



Random forest for functional data

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ECAS-SFdS course on random forest
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FRANÇAISE

*Liberté
Égalité
Fraternité*

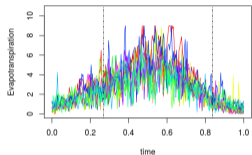
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➤ Functional data in a nutshell

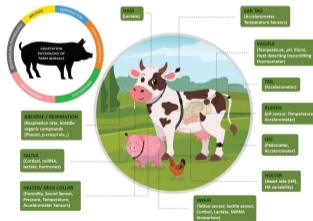
Functional data... just functions (in mathematical sense)

[Ramsay and Silverman, 2005, Ramsay and Silverman, 2002].

Examples: time series (mostly): weather, wearable sensors, chemometrics spectra, ...

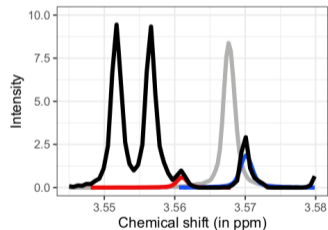


[Picheny et al., 2019]



[Neethirajan, 2020]

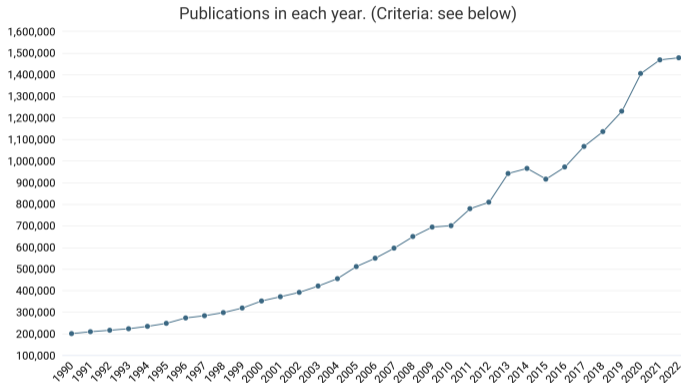
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[Lefort et al., 2021]



Time series is the new trend?



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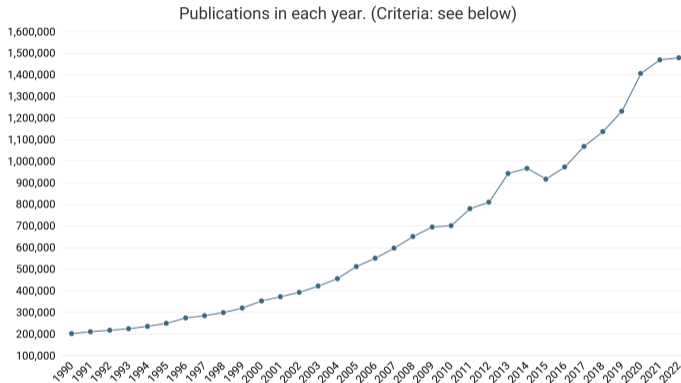
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Time series is the new trend?



Disclaimer: Forecasting is a specific case, not covered by this class



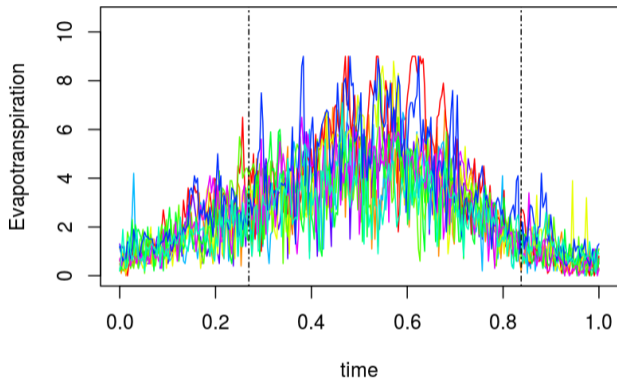
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➤ Scientific question

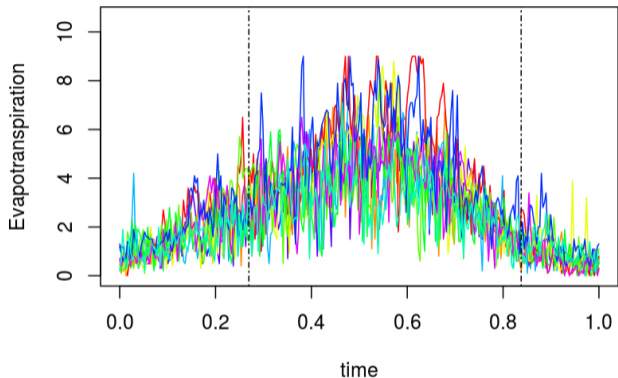


?



