Optimal Decision Trees for Complex Data

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Dolores Romero Morales[2]

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[2]Copenhagen Business School, Frederiksberg, Denmark

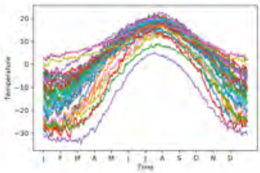
New Bridges between Mathematics and Data Science

November 9th 2021

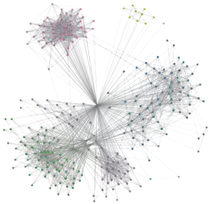
Vectorial

	name	surname	age	weight	height
0	Jorge	Perez	24	50	170
1	Pepe	Garcia	27	60	175
2	Aria	Jimenez	26	70	180
3	Maria	Ruz	25	75	181
4	Luisa	Perez	24	50	170
5	Luisa	Perez	24	50	170

Functional



Network



Image

Text


ham What you doing?how are you?
ham Ok lar... Joking wif u oni...
ham dun say so early hor... U c already then say...
ham MY NO. IN LUTON 0125698789 RING ME IF UR AROUND! H*
ham Siva is in hostel aha:-.
ham Cos i was out shopping wif darren jus now n i called him 2 ask wat present
wan lor. Then he started guessing who i was wif n he finally guessed darren lor.
spam FreeMsg: Txt: CALL to No: 86888 & claim your reward of 3 hours talk time to
use from your phone now! ubscribe6GBP/ mnth inc 3hrs 16 stop?txtStop
spam Sunshine Quiz! Win a super Sony DVD recorder if you canname the capital of
Australia? Text MQUIZ to 82277. B
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02/09/03! This is our 2nd attempt to contact YOU! Call 0871-872-9758 BOX95QU

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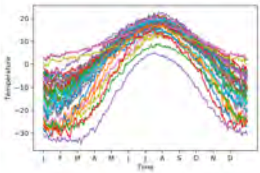

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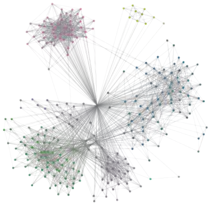

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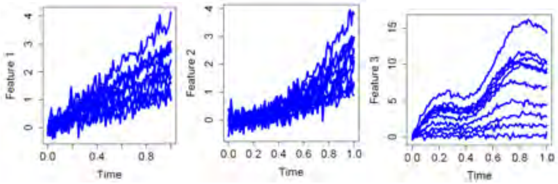

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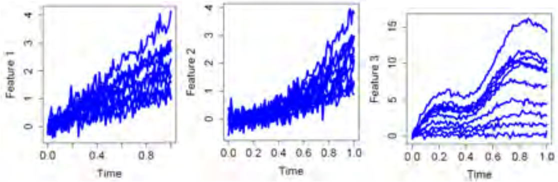

- High interest in the literature.
  - Ferraty and Vieu [2006], Goia and Vieu [2016], Ramsay and Silverman [2002]

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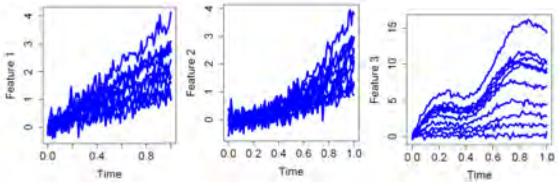


- High interest in the literature.
  - Ferraty and Vieu [2006], Goia and Vieu [2016], Ramsay and Silverman [2002]
- Real world applications:

Speech recognition

Rossi and Villa [2008]

Client segmentation

Laukaitis and Rackauskas [2005]

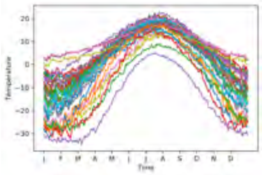
Physical processes

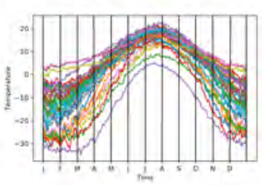
Muñoz and González [2010]

