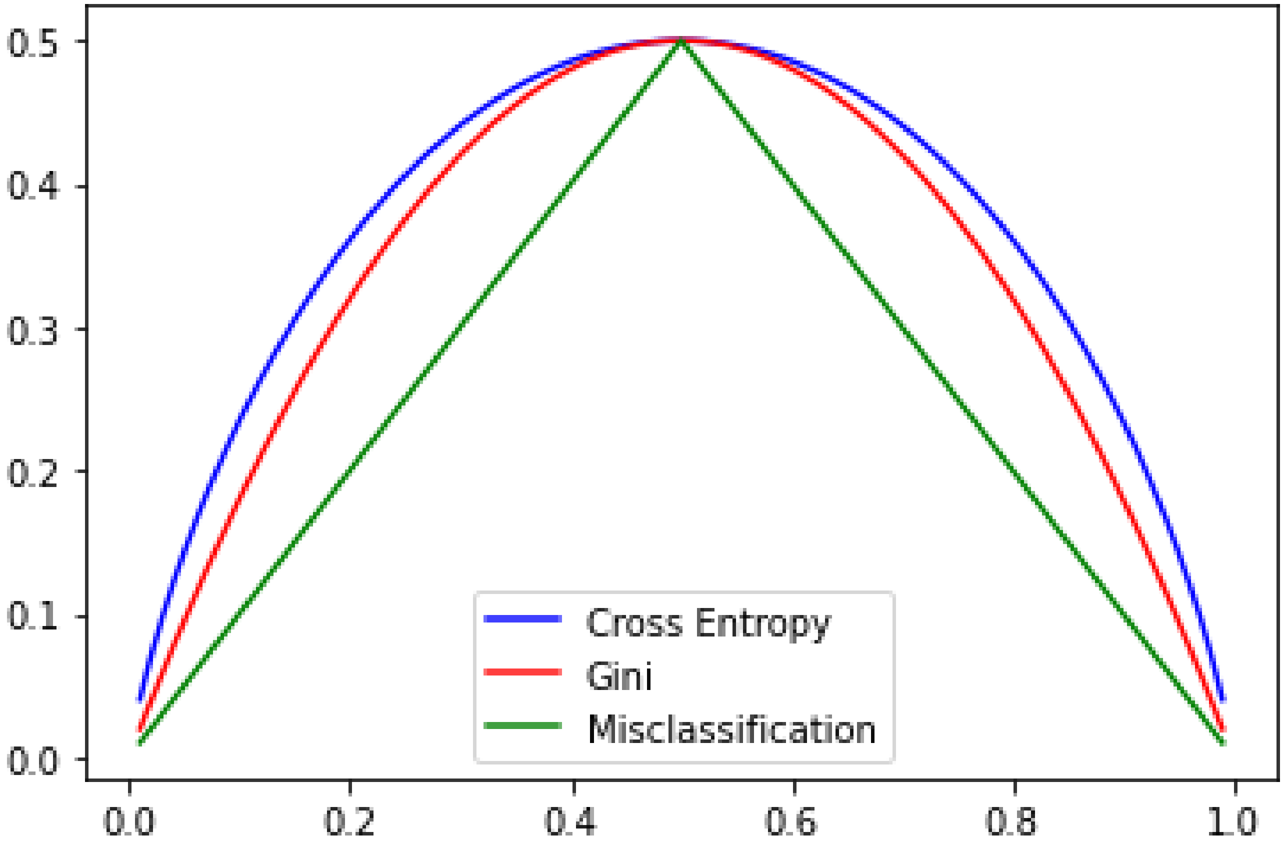
$$\frac{1}{N_m} \times \sum_{x_i \in R_m} I(y_i \neq \hat{y}_m) = 1 - \hat{p}_{m\hat{y}_m} \longrightarrow \text{Misclassification Error}$$

$$\sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk}) \longrightarrow \text{Gini Index}$$

$$-\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk} \longrightarrow \text{Cross Entropy}$$

Which error measure?

- Use Gini or Cross Entropy to grow the tree.
- For pruning use misclassification error.
- Weight the node impurity measures by the number $N_{m\ell}$ and N_{mr} of observations in the two child nodes created by splitting node m.



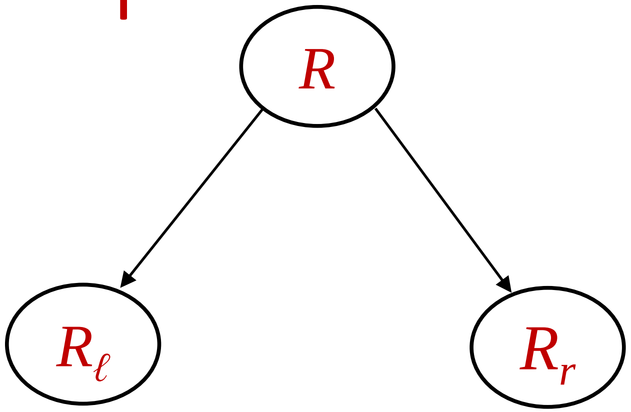
* Two class case. Cross Entropy is scaled to pass through (0.5,0.5).

$$\frac{1}{N_m} \times \sum_{x_i \in R_m} I(y_i \neq \hat{y}_m) = 1 - \hat{p}_{m\hat{y}_m} \longrightarrow \text{Misclassification Error}$$

$$\sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk}) \longrightarrow \text{Gini Index}$$

$$-\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk} \longrightarrow \text{Cross Entropy}$$

How to select a split?



$$R_\ell(j,s) = \{X \mid X_j \le s\} \qquad R_r(j,s) = \{X \mid X_j > s\}$$

Find *j* and *s* minimizing the error (or maximizing the gain of split)

$$\sum_{\{x_i \in R_\ell(j,s)\}} (y_i - \hat{y}_\ell)^2 + \sum_{\{x_i \in R_r(j,s)\}} (y_i - \hat{y}_r)^2$$

Classification Trees

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

$$\hat{y}_m = \arg\max_k \hat{p}_{mk}$$

Gini Index:

$$\sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk}) \quad \Leftrightarrow \quad \boxed{1 - \sum_{k=1}^{K} \hat{p}_{mk}^2}$$

What is the gain of a split "s"?

Gain = (Error before the split) – (Error after the split)