Purpose: prediction of a target quantity (e.g., yield) from functional data (e.g., weather time series)

➤ Scientific question



?



Purpose: prediction of a target quantity (e.g., yield) from functional data (e.g., weather time series)

Here: ? = random forest

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➤ Extensions of random forest for time series

▶ Similarity based techniques

- ▶ Proximity forest [[Lucas et al., 2019](#)] (restricted to classification)
- ▶ Fréchet forest [[Capitaine et al., 2020](#)]

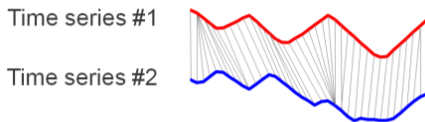


Image by courtesy of Charlotte Pelletier

➤ Extensions of random forest for time series

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▶ Interval based techniques

- ▶ Time Series Forest [[Deng et al., 2013](#)] and its extension [[Middlehurst et al., 2020](#)]
- ▶ RISE [[Lines et al., 2018](#)]



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▶ Dictionnary or symbolic representation based techniques:

- ▶ TS-CHIEF [[Shifaz et al., 2020](#)] (combines all types of splits including dictionnary based splits based on work of [[Schäfer, 2015](#)])
- ▶ (multivariate time series) symbolic representation of time series [[Baydogan and Runger, 2015](#)]



Similarity based techniques

Interval based techniques

Dictionnary or symbolic representation based techniques

Improving interpretability: interval selection



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> You don't know what to do with your time series?

Use distances! (or kernels)

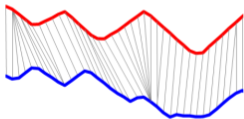
Numeric time series

DTW [Sakoe and Chiba, 1978],

Derivative DTW

[Keogh and Pazzani, 2001], ...

Time series #1



Time series #2

See: R package **TSclust**

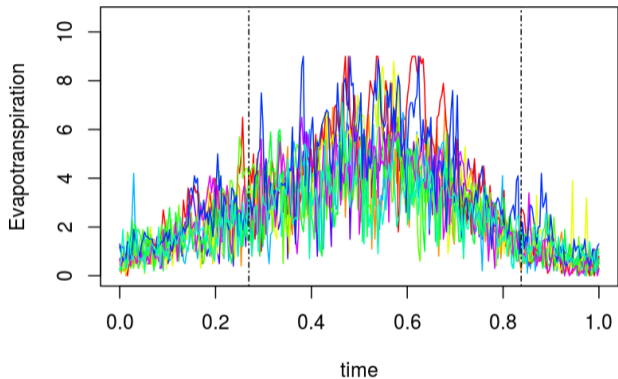
Categorical time series

χ^2 -metric, optimal matching, edit distances, ...

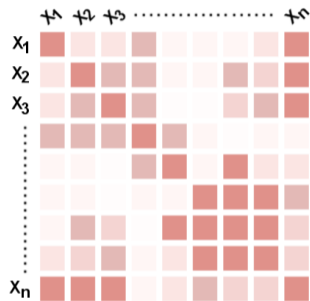
[Massoni et al., 2013, Studer and Ritschard, 2016]

Same	Different in			
	Distribution	Spell Durations	Timing	Sequencing
States				
States + Distribution	=			
Sequencing				=
Sequencing + Distribution	=			=

Use distances!



?

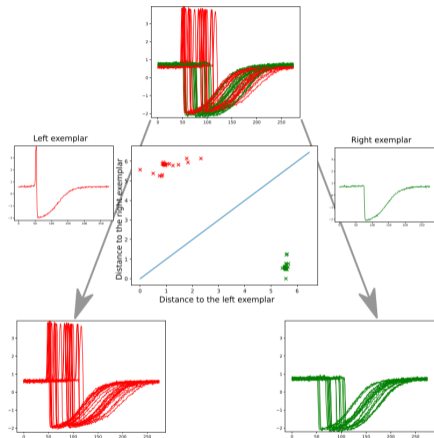


But now: I don't have variables anymore to define splits!

