

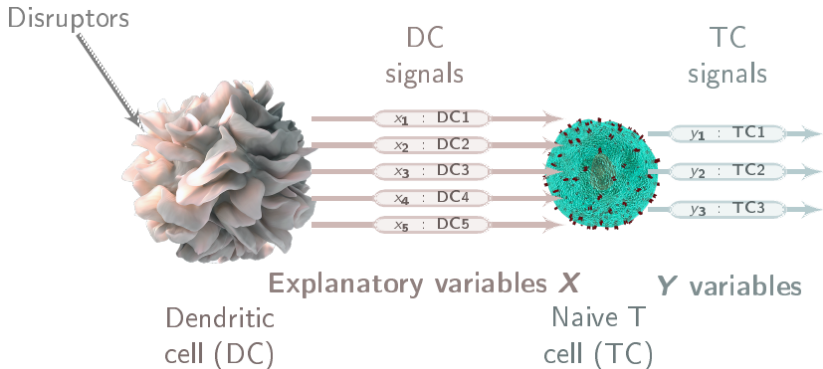
Interpretable Random Forest with Linear Models

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Dialogue between T cells and dendritic cells



Experiments on human blood

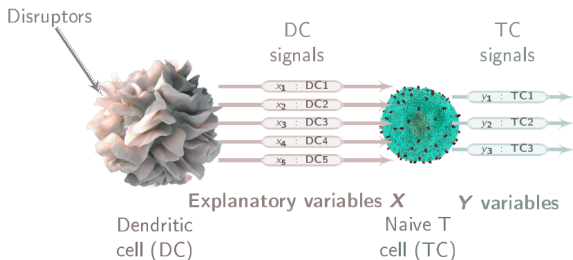


Figure: FIOUUUUUUUUUUU

Context — T cells and dendritic cells relationship

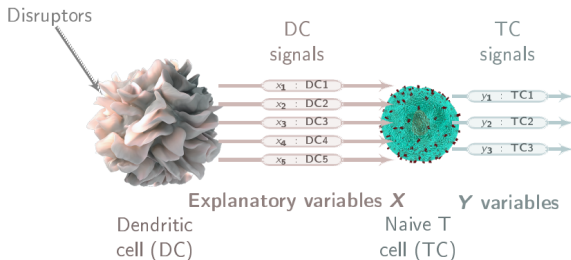
Analyze the *'language'* used by dendritic cells and T cells to communicate with each other:

- types of DC
- types of signals emitted by DC
- simultaneous signals of different natures produced by multiple DC



Project objectives: context specific model, easily interpretable and testable

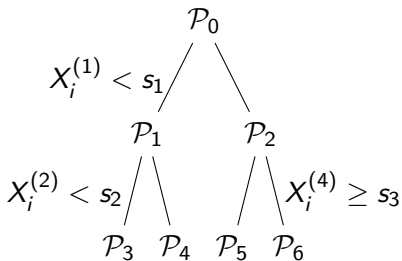
Objectives



- Context specific (relationship between response and explanatory depend on the other explanatory) **Tree ?**
- Stable rules **Forest ?**
- Easily interpretable and testable **SIRUS?**

Context specific : Decision Tree algorithm

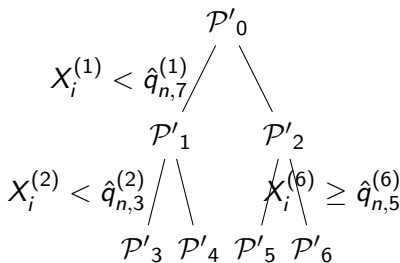
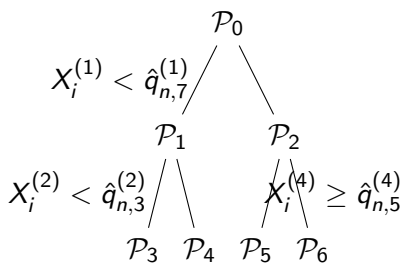
- 1 Determine the explanatory variables and the threshold that best separate the data.
- 2 Distribute data across nodes. Repeat step 1 in each node.
- 3 Stop the algorithm when the stopping criterion is reached.
- 4 Estimate \hat{y} by averaging y in each node



SIRUS: Stable and Interpretable RULE Set¹

Algorithm objective: a random forest to build a set of stable, interpretable decision rules with good predictive capabilities.