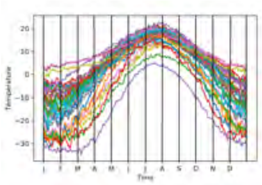
Chemical processes

Blanquero et al. [2016a,b]

Standard multivariate techniques



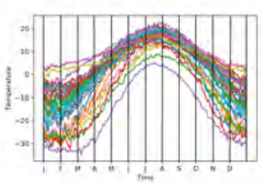

Temperature
Time
J
F
M
A
M
J
J
A
S
O
N
D



Standard multivariate techniques can be applied to *discretized* functional data

Linear Regression, SVM, Trees and RF, among others.

Standard multivariate techniques



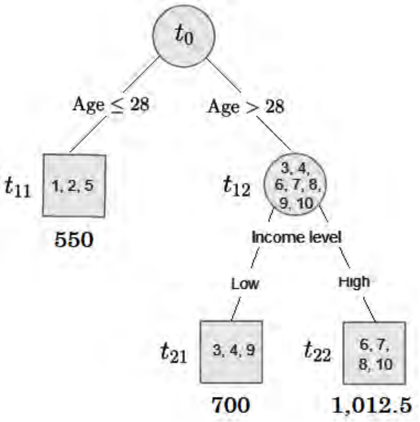
Standard multivariate techniques can be applied to *discretized* functional data

Linear Regression, SVM, Trees and RF, among others.

Serious drawbacks, Horváth and Kokoszka [2012]

- Curse of dimensionality, Vieu [2018].
- Bad representation of the data, Griswold et al. [2008].
- Lack of interpretation, Febrero et al. [2007]
- Intrinsic characteristics of functional data are not exploited, Borggaard and Thodberg [1992].

Individual	Age	Income level	Rent expense
1	22	Low	500
2	26	High	600
3	30	Low	700
4	32	Low	750
5	20	High	550
6	45	High	1100
7	60	High	900
8	54	High	1000
9	50	Low	650
10	48	High	1050



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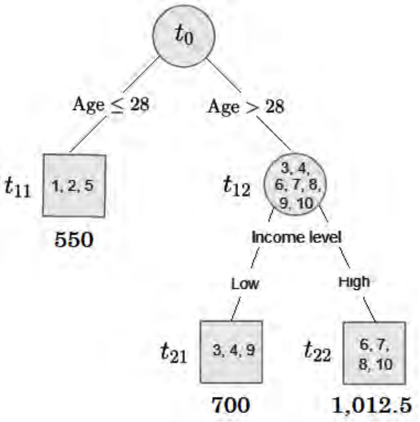

Popular tree methods are greedy:

CHAID, CART, C4.5 and C5.0, among others.

Literature review

Carrizosa et al. [2021], Mathematical optimization in classification and regression trees, TOP, 29(1):5-33.

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Mixed Integer Linear Optimization (MILO)

- Aghaei et al. [2020]
- Bertsimas and Dunn [2017]
- Firat et al. [2020]
- Günlük et al. [2021]
- Hu et al. [2019], Lin et al. [2020]
- Verwer et al. [2019]
- Zantedeschi et al. [2020]
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Optimal Classification and Regression Trees

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Constraint Programming

- Verhaeghe et al. [2019]

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Continuous Optimization

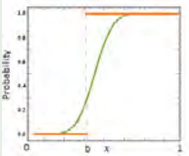
- Blanquero et al. [2021, 2020a, 2020b]

Optimal Randomized Classification and Regression Trees

Our proposal for vectorial data

Blanquero et al. [2021, 2020a, 2020b]

- We model probabilistic (as opposed to deterministic) splitting rules, defined through a CDF $F(\cdot)$:



- We seek a tradeoff between *accuracy* and *interpretability*.

Additionally:

- Local explanability.
- Counterfactual explanability.
- Cost sensitivity.
- Fairness.