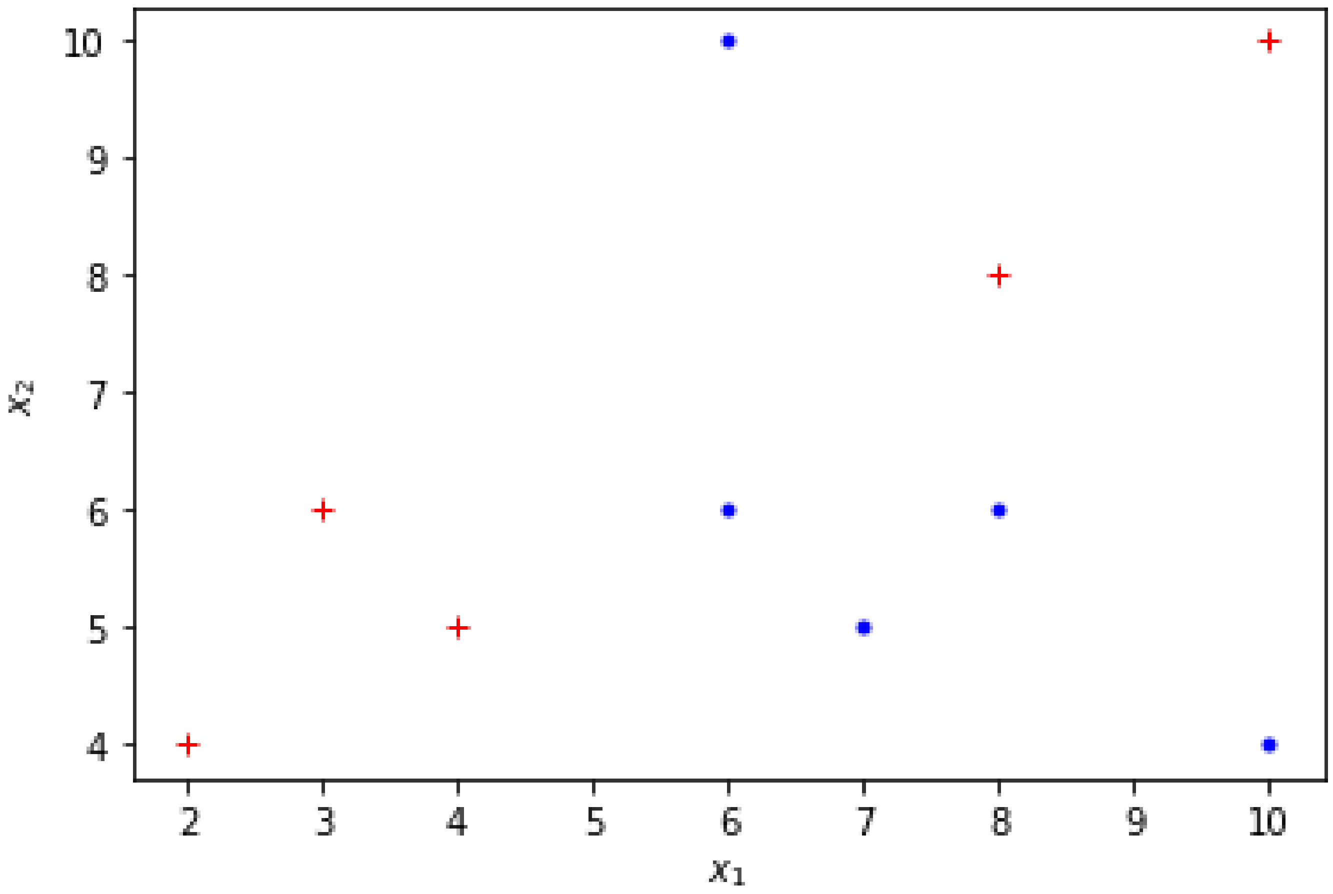
$$G(s) = \boxed{E(R)} - \boxed{E(s)}$$

$$\boxed{E(s) = \frac{N_{ml}}{N_m} E(R_l) + \frac{N_{mr}}{N_m} E(R_r)}$$

Error at node R

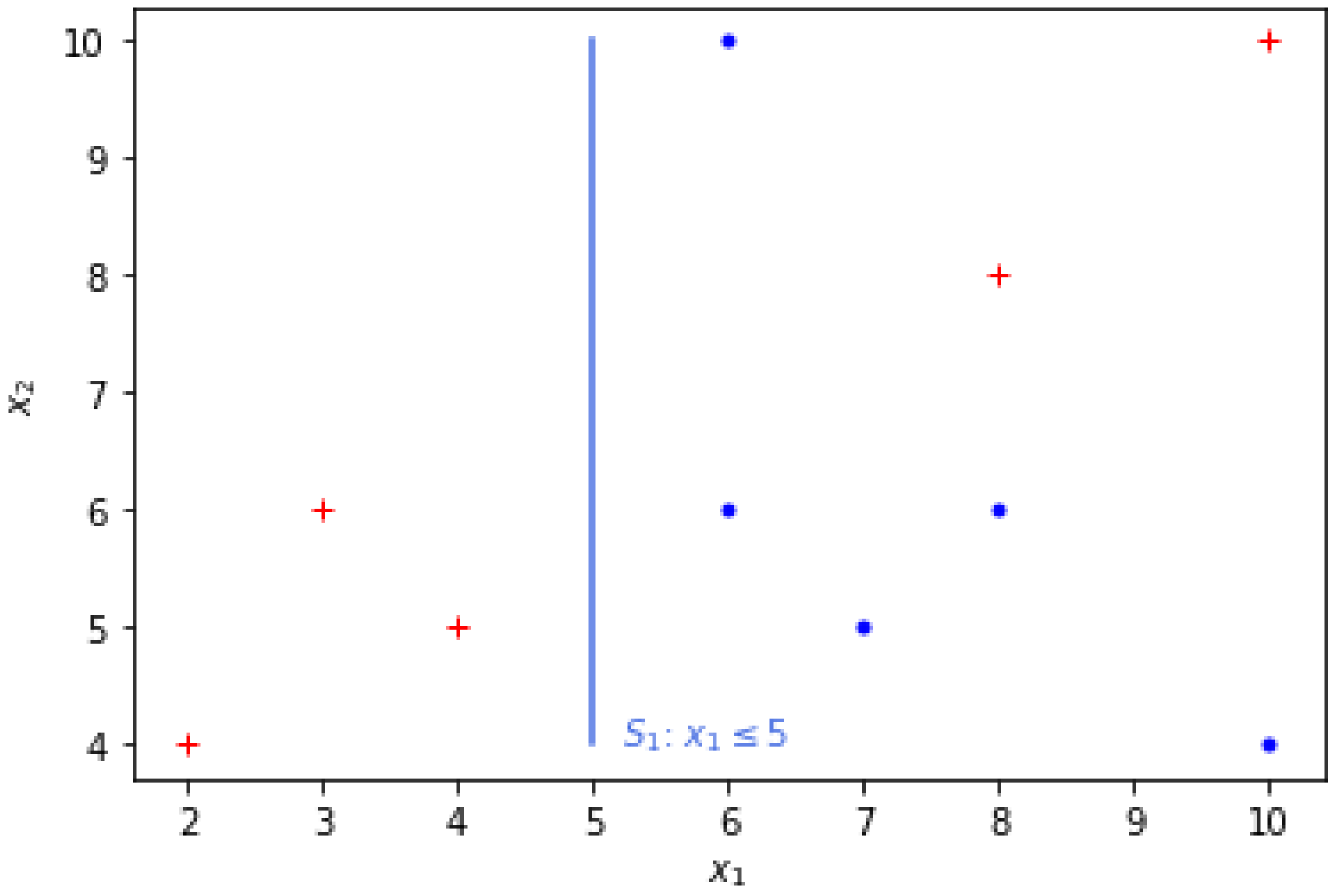
Error of split s

Classification – { +, • }



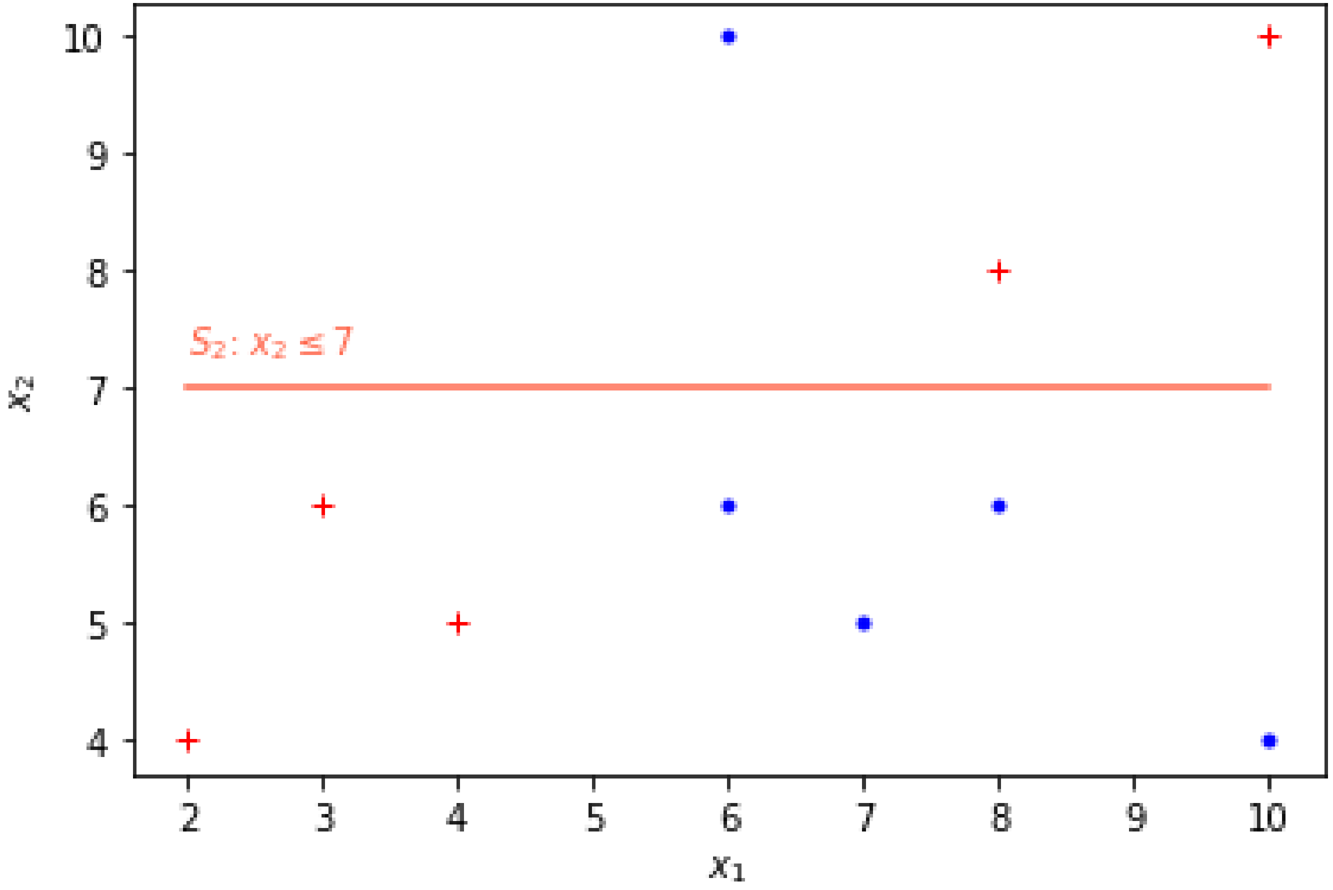
Classification – { +, • }

Split #1: $x_1 \leq 5$



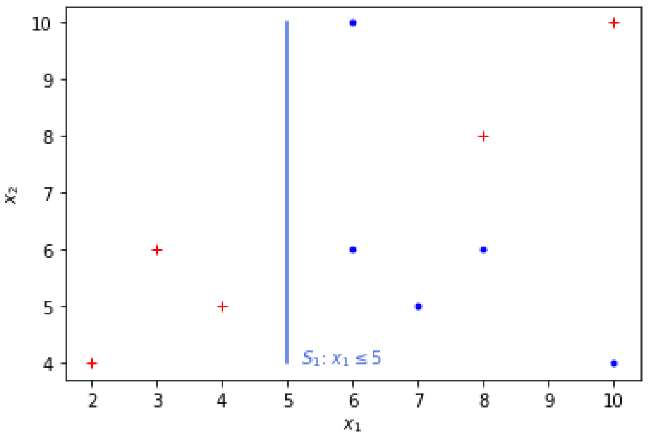
Classification – { +, • }

Split #2: $x_2 \leq 7$



Classification – { +, • }

Gini Index: $1 - \sum_{k=1}^{K} \hat{p}_{mk}^2$



Split #1: $x_1 \leq 5$

S_1

$$\boxed{E(R) = 1-(0.5)^2-(0.5)^2 = 0.5}$$

+++++
•••••
R

$R_\ell(x_1, 5) = \{x | x_1 \leq 5\}$

$R_r(x_1, 5) = \{x | x_1 > 5\}$

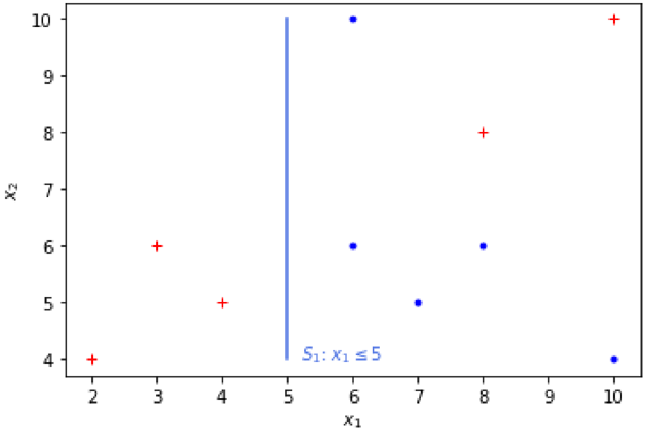
+++ R_ℓ

R_r •••••
++

Classification – { +, • }

Gini Index: $1 - \sum_{k=1}^{K} \hat{p}_{mk}^2$

Split #1: $x_1 \leq 5$



$E(R) = 1\text{-}(0.5)^2\text{-}(0.5)^2 = 0.5$

+++++ ••••• R

$R_\ell(x_1, 5) = \{x | x_1 \leq 5\}$

$R_r(x_1, 5) = \{x | x_1 > 5\}$

+++ R_ℓ

R_r ••••• ++

$E(R_\ell) = 1\text{-}(1.0)^2\text{-}(0.0)^2 = 0.0$

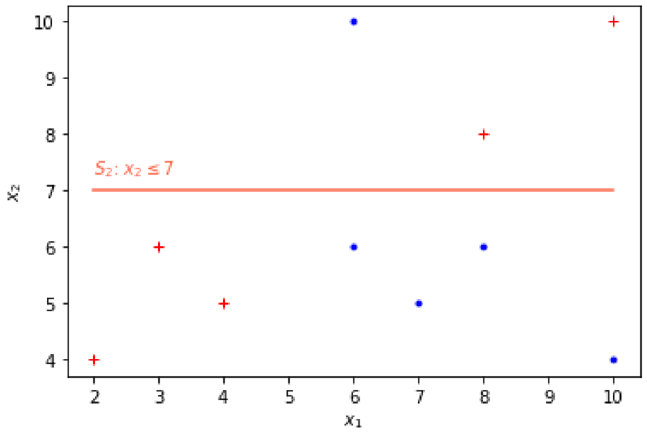
$E(R_r) = 1\text{-}(2/7)^2\text{-}(5/7)^2 = 0.41$

$$
\begin{aligned}
E(S_1) &= (3/10)\cdot E(R_\ell) + (7/10)\cdot E(R_r) \\
&= 0.3 \cdot 0.0 + 0.7 \cdot 0.41 \\
&= 0.29
\end{aligned}
$$

$$
\begin{aligned}
G(S_1) &= E(R) - E(S_1) \\
&= 0.5 - 0.29 \\
&= 0.21