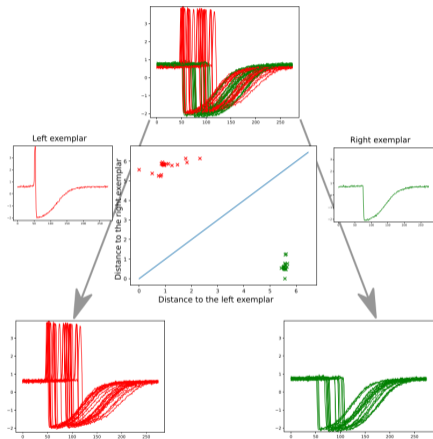


➤ Proximity forest [Lucas et al., 2019] (classification only)

Splits defined by **splitter pairs** and distances.



Proximity forest [Lucas et al., 2019] (classification only)

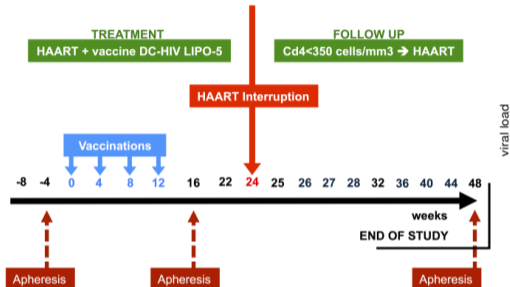


Splits defined by **splitter pairs** and distances.

In practice: select best “splitter” pair among R (5) randomly chosen splitter pairs using Gini.

➤ Generalization: Fréchet forests [Capitaine et al., 2020]

Inputs: repeated time series



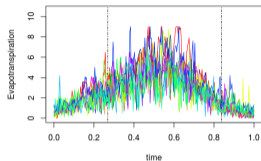
Example: $n = 17$ patients \times $p = 5,398$ gene expression time series

Goal: predict viral load (also time series)

Notation: $X_i = (X_i^{(1)}, \dots, X_i^{(p)})$ where $X_i^{(j)} \in (\mathcal{X}_j, d_j)$ (metric space)
 $Y_i \in (\mathcal{Y}, d)$ (also a metric space)

some slides by courtesy of R. Genuer

Basics on Fréchet things... (similar to kernels)



?



Can I compute distances and variance just using d_j ?



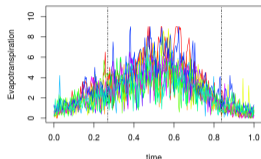
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➤ Basics on Fréchet things... (similar to kernels)



?



Can I compute distances and variance just using d_j ?

Yes! [Fréchet, 1906, Peterson and Müller, 2019]:

- ▶ empirical Fréchet mean of $(X_i^{(j)})_{i \in \mathcal{C}}$:

$$\overline{X^{(j)}} \in \arg \min_{z \in (\mathcal{X}_j, d_j)} \frac{1}{|\mathcal{C}|} \sum_{i \in \mathcal{C}} d_j^2(X_i^{(j)}, z)$$

- ▶ empirical Fréchet variance:

$$\mathcal{V}_{\mathcal{C}} = \frac{1}{|\mathcal{C}|} \sum_{i \in \mathcal{C}} d_j^2(X_i^{(j)}, \overline{X^{(j)}})$$

> In short: Fréchet split for $X^{(j)}$

1. Fréchet 2-means [Genolini et al., 2016] \rightarrow partition of $(X_i^{(j)})_{i \in \mathcal{C}}$ into \mathcal{C}_L^j and \mathcal{C}_R^j

➤ In short: Fréchet split for $X^{(j)}$

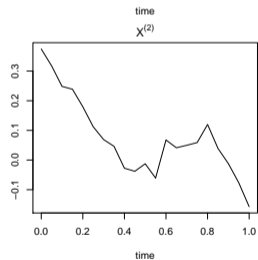
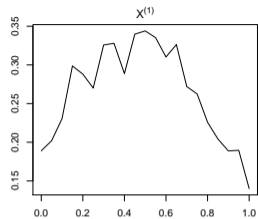
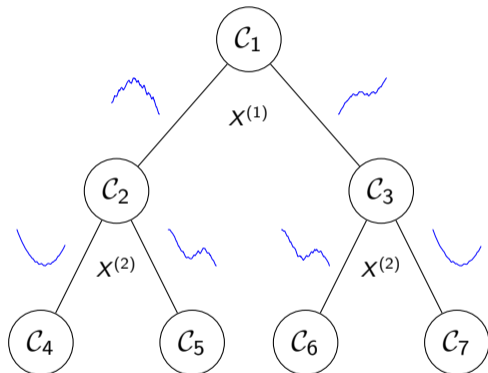
1. Fréchet 2-means [Genolini et al., 2016] → partition of $(X_i^{(j)})_{i \in \mathcal{C}}$ into \mathcal{C}_L^j and \mathcal{C}_R^j
2. Quality of split:

$$\Phi^{(j)}(\mathcal{C}) = \left(\frac{|\mathcal{C}_L^j|}{|\mathcal{C}|} \Phi(\mathcal{C}_L^j) + \frac{|\mathcal{C}_R^j|}{|\mathcal{C}|} \Phi(\mathcal{C}_R^j) \right)$$

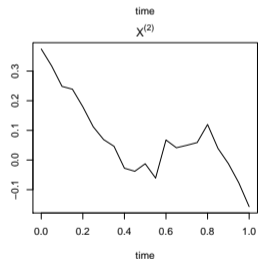
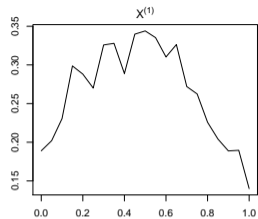
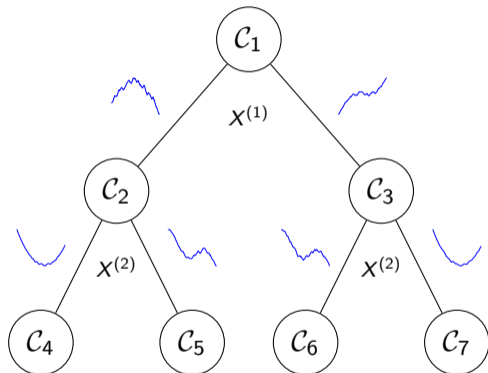
with Φ : Fréchet variance of Y



> In short: Fréchet tree



➤ In short: Fréchet tree



prediction: Fréchet mean of Y in C_5



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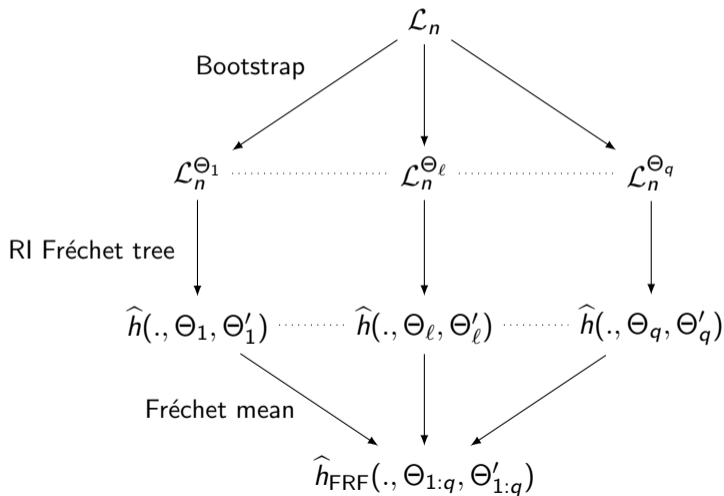
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➤ Summary: Fréchet random forests

<https://github.com/Lcapitaine/FrechForest/tree/master> (R package)



➤ Take home message of similarity based RF

▶ Proximity forest

- ▶ splits based on random draw of two functions (X)
- ▶ nodes based on distances between functions
- ▶ restricted to classification

▶ Fréchet forest

- ▶ splits and nodes based on distance based 2-means
- ▶ more suited for multivariate function inputs
- ▶ adapted to any type of outputs