Optimal Randomized Classification and Regression Trees

Aim

Adapt previous models to deal with **functional data**

Blanquero et al. [2021, 2020a, 2020b]

with two additional goals:

- Detection of *critical intervals* for prediction.
- Use of a *small number of critical intervals*, as well as a *small proportion of the curves*.

- A sample of N individuals represented by

$$\left(x_{i1}, \dots, x_{ip_1}, x_{ip_1+1}(\cdot), \dots, x_{ip_1+p_2}(\cdot), y_i\right), \quad i = 1, \dots, N,$$

where

$x_{ij} \in \mathbb{R}, \ j = 1, \dots, p_1$ *Vectorial*

$x_{ij}(\cdot) : [0,1] \to \mathbb{R}, \ j = p_1 + 1, \dots, p_1 + p_2$ *Functional*

$y_i \in \mathbb{R}$ *Response*

Jiménez-Cordero and Maldonado, 2021.

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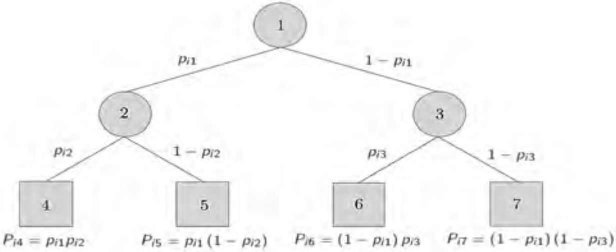
- A maximal binary tree of depth D, with branch τ_B and leaf τ_L nodes.



- *Oblique splits* at branch nodes $t \in \tau_B$:

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$$\sum_{j=1}^{p_1} a_{jt} x_{ij} \qquad + \; \mu_t, \; i = 1, \ldots, N$$

a_{jt}	coefficient of vectorial variable $j = 1, \ldots, p_1$,
μ_t	intercept,

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$$\sum_{j=1}^{p_1} a_{jt} x_{ij} + \sum_{j=p_1+1}^{p_1+p_2} \int_0^1 a_{jt}(s) x_{ij}(s) ds + \mu_t, \; i = 1, \ldots, N$$

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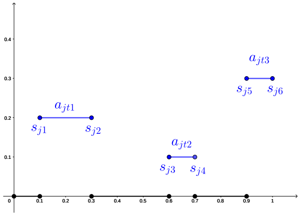

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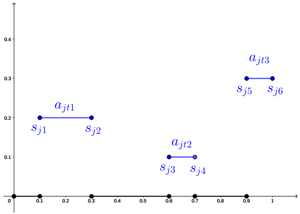

$$a_{jt}(s) = \begin{cases} 0, & \text{if } s \notin \bigcup_{k=1}^{K} [s_{j,2k-1}, s_{j,2k}] \\ \dfrac{a_{jtk}}{s_{j,2k} - s_{j,2k-1}}, & \text{if } s \in [s_{j,2k-1}, s_{j,2k}], \\ & k = 1, \ldots, K \end{cases}$$

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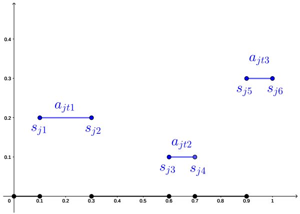

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Notation

- *Oblique splits* at branch nodes $t \in \tau_B$:

$$\sum_{j=1}^{p_1} a_{jt} x_{ij} + \sum_{j=p_1+1}^{p_1+p_2} \sum_{k=1}^{K} \frac{a_{jtk}}{s_{2k} - s_{2k-1}} \int_{s_{j,2k-1}}^{s_{j,2k}} x_{ij}(s)ds + \mu_t, \ \ i = 1, \dots, N$$

a_{jt}	coefficient of vectorial variable $j = 1, \dots, p_1$,
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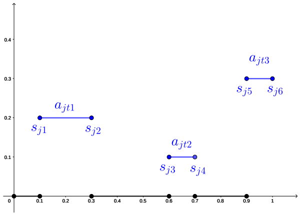