\end{aligned}
$$

Classification – { +, • }

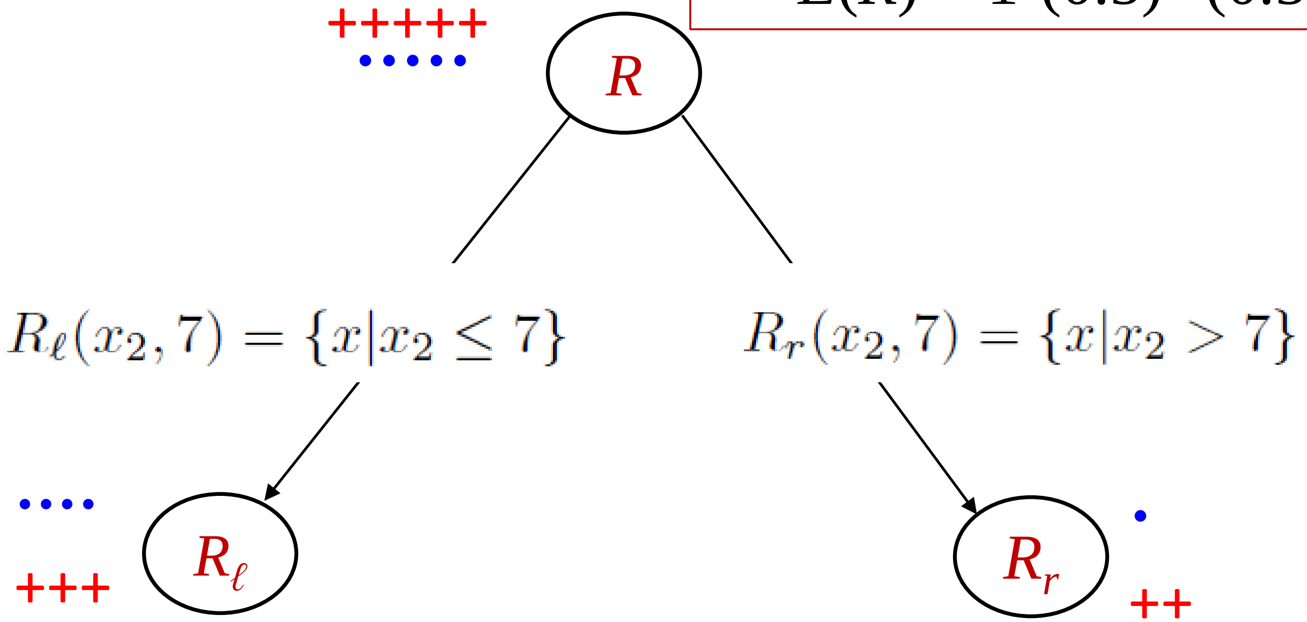
Gini Index: $1 - \sum_{k=1}^{K} \hat{p}_{mk}^2$



Split #2: $x_2 \leq 7$

S_2

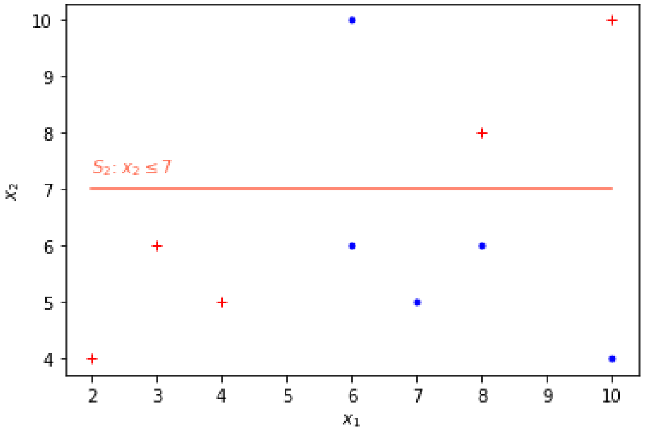
$E(R) = 1\text{-}(0.5)^2\text{-}(0.5)^2 = 0.5$



Classification – { +, • }

Gini Index: $1 - \sum_{k=1}^{K} \hat{p}_{mk}^2$

Split #2: $x_2 \leq 7$



$E(R) = 1\text{-}(0.5)^2\text{-}(0.5)^2 = 0.5$

+++++
•••••

R

$R_\ell(x_2, 7) = \{x | x_2 \leq 7\}$

$R_r(x_2, 7) = \{x | x_2 > 7\}$

••••
+++

R_ℓ

R_r

•
++

$E(R_\ell) = 1\text{-}(4/7)^2\text{-}(3/7)^2 = 0.49$

$E(R_r) = 1\text{-}(1/3)^2\text{-}(2/3)^2 = 0.44$

$$
\begin{aligned}
E(S_2) &= (7/10)\cdot E(R_\ell) + (3/10)\cdot E(R_r) \\
&= 0.7 \cdot 0.49 + 0.3 \cdot 0.44 \\
&= 0.343 + 0.132 \\
&= 0.48
\end{aligned}
$$

$$
\begin{aligned}
G(S_2) &= E(R) - E(S_2) \\
&= 0.5 - 0.48 \\
&= 0.02
\end{aligned}
$$

Optimization Models?

Generic Model

$$\begin{array}{ll} \text{minimize} & f(\boldsymbol{x}) \\ \text{subject to} & g(\boldsymbol{x}) \geq \mathbf{0}. \end{array}$$

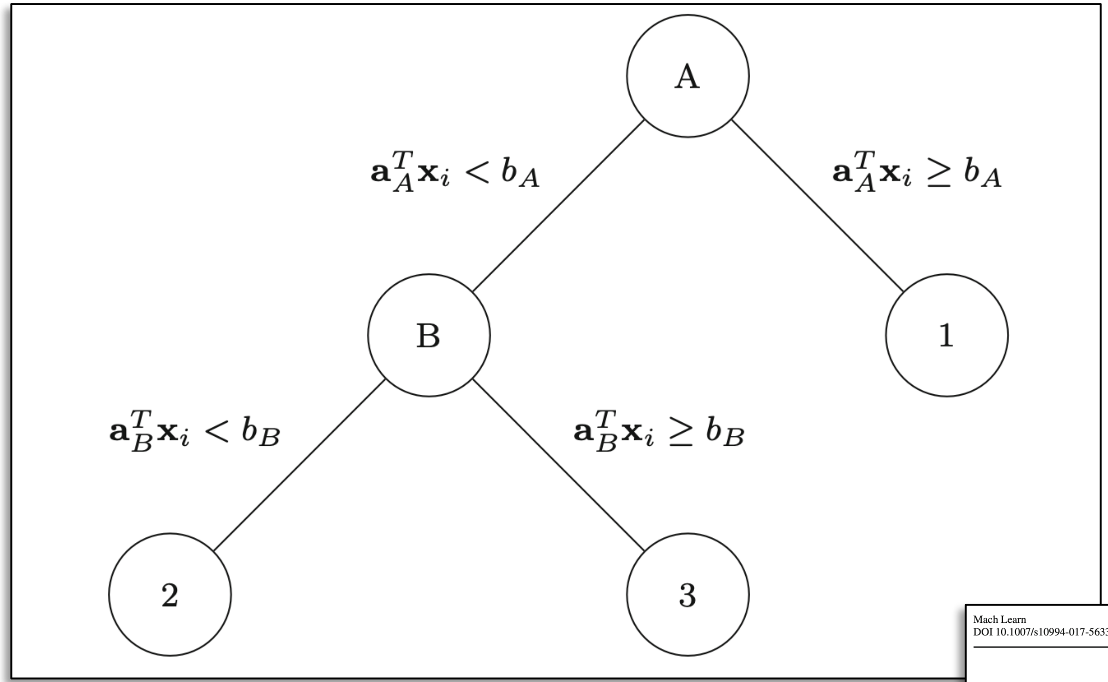
Integer Programming Model

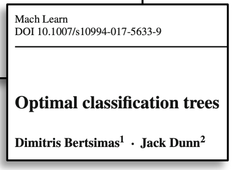
$$\begin{array}{ll} \text{minimize} & \boldsymbol{c}^\top \boldsymbol{x} \\ \text{subject to} & \boldsymbol{A}\boldsymbol{x} \geq \boldsymbol{b}, \\ & \boldsymbol{x} \in \{\mathbf{0}, \mathbf{1}\}. \end{array}$$