- **Step 1: build a forest** (with empirical decile as split values).
- Step 2: select rules according to their appearance frequency in the forest
- Step 3: post-processing : remove rules that are linear combination of more frequent rules (and equal rules).
- Step 4: rules agregation.

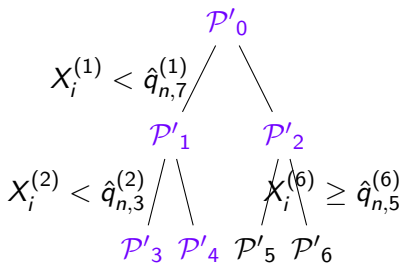
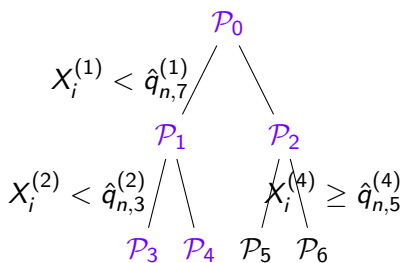


¹Bénard, Biau, Da Veiga, Scornet (2021)

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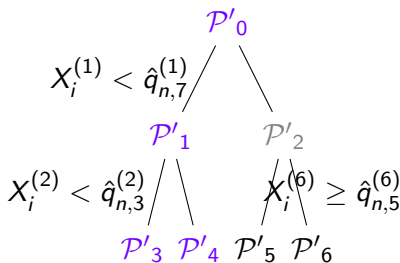
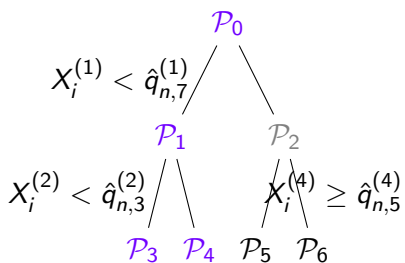


²Bénard, Biau, Da Veiga, Scornet (2021)

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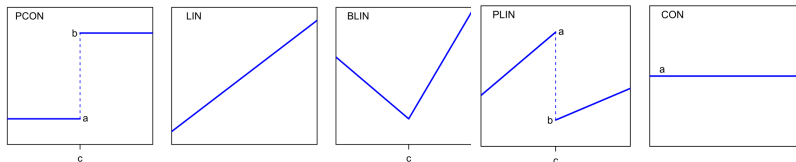
$$(\hat{\beta}_0, \hat{\beta}) = \operatorname{argmin}_{\beta, \beta_0} \|Y - \beta_0 \mathbf{1}_n - \beta \Gamma_{n, p_0}\| + \lambda \|\beta\|_2^2,$$

with Γ_{n, p_0} a $n \times R$ matrix containing the rules values.

⁴Bénard, Biau, Da Veiga, Scornet (2021)

Decision Tree, PILOT algorithm

PILOT⁵: Piecewise Linear Organic Tree, decision tree in which each node can be associated with a different model.



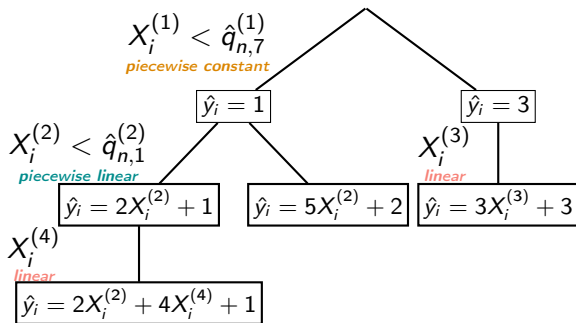
For each node choose the variable $X^{(j)}$ and type t that minimise

$$n \log \left(\frac{RSS(X^{(j)}, t)}{n} \right) + \nu \log(n), \text{ with}$$

- $RSS(X^{(j)}, t)$ residuals sum of square after the node
- ν a penalty parameters depending on t

⁵Raymaekers, Rousseeuw, Verdonck, Yao (2024)

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Decision tree: simple structure but instability.

Random Forest: set of decision trees.

- each tree is built on a subsample of the data
- for each node, the algorithm selects a subset of the explanatory variables

⇒ Powerful predictivity, less instability.

⇒ BUT *black box*: high number of operations.

Random Forest with PILOT tree: Random Forest Featuring Linear Extensions (RaFFLE) ⁷.

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Stable Piecewise Linear Interpretable Model

Main idea Extract interpretable rules from a forest of PILOT trees.