Similarity based techniques

Interval based techniques

Dictionary or symbolic representation based techniques

Improving interpretability: interval selection



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> Time Series Forest

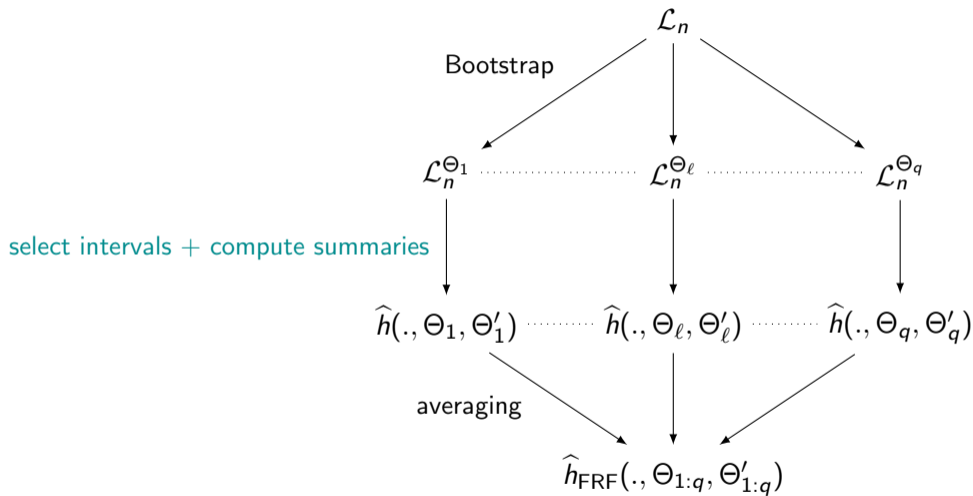
Basic principles:

1. for a given tree: random sampling of intervals
2. for a given tree: compute summaries (mean, sd, slope for [Deng et al., 2013])
3. define splits as usual based on these summaries

Implemented in Python package **ptys** (contains also most transformations or preprocessings described in this class).

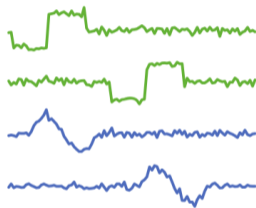


Time Series Forest



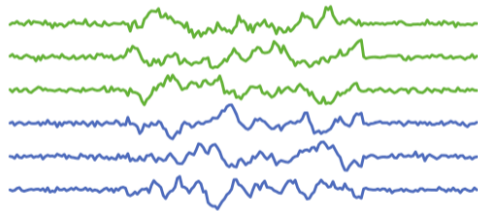
➤ More on summaries for time-series

- ▶ add more summaries: catch22 [Middlehurst et al., 2020]
- ▶ use basis decomposition, power spectrum (Fourier) or auto-correlation features [Lines et al., 2018] (HIVE-COTE)



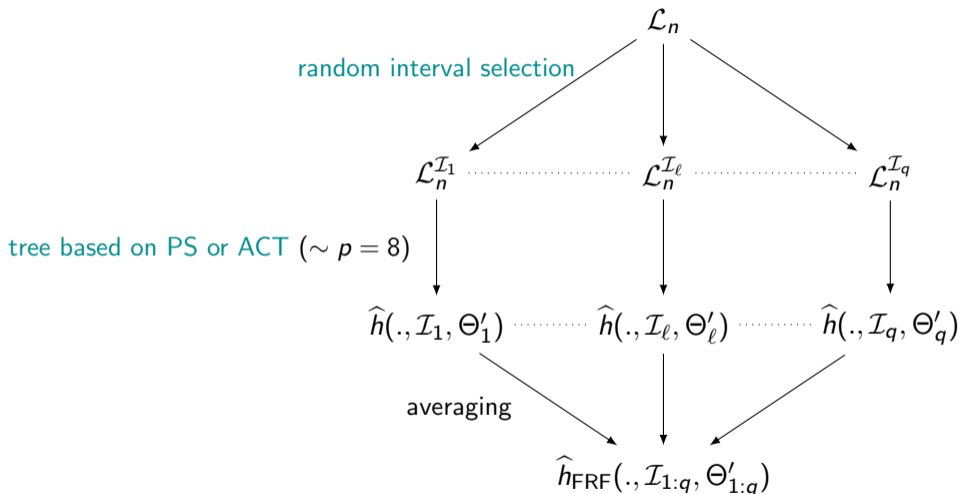
$$X(t) = \sum_{j=1}^P \beta_j \phi_j(t)$$

(ϕ_j : basis functions)
 $\rightarrow (\beta_j)_j \subset \mathbb{R}^P$



$$X_i \rightarrow \text{FFT} \in \mathbb{R}^T$$

Random Interval Spectral Ensemble (RISE) [Lines et al., 2018]