Linear Programming Model

$$\begin{array}{ll} \text{minimize} & \boldsymbol{c}^\top \boldsymbol{x} \\ \text{subject to} & \boldsymbol{A}\boldsymbol{x} \geq \boldsymbol{b}, \\ & \boldsymbol{x} \geq \mathbf{0}. \end{array}$$

Optimal Classification Trees (OCT)




Mach Learn
DOI 10.1007/s10994-017-5633-9

Optimal classification trees

Dimitris Bertsimas[1] · Jack Dunn[2]

$$\boldsymbol{x}_i \in \mathbb{R}^p, y_i \in \{1, \ldots, K\},\ i = 1, \ldots, n$$

classification error

number of branches in T

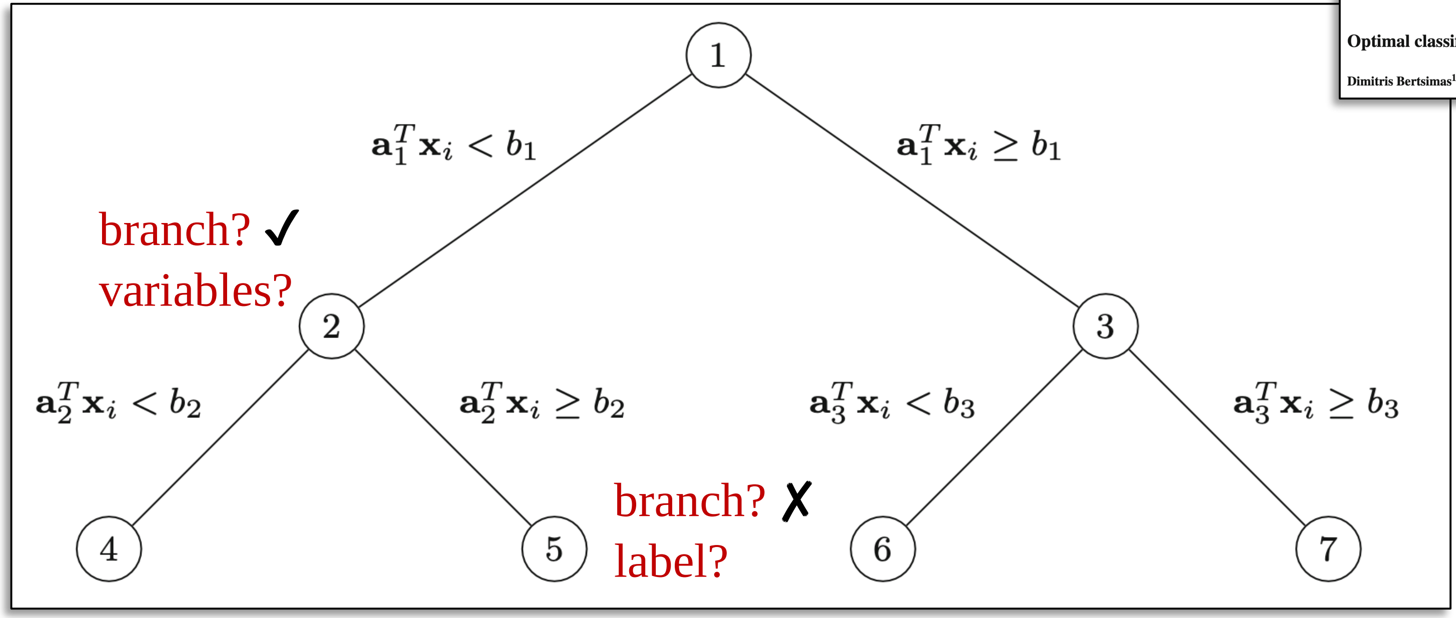
tree

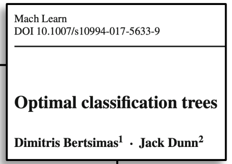
$$\begin{aligned} &\text{minimize} && R_{xy}(T) + \alpha|T| \\ &\text{subject to} && N_x(l) \geq N_{\min}, \quad l \in \text{leaves of } T \end{aligned}$$

number points in leaf l

minimum number of samples in any leaf

OCT - Setup

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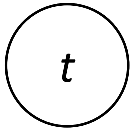
Optimal classification trees

Dimitris Bertsimas[1] · Jack Dunn[2]

$\mathcal{T}_B$: branch nodes

$\mathcal{T}_l$: leaf nodes



$p(t)$: parent node of t

$A(t)$: set of ancestors of node t

$A_L(t)$: "left" ancestors of node t

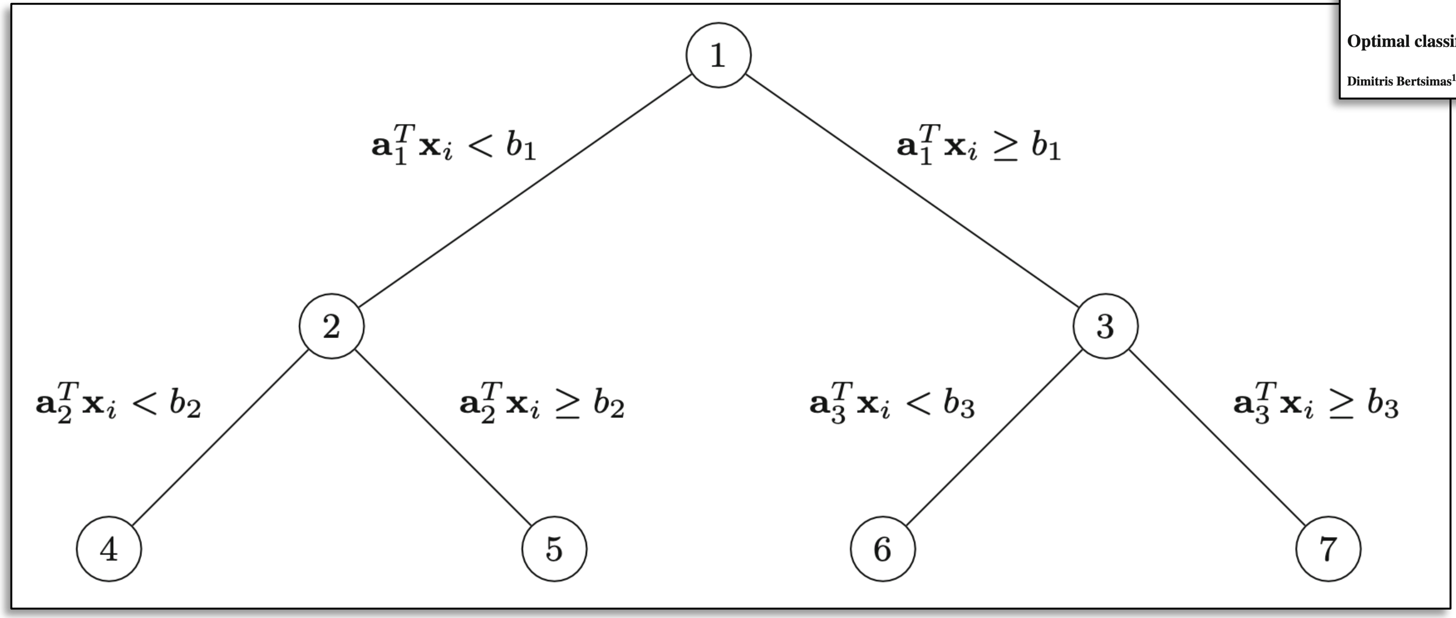
$A_R(t)$: "right" ancestors of node t

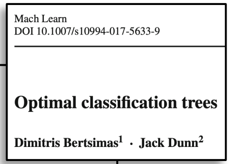
$$A_L(5) = \{1\},\ A_R(5) = \{2\}$$

$$A(t) = A_L(t) \cup A_R(t)$$

OCT – Splitting Constraints

Univariate Trees





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Optimal classification trees

Dimitris Bertsimas[1] · Jack Dunn[2]

$$\sum_{j=1}^{p} a_{jt} = d_t, \quad t \in \mathcal{T}_B$$

$\boldsymbol{a}_t$: unit vector

$$0 \leq b_t \leq d_t, \quad t \in \mathcal{T}_B$$

$d_t \in \{0, 1\}$: split or not

$$a_{jt} \in \{0, 1\}, \quad j = 1, \ldots, p; \; t \in \mathcal{T}_B$$

$$d_t \leq d_{p(t)}, \; t \in \mathcal{T}_B \backslash \{1\}$$

OCT – Sample Tracking Constraints

Univariate Trees

z_{it} : $\boldsymbol{x}_i$ is in node t or not

l_t : leaf t contains points or not

$$
\begin{aligned}
& z_{it} \le l_t, && t \in \mathcal{T}_L \\
& \textstyle\sum_{i=1}^{n} z_{it} \ge N_{\min} l_t, && t \in \mathcal{T}_L \\
& \textstyle\sum_{t \in \mathcal{T}_L} z_{it} = 1, && i = 1, \dots, n
\end{aligned}
$$

$$
\begin{aligned}
& \boldsymbol{a}_m^{\intercal} \boldsymbol{x}_i + \varepsilon \le b_m + M_1(1 - z_{it}) && i = 1, \dots, n; t \in \mathcal{T}_L \;;\; m \in A_L(t) \\
& \boldsymbol{a}_m^{\intercal} \boldsymbol{x}_i \ge b_m - M_2(1 - z_{it}) && i = 1, \dots, n; t \in \mathcal{T}_L \;;\; m \in A_R(t)
\end{aligned}
$$