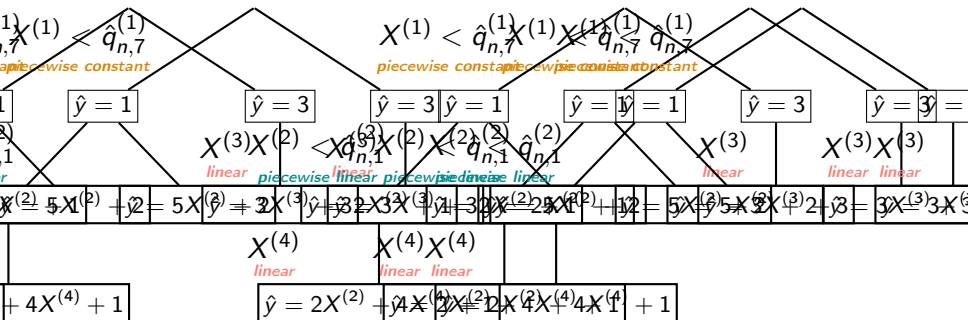
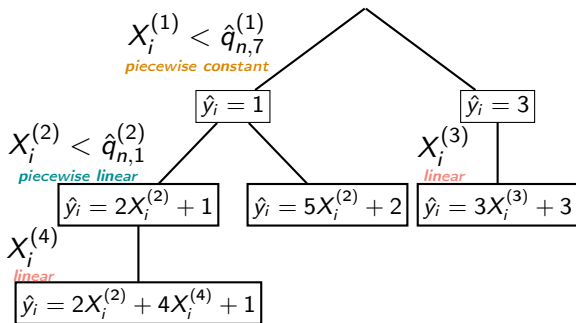


Figure: Glouups on n'y voit rien !

Difference from SIRUS : rules are not piecewise constant.

Rules extraction from PILOT Trees



Rules (Variables)

- $\mathbb{1}_{X^{(1)} < \hat{q}_{n,7}^{(1)}}$
- $\mathbb{1}_{X^{(1)} < \hat{q}_{n,7}^{(1)}} \mathbb{1}_{X^{(2)} < \hat{q}_{n,1}^{(2)}}$
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- $\mathbb{1}_{X^{(1)} < \hat{q}_{n,7}^{(1)}} \mathbb{1}_{X^{(2)} < \hat{q}_{n,1}^{(2)}} X^{(4)}$
- $\mathbb{1}_{X^{(1)} < \hat{q}_{n,7}^{(1)}} \mathbb{1}_{X^{(2)} \geq \hat{q}_{n,1}^{(2)}} X^{(2)}$
- $\mathbb{1}_{X^{(1)} \geq \hat{q}_{n,7}^{(1)}}$
- $\mathbb{1}_{X^{(1)} \geq \hat{q}_{n,7}^{(1)}} X^{(3)}$

Stable Piecewise Linear Interpretable Model

Algorithm 1 SPLIM

Require: Training data $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$, number of trees T , frequency threshold s

Output: Aggregated predictor $\hat{m}(\cdot)$

- 1: Initialize an empty multiset of rules \mathcal{R}
 - 2: **for** $t = 1$ to T **do**
 - 3: Draw a bootstrap sample \mathcal{D}_t from \mathcal{D}
 - 4: Fit a PILOT tree on \mathcal{D}_t
 - 5: Extract all rules from the fitted tree and add them to \mathcal{R}
 - 6: **end for**
 - 7: Compute the empirical frequency of each rule $r \in \mathcal{R}$
 - 8: Retain rules whose empirical frequency exceeds s
 - 9: Decompose retained rules into sub-rules and fit a ridge regression
-

EXPERIMENTS

$$X \in \mathbb{R}^{n,p} \quad , X \sim \mathcal{N}(0, \Sigma)$$
$$Y = f(X) + \epsilon \quad , \epsilon \sim \mathcal{N}(0, \sigma)$$

Parameters:

- n number of observations, p number of explanatory variables
- σ noise on Y , correlation matrix Σ
- data simulation configuration (function f)

Simulation study — Framework

with $f(X)$ corresponding to several configurations:

Scheme name	Definition of $f(X)$
CSTE	$\begin{cases} 1, & \text{if } X_1 > q_{0.5, X_1}, \\ 0, & \text{otherwise.} \end{cases}$
REG3	$\begin{cases} X_3 + 1.2, & \text{if } X_1 > q_{0.5, X_1} \text{ and } X_2 > q_{0.5, X_2}, \\ 0.7, & \text{otherwise.} \end{cases}$
REG5	$\begin{cases} X_1 + X_2 + 1.2, & \text{if } X_1 > q_{0.5, X_1}, \\ X_3, & \text{otherwise.} \end{cases}$
EXP	$\begin{cases} \exp(X^{(2)}) + 1.2, & \text{if } X^{(1)} > q_{0.5, X_1}, \\ \exp(X^{(3)}), & \text{otherwise.} \end{cases}$

RMSE: Root Mean Square Error on test sample.