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- *Probabilities* tailored to each individual $i = 1, \ldots, N$:

$$p_{it}\left(\boldsymbol{a}_t, \mu_t, \boldsymbol{s}\right) = F\left(\sum_{j=1}^{p_1} a_{jt}x_{ij} + \sum_{j=p_1+1}^{p_1+p_2}\sum_{k=1}^{K} \frac{a_{jtk}}{s_{j,2k} - s_{j,2k-1}} \int_{s_{j,2k-1}}^{s_{j,2k}} x_{ij}(s)ds + \mu_t\right), \;\; t \in \tau_B.$$

$$P_{it}\left(\boldsymbol{a}, \boldsymbol{\mu}, \boldsymbol{s}\right) = \prod_{t_l \in \mathcal{N}_L(t)} p_{it_l}\left(\boldsymbol{a}_{t_l}, \mu_{t_l}, \boldsymbol{s}\right) \prod_{t_r \in \mathcal{N}_R(t)} \left(1 - p_{it_r}\left(\boldsymbol{a}_{t_r}, \mu_{t_r}, \boldsymbol{s}\right)\right), \;\; t \in \tau_L.$$

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- *Linear predictions* at leaf nodes $t \in \tau_L$:

$$\varphi_{it}\left(\tilde{\boldsymbol{a}}_t, \tilde{\mu}_t, \boldsymbol{s}\right) = \sum_{j=1}^{p_1} \tilde{a}_{jt} x_{ij} + \sum_{j=p_1+1}^{p_1+p_2} \sum_{k=1}^{K} \frac{\tilde{a}_{jtk}}{s_{j,2k} - s_{j,2k-1}} \int_{s_{j,2k-1}}^{s_{j,2k}} x_{ij}(s) ds + \mu_t, \; i = 1, \ldots, N$$

$\tilde{a}_{jt}$ coefficient of vectorial variable $j = 1, \ldots, p_1$,
$\tilde{a}_{jtk}$ coefficient of functional variable $j = p_1 + 1, \ldots, p_1 + p_2$, $k = 1, \ldots, K$,
$\tilde{\mu}_t$ intercept.

$$
\begin{aligned}
\underset{\substack{(\boldsymbol{a},\boldsymbol{\mu})\in\mathbb{R}^{(p_1+p_2K+1)|\tau_B|}\\ (\tilde{\boldsymbol{a}},\tilde{\boldsymbol{\mu}})\in\mathbb{R}^{(p_1+p_2K+1)|\tau_L|}\\ \boldsymbol{s}\in\mathbb{R}^{2p_2K}}}{\text{minimize}} \quad & \frac{1}{N}\sum_{i=1}^{N}\left(\sum_{t\in\tau_L} P_{it}\left(\boldsymbol{a},\boldsymbol{\mu},\boldsymbol{s}\right)\varphi_{it}\left(\tilde{\boldsymbol{a}}_t,\tilde{\mu}_t,\boldsymbol{s}\right)-y_i\right)^2 \text{ (MSE)}\\
& +\lambda^{\text{local}}\sum_{j=1}^{p_1+p_2}\left\|(\boldsymbol{a}_j,\tilde{\boldsymbol{a}}_j)\right\|_1 \text{ (less coefficients)}\\
& +\lambda^{\text{global}}\sum_{j=1}^{p_1+p_2}\left\|(\boldsymbol{a}_j,\tilde{\boldsymbol{a}}_j)\right\|_\infty \text{ (less variables)}\\
& +\lambda^{\text{interval}}\sum_{j=p_1+1}^{p_1+p_2}\sum_{k=1}^{K}\left\|(\boldsymbol{a}_{jk},\tilde{\boldsymbol{a}}_{jk})\right\|_\infty \text{ (less intervals)}\\
& +\lambda^{\text{length}}\sum_{j=p_1+1}^{p_1+p_2}\sum_{k=1}^{K}\left(s_{j,2k}-s_{j,2k-1}\right) \text{ (less proportion of curves)}\\
\text{s.t.} \quad & s_{j,k}\leq s_{j,k+1},\ j=p_1+1,\ldots,p_1+p_2,\ k=1,\ldots,K-1
\end{aligned}
$$