OCT – Objective Function

Univariate Trees

$$Y_{ik} = \begin{cases} +1, & \text{if } y_i = k; \\ -1, & \text{otherwise} \end{cases}$$

$$N_{kt} = \frac{1}{2}\sum_{i=1}^{n}(1+Y_{ik})z_{it}, \;\; k=1,\ldots,K; \;\; t \in \mathcal{T}_L$$

$$c_t = \arg\max_{k=1,\ldots,K}\{N_{kt}\} \quad \text{and} \quad c_{kt} = \begin{cases} 1, & \text{if } c_t = k; \\ 0, & \text{otherwise} \end{cases}$$

$$N_t = \sum_{i=1}^{n} z_{it}, \;\; t \in \mathcal{T}_L$$

$$L_t = N_t - \max_{1,\ldots,K}\{N_{kt}\} = \min_{k=1,\ldots,K}\{N_t - N_{kt}\}$$

$$\begin{aligned} L_t &\geq N_t - N_{kt} - M(1-c_{kt}), && k=1,\ldots,K; t \in \mathcal{T}_L, \\ L_t &\leq N_t - N_{kt} + Mc_{kt}, && k=1,\ldots,K; t \in \mathcal{T}_L, \\ L_t &\geq 0, && t \in \mathcal{T}_L \end{aligned}$$

$$(M = n)$$

OCT – Overall Model

Univariate Trees

$$
\begin{aligned}
\text{minimize} \quad & \frac{1}{\hat{L}} \sum_{t \in \mathcal{T}_L} L_t + \alpha \sum_{t \in \mathcal{T}_B} d_t \\
\text{subject to} \quad & L_t \geq N_t - N_{kt} - M(1 - c_{kt}), \quad k = 1, \ldots, K; t \in \mathcal{T}_L, \\
& L_t \leq N_t - N_{kt} + M c_{kt}, \quad k = 1, \ldots, K; t \in \mathcal{T}_L, \\
& L_t \geq 0, \quad t \in \mathcal{T}_L \\
& N_{kt} = \frac{1}{2} \sum_{i=1}^{n} (1 + Y_{ik}) z_{it}, \; k = 1, \ldots, K; \; t \in \mathcal{T}_L \\
& N_t = \sum_{i=1}^{n} z_{it}, \; t \in \mathcal{T}_L \\
& \boldsymbol{a}_m^\intercal \boldsymbol{x}_i + \varepsilon \leq b_m + M_1(1 - z_{it}) \quad i = 1, \ldots, n; \; t \in \mathcal{T}_B; \; m \in A_L(t) \\
& \boldsymbol{a}_m^\intercal \boldsymbol{x}_i \geq b_m - M_2(1 - z_{it}) \quad i = 1, \ldots, n; \; t \in \mathcal{T}_B; \; m \in A_R(t) \\
& z_{it} \leq l_t, \quad t \in \mathcal{T}_L \\
& \textstyle\sum_{i=1}^{n} z_{it} \geq N_{\min} l_t, \quad t \in \mathcal{T}_L \\
& \textstyle\sum_{i=1}^{n} z_{it} = 1, \quad i = 1, \ldots, n \\
& \textstyle\sum_{j=1}^{p} a_{jt} = d_t, \quad t \in \mathcal{T}_B \\
& 0 \leq b_t \leq d_t, \quad t \in \mathcal{T}_B \\
& d_t \leq d_{p(t)}, \; t \in \mathcal{T}_B \backslash \{1\} \\
& z_{it}, l_t \in \{0, 1\}, i = 1, \ldots, n; t \in \mathcal{T}_L, \\
& a_{jt}, d_t \in \{0, 1\}, i = 1, \ldots, n; t \in \mathcal{T}_B
\end{aligned}
$$

$$
\begin{aligned}
\text{minimize} \quad & R_{xy}(T) + \alpha |T| \\
\text{subject to} \quad & N_x(l) \geq N_{\min}, \quad l \in \text{leaves of } T
\end{aligned}
$$

Number of Binary Variables

$$\mathcal{O}(n 2^{D})$$

tree depth

OCT – Take Away Messages

- A large-scale mixed integer optimization model
- Relies heavily on the speed of state-of-the-art solvers (*e.g.*, Gurobi)
- Can be easily extended to splits with hyperplanes (multivariate trees)
- Empirically shown that overfitting does not occur
- The solution time increases drastically with the number of samples and the tree depth
- Random Forest still performs better when it comes to accuracy

Mach Learn
DOI 10.1007/s10994-017-5633-9

Optimal classification trees

Dimitris Bertsimas[1] · Jack Dunn[2]

State-of-the-art

Mach Learn
DOI 10.1007/s10994-017-5633-9

Optimal classification trees

Dimitris Bertsimas[1] · Jack Dunn[2]

n = 5456 ; p = 2 ; K = 4 ; (2017)

Strong Optimal Classification Trees

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n = 3196 ; p = 38 ; K = 2 ; (2021)

The Thirty-Third AAAI Conference on Artificial Intelligence (AAAI-19)

Learning Optimal Classification Trees Using a Binary Linear Program Formulation

Sicco Verwer   Yingqian Zhang

n = 4601 ; p = 57 ; K = 2 ; (2019)

arXiv version 1 (2020) 1-48   Submitted 4/00; Published 10/00

MurTree: Optimal Classification Trees via Dynamic Programming and Search

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Melbourne, Australia

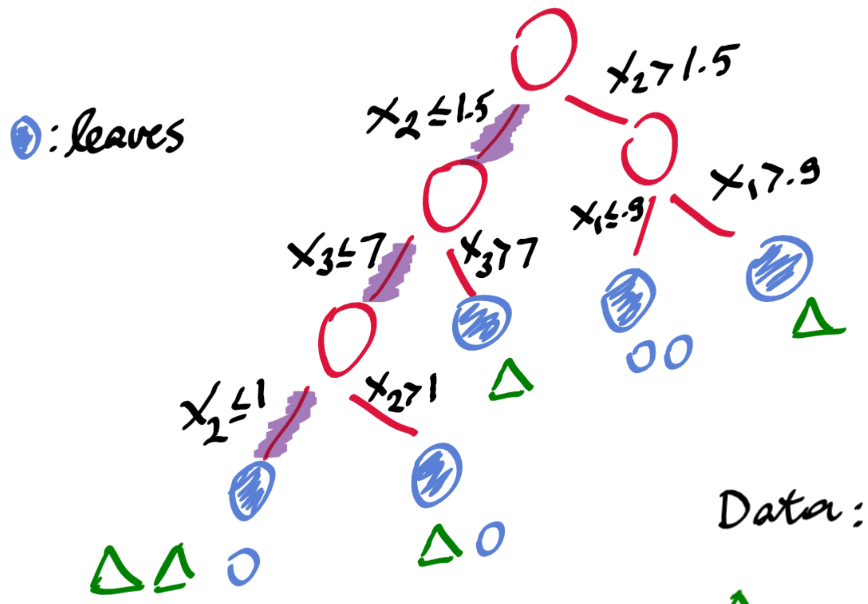
n = 43500 ; p = 181 ; K = 7 ; (2020)

Rules and Rule Set Generation?

RULE-BASED METHODS USING OPTIMIZATION

IF AGE > 25 AND PASTCREDIT = TRUE THEN ACCEPT

DECISION TREES



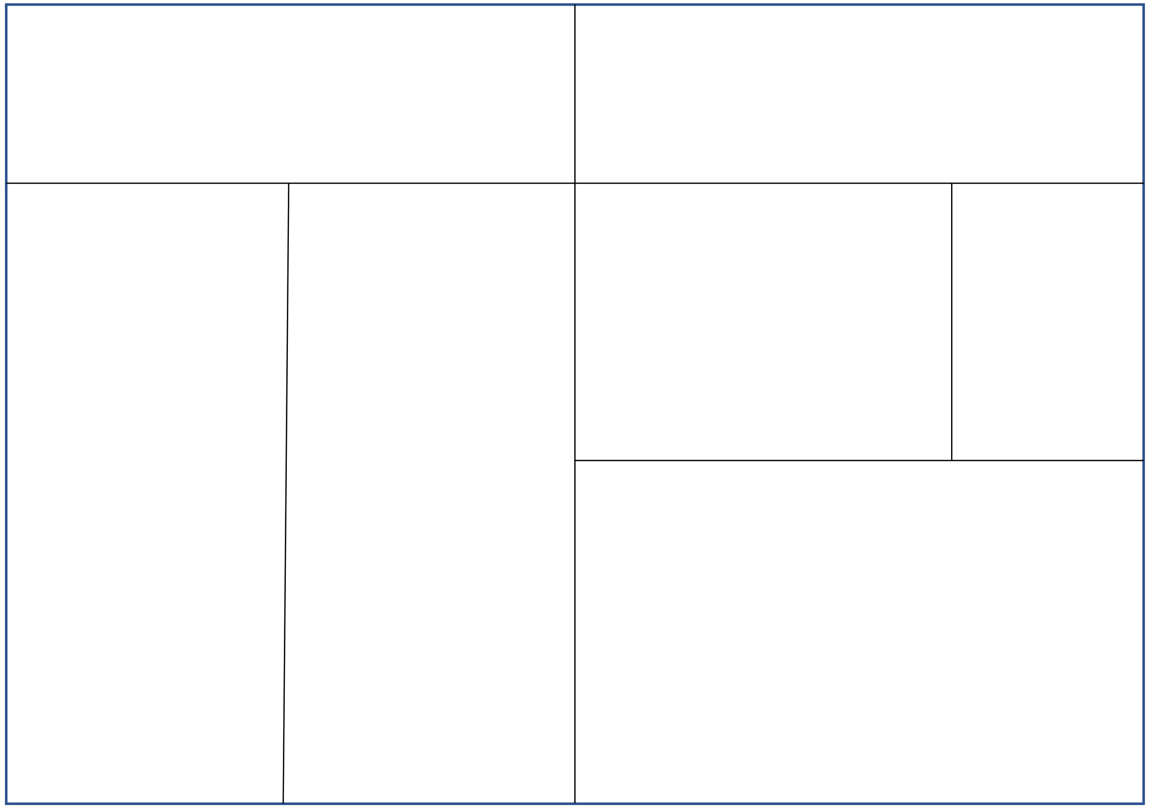
Rule j (leaf) : $X_2 \le 1$ & $X_3 \le 7$