True Positive Rate: proportion of variables correctly included in the model.

False Positive Rate: ... wrongly ...

Simulation study — RMSE comparison

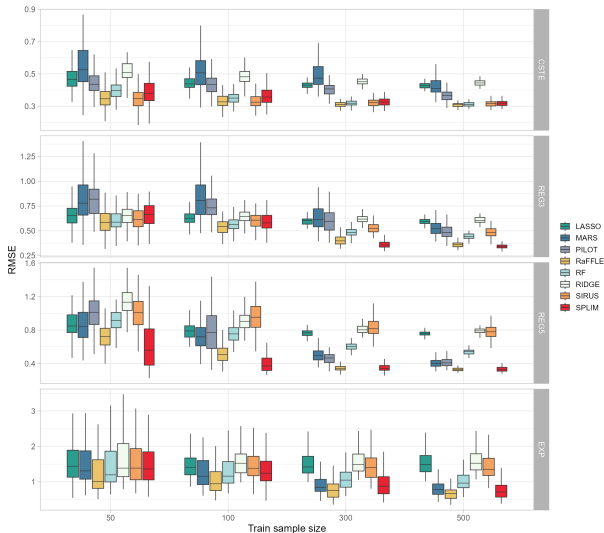


Figure: Root Mean Square Error (RMSE) on test samples across 100 batches, comparing different algorithms.

Simulation study — TPR/FPR comparison

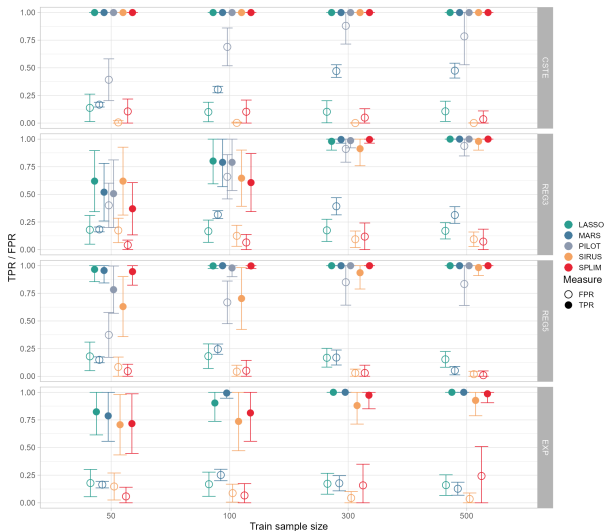


Figure: True and False Positive Rates on test samples across 100 batches, comparing different algorithms.

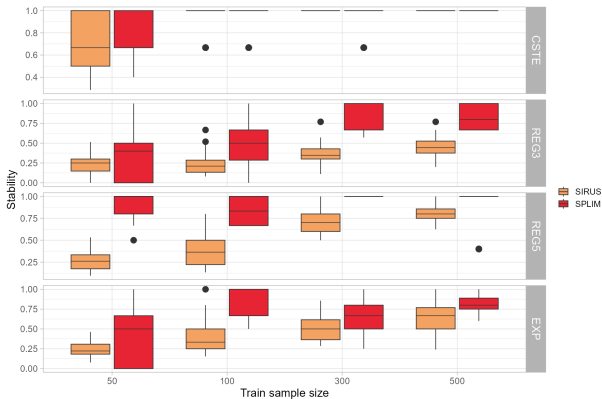


Figure: Stability on 10 fold CV dataset.

$$S(\mathcal{R}_1, \mathcal{R}_2) = \frac{2 \times |\mathcal{R}_1 \cap \mathcal{R}_2|}{|\mathcal{R}_1| + |\mathcal{R}_2|}$$

Conclusions:

- SPLIM is well-suited to the problem, and perform similarly to or better than SIRUS and RaFFLE.

Perspectives:

- Wait for feedback from the biologists
- Build a multivariate algorithm

Thank you for your attention!