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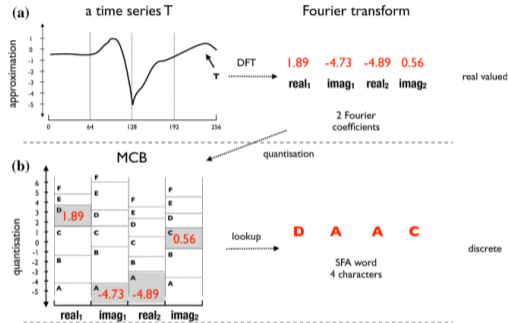
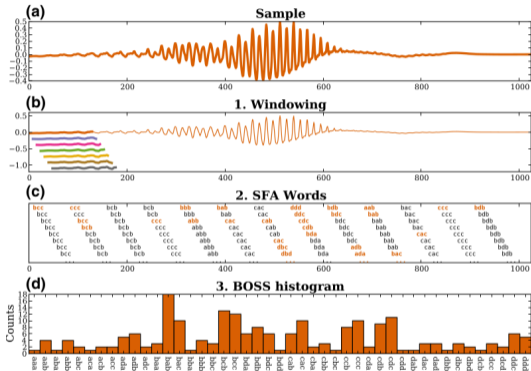
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Symbolic representations based on FFT and windowing

BOSS [Schäfer, 2015]



Based on: Fourier transform then symbolic representation.

A Java implementation exists.



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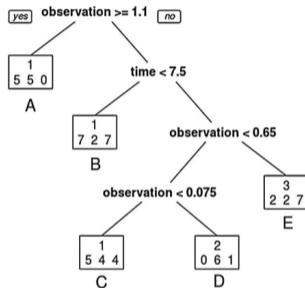
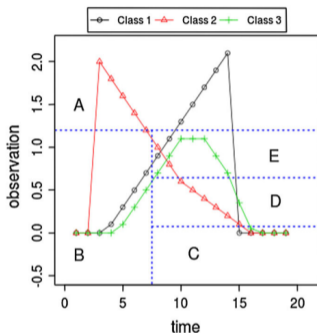
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Symbolic representation based on trees

[Baydogan and Runger, 2015]



Recode $X_i(t_k)$ using the tree partitionning (A, B, C, D, E) = proportion of the time series in each class.

$X_i \rightarrow \mathbb{R}^{\sum_{t=1}^T N_t}$ (N_t : number of partitions induced by tree t).

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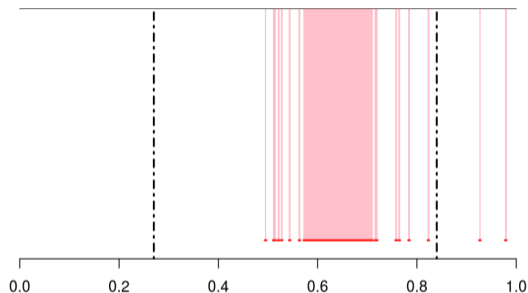
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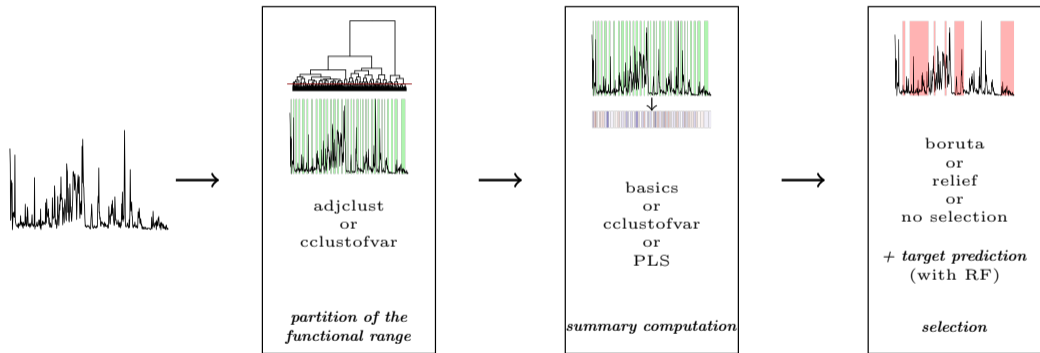
> Scientific question



Purpose: Improve interpretability by selecting the most predictive intervals.