Data: {Δ, Δ, O, Δ, O, O}

Δ ← labels

O ↙

DECISION TREES vs RULES

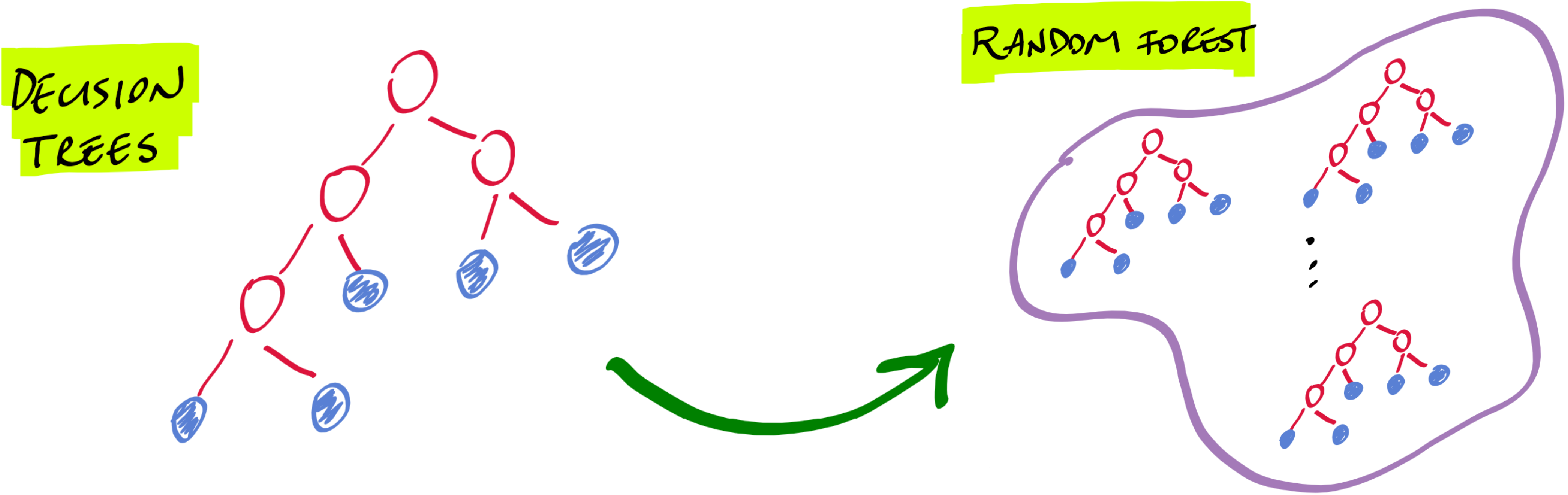


Rules are simple and easy to understand. In some cases they are easier to understand than the decision trees.

What are possible measures for interpretability?

- Set Size (number of rules)
- Rule length (number of clauses)
- Cover (number of samples covered)
- Overlap (between two rules)

Rule Generation



Variance ↓ Accuracy ↑

Interpretability ↓

Rule Generation for Classification: Scalability, Interpretability, and Fairness

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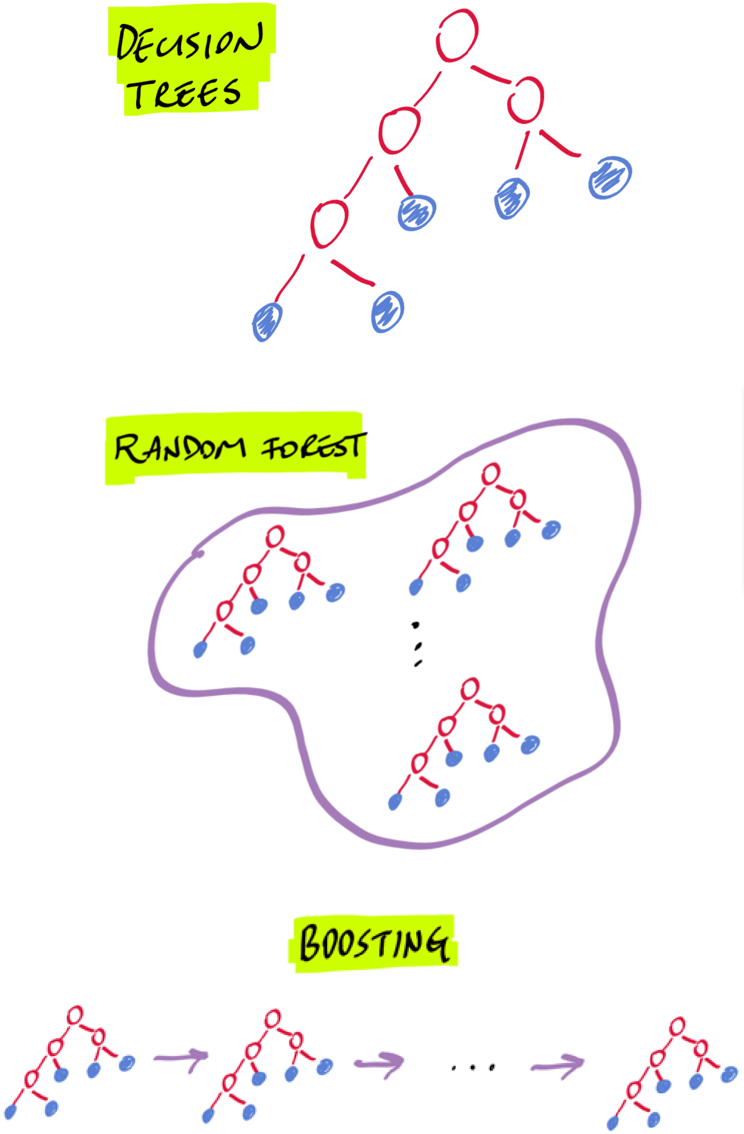
**University of Amsterdam, 11018 TV, Amsterdam P.O. Box 15953, The Netherlands

Scalability

Rules
Rules
Rules
…



Optimization
with
Constraints

$$\cancel{\begin{array}{ll} \text{minimize} & f(\boldsymbol{x}) \\ \text{subject to} & g(\boldsymbol{x}) \geq \mathbf{0}. \end{array}}$$

$$\begin{array}{ll} \text{minimize} & \boldsymbol{c}^\mathsf{T}\boldsymbol{x} \\ \text{subject to} & \boldsymbol{A}\boldsymbol{x} \geq \boldsymbol{b}, \\ & \cancel{\boldsymbol{x} \in \{\mathbf{0}, \mathbf{1}\}}. \end{array}$$

$$\boxed{\begin{array}{ll} \text{minimize} & \boldsymbol{c}^\mathsf{T}\boldsymbol{x} \\ \text{subject to} & \boldsymbol{A}\boldsymbol{x} \geq \boldsymbol{b}, \\ & \boldsymbol{x} \geq \mathbf{0}. \end{array}}$$

LP!

Scalable Rule Generation for Learning

Modeling

$\mathcal{D} = \{(\boldsymbol{x}_i, y_i) : i \in \mathcal{I}\}$

$\boldsymbol{x}_i \in \mathbb{R}^p, y_i \in \{1, \dots, K\}$

$$y_i = k \implies \boldsymbol{y}_i = \Big(-\frac{1}{K-1}, -\frac{1}{K-1}, \dots, \overset{k^{\text{th}}}{1}, \dots, -\frac{1}{K-1}\Big)^\intercal \in \mathbb{R}^K$$

prediction of rule *j* for sample *i* → $\boldsymbol{R}_j(\boldsymbol{x}_i) \in \mathbb{R}^K$

prediction for sample *i* → $$\hat{\boldsymbol{y}}_i(\boldsymbol{w}) = \sum_{j \in J} a_{ij} \boldsymbol{R}_j(\boldsymbol{x}_i) w_j$$

classification loss for sample *i* → $$\mathcal{L}(\hat{\boldsymbol{y}}_i(\boldsymbol{w}), \boldsymbol{y}_i) = \max\{1 - \kappa \hat{\boldsymbol{y}}_i(\boldsymbol{w})^\intercal \boldsymbol{y}_i, 0\}$$

Total Loss → $$\sum_{i \in \mathcal{I}} \underbrace{\mathcal{L}(\hat{\boldsymbol{y}}_i(\boldsymbol{w}), \boldsymbol{y}_i)}_{v_i}$$

set of rules

rule *j* covers sample *i* or not

weight of rule *j*

$\kappa = (K-1)/K$

auxiliary variables

Master Problem

$$\boxed{v_i \geq \max\{1 - \kappa \hat{\boldsymbol{y}}_i(\boldsymbol{w})^\intercal \boldsymbol{y}_i, 0\}}$$

$$\begin{array}{lll}
\text{minimize} & \overbrace{\lambda \sum_{j \in \mathcal{J}} c_j w_j}^{(i)} + \overbrace{\sum_{i \in \mathcal{I}} v_i}^{(ii)} & \\
\text{subject to} & \sum_{j \in \mathcal{J}} \hat{a}_{ij} w_j + v_i \geq 1, & i \in \mathcal{I}, \\
& v_i \geq 0, & i \in \mathcal{I}, \\
& w_j \geq 0, & j \in \mathcal{J}
\end{array}$$

$$\hat{a}_{ij} = \kappa a_{ij} \boldsymbol{R}_j(\boldsymbol{x}_i)^\intercal \boldsymbol{y}_i$$