➤ Overview of SFCB (Selection Forest for funCtion Based predictions)

[Servien and Vialaneix, 2023], R package **SISIR**



➤ A focus on partition of the functional range

Two unsupervised and data-driven methods:

- ▶ **Constrained hierarchical clustering** [[Randriamihamison et al., 2021](#)] as in R package **adjclust** [[Ambroise et al., 2019](#)]: correlations between time steps + kernel based HC



> A focus on partition of the functional range

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- ▶ **Clustering of variables** (**ClustOfVar**, [[Chavent et al., 2012](#)]; also hierarchical and also based on correlation but using PCA-like criterion) but constrained to contiguity (implementation available in **SISIR**)

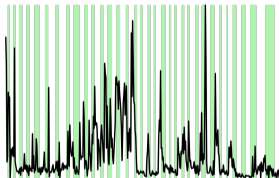
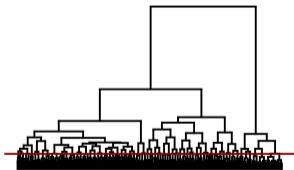


➤ A focus on partition of the functional range

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Output: dendrogram + cut \Rightarrow intervals (or hierarchy or intervals)



➤ A focus on summary of intervals

Three methods:

- ▶ **Unsupervised**: mean and sd

➤ A focus on summary of intervals

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- ▶ **Unsupervised**: mean and sd
- ▶ **Supervised**: 1st PLS component (same idea in [[Poterie et al., 2019](#)] for group-based RF; or other authors ...)

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- ▶ **for cClustOfVar only**: composite variable obtained from **ClustOfVar** (similar to PC)

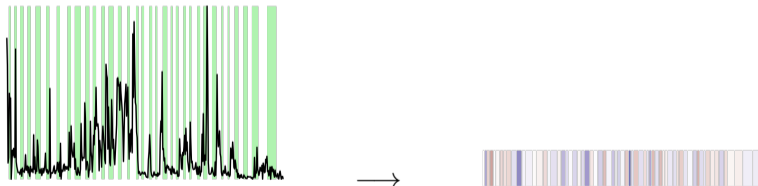


➤ A focus on summary of intervals

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Output: \mathbb{R}^K vector



> A focus on variable selection

Two methods:

- ▶ RF based variable selection: Boruta [[Kursa and Rudnicki, 2010](#)] (other methods available like the excellent **VSURF** [[Genuer et al., 2015](#)], see [[Speiser et al., 2019](#), [Degenhardt et al., 2019](#)])

I am so eager to know more!!



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- ▶ a standard VS method: Relief (extended to regression [[Kira and Rendell, 1992](#), [Robnik-Šikonja and Kononenko, 1997](#)])

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➤ A focus on variable selection

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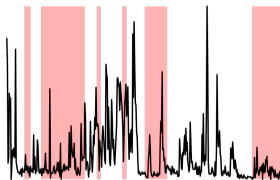
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- ▶ a standard VS method: Relief (extended to regression [[Kira and Rendell, 1992](#), [Robnik-Šikonja and Kononenko, 1997](#)])

I am so eager to know more!!

Output: selected summaries corresponding to intervals

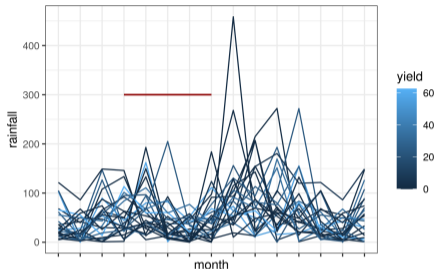




Application to black truffle & weather time series



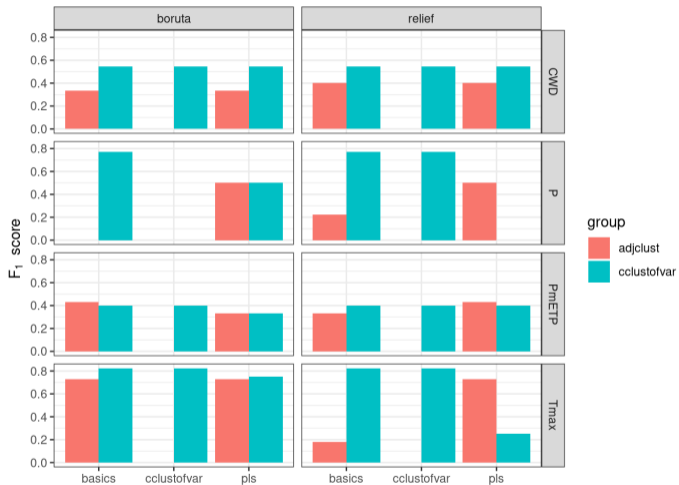
Dataset courtesy from authors of [Baragatti et al., 2019] and fully available at <https://doi.org/10.57745/KMH2GP>.



- ▶ X : $p = 15$ monthly measures (4: rainfall, sun, ...) from January of year N to March of year $N + 1$ for $N \in \llbracket 1925, 1949 \rrbracket$ ($n = 25$)
- ▶ Y : yield of truffles year $N + 1$
- ▶ expert knowledge of important periods for each weather measurement



A brief overview of the comparison between variants

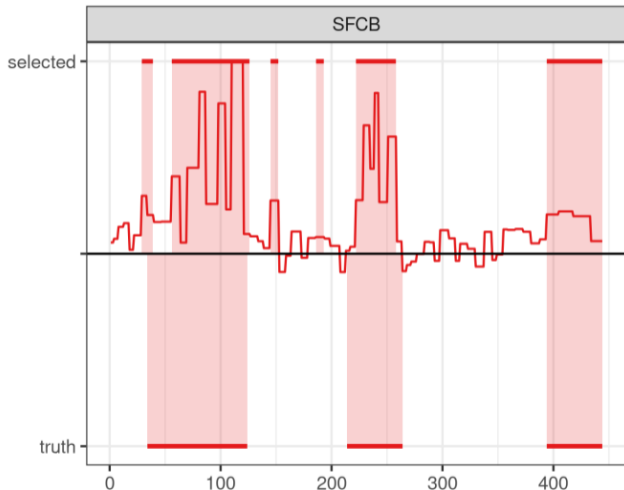


➤ On simulated dataset

- ▶ X : 1,000 weather daily time series (WACSGen simulator [Flecher et al., 2010]) –
 $p = 444$
- ▶ Y :

$$y_i = \log(1 + |\langle x_i, \beta \rangle|) + \epsilon_i,$$

- ▶ β : piecewise constant as “truth” on the left
- ▶ $\epsilon_i \sim \mathcal{N}(0, 0.5)$



End of the story!

Questions?

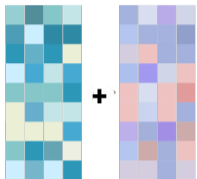


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RF + VI computation

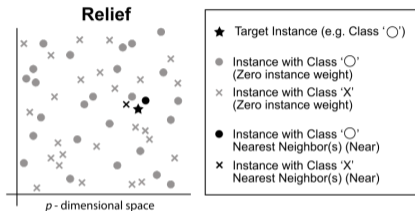


compare:

$VI(j)$ $\max_j VI(j)$

- 1: **repeat**
- 2: augment dataset with randomized shadow copies
- 3:
- 4: train random forest and compute VI
- 5: compute $ZMOCK := \max_{j: \text{copies}} VI(j)$
- 6: Decision: for j in initial variables
- 7: **if** $VI(j) > ZMOCK$ **then**
- 8: j is selected
- 9: **else**
- 10: **if** $VI(j)$ rejected by Student's test for ZMOCK **then**
- 11: j is rejected
- 12: **end if**
- 13: **end if**
- 14: **until** all variables have been given a decision or Tmax iterations have been performed





Iterative computation of weights:

1. pick an observation i at random
2. update weights of variable j :

$$w_j = w_j - (x_{ij} - x_{\text{nearest hit},j})^2 + (x_{ij} - x_{\text{nearest miss},j})^2$$

Back

> Credits

- ▶ Evolution of the number of publications on time series has been obtained from <https://app.dimensions.ai>
- ▶ corn harvest image is “récolte du maïs à Épône (Yvelines)” by Spedona, from [Wikimedia Commons](#)
- ▶ DTW image is courtesy of Charlotte Pelletier
- ▶ Proximity forest split image is taken from [[Lucas et al., 2019](#)]
- ▶ Design of experiment image for vaccine trial is taken from [[Capitaine et al., 2020](#)]
- ▶ Fréchet tree, related time series and Fréchet forest images are courtesy of Robin Genuer (and adapted to my needs)
- ▶ BOSS images are taken from [[Schäfer, 2015](#)]
- ▶ tree recoding image is taken from [[Baydogan and Runger, 2015](#)]
- ▶ black truffle basket image is “A basket of Summer black truffles from Mercato Gourmet by Giando” by Peachyeung316, from [Wikimedia Commons](#)
- ▶ Relief method image is “Illustration of Relief neighbor selection for scoring.” by Docurbs from [Wikimedia Commons](#)

The rest is my own work.

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