(i) total **weighted** cost of using rules

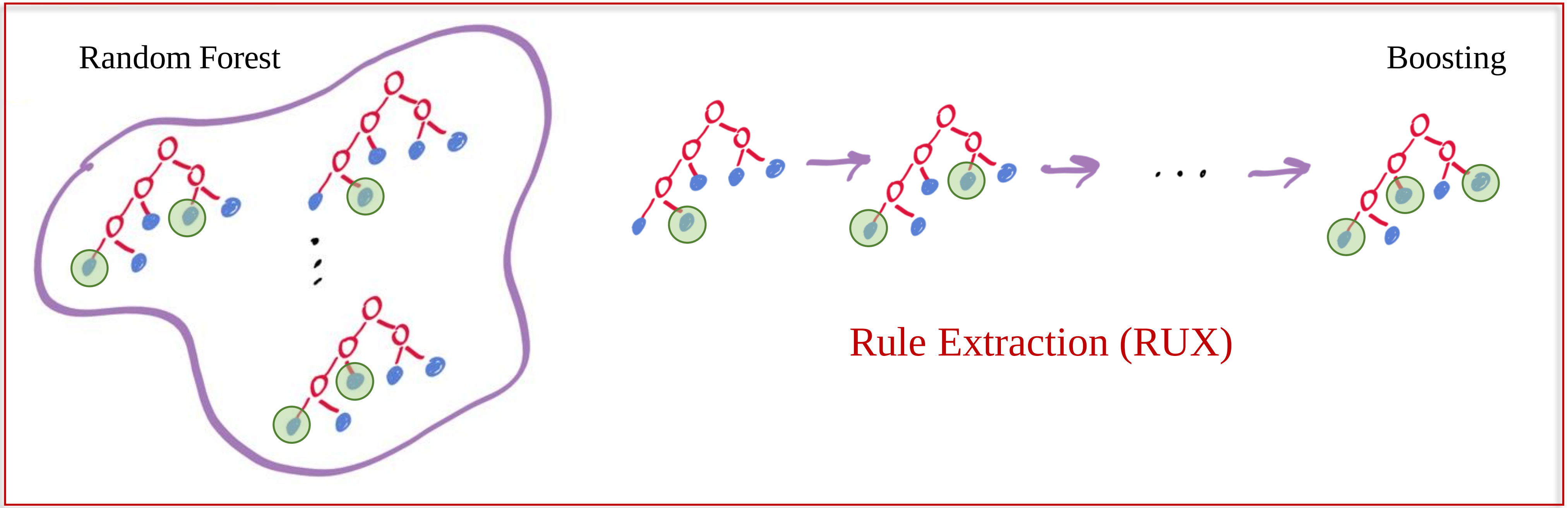
(ii) total loss from misprediction

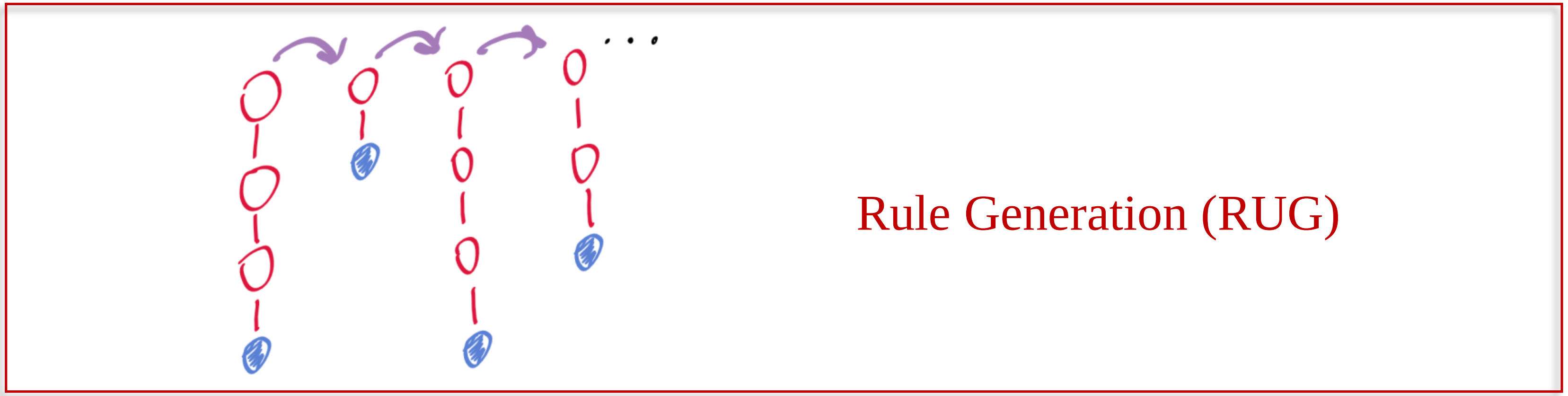
scaling hyperparameter

Set of rules (aka columns)?

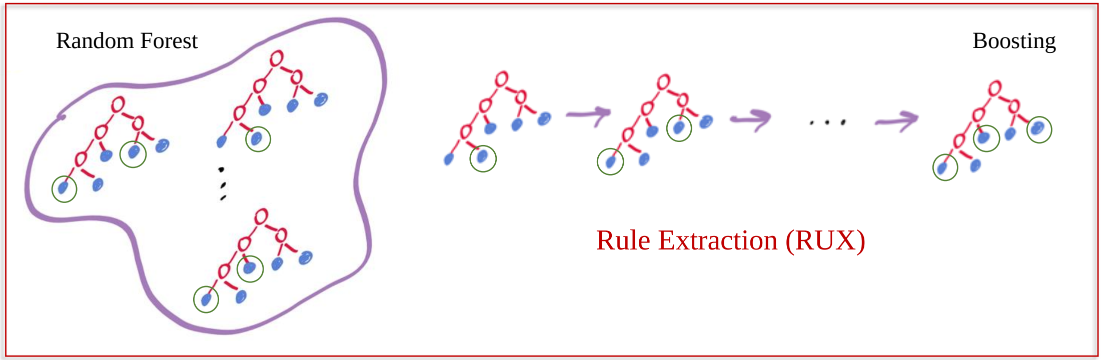
Rule Discovery

Set of rules (aka columns)?





RUX



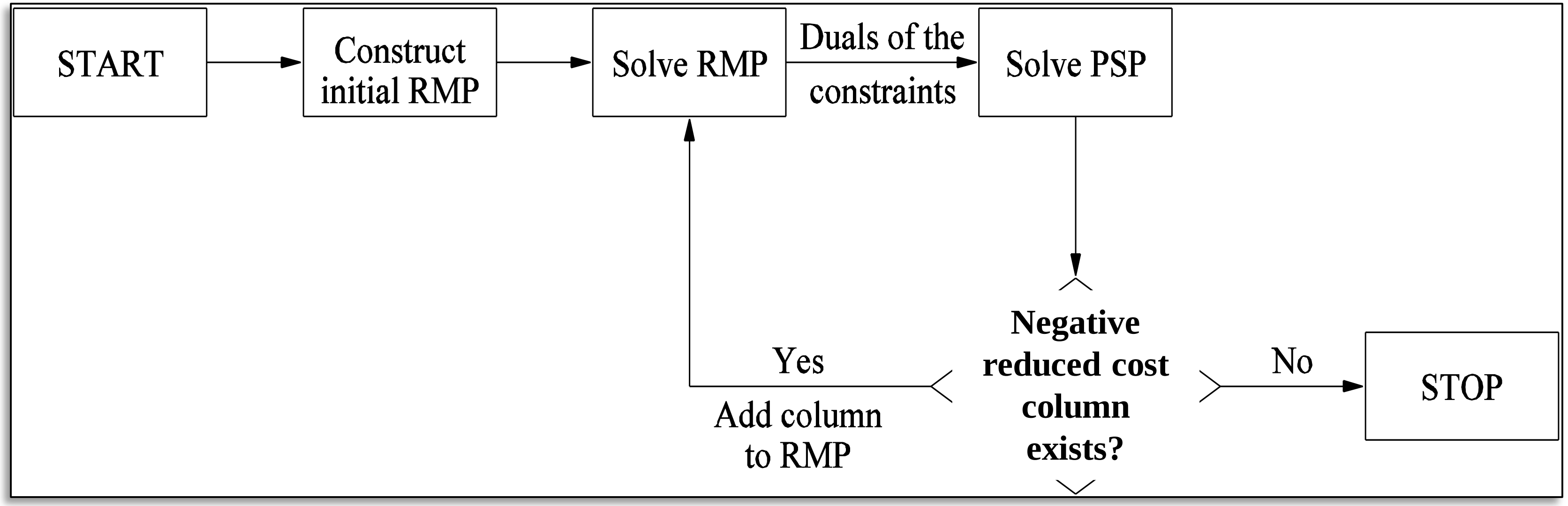
Master Problem

$$
\begin{array}{lll}
\text{minimize} & \lambda \sum_{j\in\mathcal{J}} c_j w_j + \sum_{i\in\mathcal{I}} v_i & \\
\text{subject to} & \sum_{j\in\mathcal{J}} \hat{a}_{ij} w_j + v_i \geq 1, & i \in \mathcal{I}, \\
& v_i \geq 0, & i \in \mathcal{I}, \\
& w_j \geq 0, & j \in \mathcal{J}
\end{array}
$$

Algorithm - Rule Extraction

1: **Input:** training data, $\mathcal{D} = \{(\boldsymbol{x}_i, y_i) : i \in \mathcal{I}\}$
2: Train a tree ensemble to construct rule pool $\mathcal{J}$
3: $\mathcal{J}^* \leftarrow$ Solve master problem using $\mathcal{J}$
4: **return** $\mathcal{J}^*$ and w_j, $j \in \mathcal{J}^*$

Column Generation

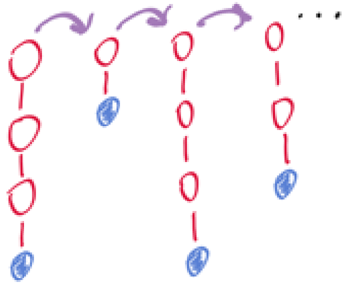


RMP*

$$
\begin{array}{lll}
\text{minimize} & \lambda \sum_{j \in \mathcal{J}_t} c_j w_j + \sum_{i \in \mathcal{I}} v_i & \\
\text{subject to} & \sum_{j \in \mathcal{J}_t} \hat{a}_{ij} w_j + v_i \geq 1, & i \in \mathcal{I}, \\
 & v_i \geq 0, & i \in \mathcal{I}, \\
 & w_j \geq 0, & j \in \mathcal{J}_t
\end{array}
$$

* restricted master problem

RUG



Rule Generation (RUG)

Dual Problem (J_t)

$$
\begin{array}{lll}
\text{maximize} & \sum_{i\in\mathcal{I}} \beta_i & \\
\text{subject to} & \sum_{i\in\mathcal{I}} \hat{a}_{ij}\beta_i \leq \lambda c_j, & j \in \mathcal{J}_t, \\
& 0 \leq \beta_i \leq 1, & i \in \mathcal{I}
\end{array}
$$

PSP*

$$
\min_{j\in\mathcal{J}/\mathcal{J}_t} \left\{ \lambda c_j - \sum_{i\in\mathcal{I}} \hat{a}_{ij}\beta_i^{(t)} \right\}
$$

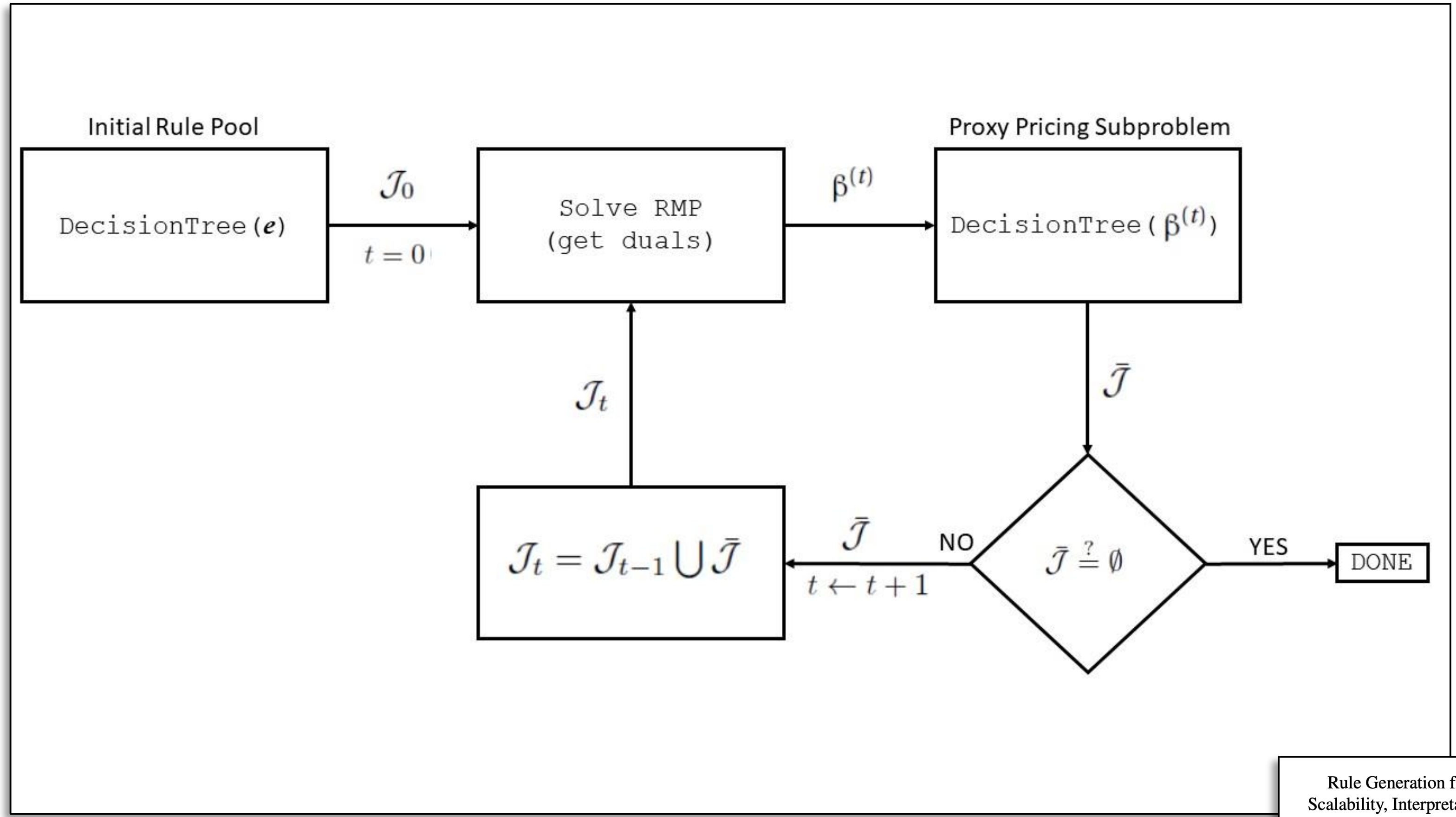
Proposition. *PSP is NP-hard*

* pricing subproblem

Proxy PSP

PSP

$$\min_{j \in \mathcal{J}/\mathcal{J}_t} \left\{ \lambda c_j - \sum_{i \in \mathcal{I}} \hat{a}_{ij} \beta_i^{(t)} \right\}$$



Rule Generation for Classification:
Scalability, Interpretability, and Fairness

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Extensions: Fairness

- Sensitive Attribute (female/male, race, age etc., G)
- Additional constraints are needed.
- There are more than 20 fairness definitions (Verma and Rubin, 2018).
  - Group fairness (Statistical parity):
    $P(\hat{Y}=1 \mid G=m) = P(\hat{Y}=1 \mid G=f)$.
  - Predictive parity:
    $P(Y=1 \mid \hat{Y}=1, G=m) = P(Y=1 \mid \hat{Y}=1, G=f)$.
  - Equal opportunity (False negative rate):
    $P(\hat{Y}=0 \mid Y=1, G=m) = P(\hat{Y}=0 \mid Y=1, G=f)$.
  - Equalized Odds (Disparate Mistreatment):
    $P(\hat{Y}=1 \mid Y=i, G=m) = P(\hat{Y}=1 \mid Y=i, G=f),\ i \in 0, 1$.
  - Overall accuracy equality:
    $P(\hat{Y}=Y, G=m) = P(\hat{Y}=Y, G=f)$.

Binary classification

What happens when there are multiple classes?

Equalized Odds:

$$P(\hat{y}_i \neq y_i | y_i = k, G = g) = P(\hat{y}_j \neq y_j | y_j = k, G = g'), \qquad \forall i, j \in \mathcal{I}, \forall k \in \mathcal{K} \text{ and } \forall g, g' \in \mathcal{G}$$

$$\begin{array}{lll}
\text{minimize} & \lambda \sum_{j \in \mathcal{J}} c_j w_j + \sum_{i \in \mathcal{I}} v_i & \\
\text{subject to} & \sum_{j \in \mathcal{J}} \hat{a}_{ij} w_j + v_i \geq 1, & i \in \mathcal{I}, \\
& v_i \geq 0, & i \in \mathcal{I}, \\
& w_j \geq 0, & j \in \mathcal{J}
\end{array}$$

Fairness Constraints

$$\left\{\begin{array}{ll}
\sum_{i \in \mathcal{P}_{k,1}} v_i - \sum_{i \in \mathcal{P}_{k,2}} v_i \leq \epsilon & \forall k \in \mathcal{K} \text{ and } \forall g, g' \in \mathcal{G} \\
\sum_{i \in \mathcal{P}_{k,2}} v_i - \sum_{i \in \mathcal{P}_{k,1}} v_i \leq \epsilon & \forall k \in \mathcal{K} \text{ and } \forall g, g' \in \mathcal{G}
\end{array}\right.$$

FairRUX

FairRUG

$$\boxed{\mathcal{P}_{k,g} = \{i \in \mathcal{I} : y_i = k, G = g\}}$$

Equal Overall Mistreatment:

$$\sum_{k\in\mathcal{K}} P(\hat{y}_i \neq y_i = k | G = g) = \sum_{k\in\mathcal{K}} P(\hat{y}_i \neq y_i = k | G = g'), \qquad \forall i \in \mathcal{I} \text{ and } \forall g, g' \in \mathcal{G}$$

$$\begin{array}{lll} \text{minimize} & \lambda \sum_{j\in\mathcal{J}} c_j w_j + \sum_{i\in\mathcal{I}} v_i & \\ \text{subject to} & \sum_{j\in\mathcal{J}} \hat{a}_{ij} w_j + v_i \geq 1, & i \in \mathcal{I}, \\ & v_i \geq 0, & i \in \mathcal{I}, \\ & w_j \geq 0, & j \in \mathcal{J} \end{array}$$

Fairness Constraints

$$\sum_{i\in\mathcal{I}_g} v_i - \sum_{i\in\mathcal{I}_{g'}} v_i \leq \epsilon$$

$$\sum_{i\in\mathcal{I}_{g'}} v_i - \sum_{i\in\mathcal{I}_g} v_i \leq \epsilon$$

FairRUX

$$\forall k \in \mathcal{K} \text{ and } \forall g, g' \in \mathcal{G}$$

$$\forall k \in \mathcal{K} \text{ and } \forall g, g' \in \mathcal{G}$$

FairRUG

$$\mathcal{I}_g = \{i \in \mathcal{I} : G = g\}$$

Rule Generation – Take Aways

- Linear programming brings in scalability
- The generated rules come with their associated weights
- Proxy PSP can be solved very fast
- Fairness constraints can be easily added
- There could still be too many rules leading to a less interpretable model
- Accuracy can be inferior compared against ensemble methods

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$n = 245057$; $p = 3$; $K = 2$;
$n = 58509$; $p = 48$; $K = 11$; (2022)

Optional Readings

Interpretable and Fair Boolean Rule Sets via Column Generation

Connor Lawless[1] Sanjeeb Dash[2] Oktay Günlük[1] Dennis Wei[2]

Mach Learn
DOI 10.1007/s10994-017-5633-9

Optimal classification trees

Dimitris Bertsimas[1] · Jack Dunn[2]

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