The model

$$
\begin{aligned}
\underset{\substack{(\boldsymbol{a},\boldsymbol{\mu})\in\mathbb{R}^{(p_1+p_2K+1)|\tau_B|}\\ (\tilde{\boldsymbol{a}},\tilde{\boldsymbol{\mu}})\in\mathbb{R}^{(p_1+p_2K+1)|\tau_L|}\\ \boldsymbol{s}\in\mathbb{R}^{2p_2K}}}{\text{minimize}} \quad & \frac{1}{N}\sum_{i=1}^{N}\left(\sum_{t\in\tau_L} P_{it}\left(\boldsymbol{a},\boldsymbol{\mu},\boldsymbol{s}\right)\varphi_{it}\left(\tilde{\boldsymbol{a}}_t,\tilde{\mu}_t,\boldsymbol{s}\right) - y_i\right)^2 \text{ (MSE)}\\
& + \lambda^{\text{local}}\sum_{j=1}^{p_1+p_2}\left\|\left(\boldsymbol{a}_j,\tilde{\boldsymbol{a}}_j\right)\right\|_1 \text{ (less coefficients)}\\
& + \lambda^{\text{global}}\sum_{j=1}^{p_1+p_2}\left\|\left(\boldsymbol{a}_j,\tilde{\boldsymbol{a}}_j\right)\right\|_\infty \text{ (less variables)}\\
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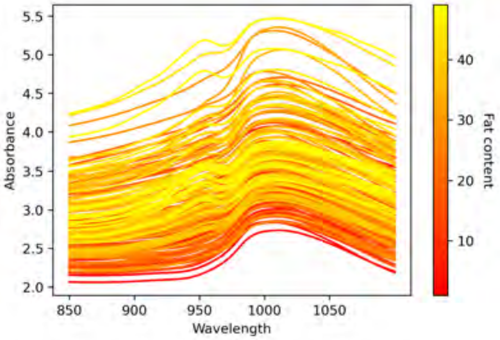
\end{aligned}
$$

- There exists an equivalent nonlinear smooth formulation with linear constraints.

- Tecator data set: the near-infrared absorbance spectra of 215 samples of finely chopped pork. The response variable is the fat content.



Implementation details

- Logistic CDF.
- SLSQP solver in the `scipy.optimize` package in Python 3.7.
- Intel® Core™ i7-8550U CPU 1.80GHz with 8 GB RAM.

Implementation details

- Logistic CDF.
- SLSQP solver in the `scipy.optimize` package in Python 3.7.
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Comparison using 10-fold cross-validation

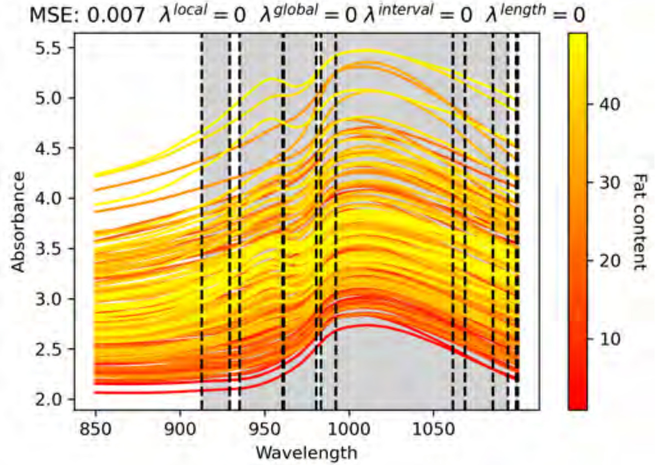
Optimal Randomized Regression Trees with $D = 1$ and $\lambda^{\text{local}} = \lambda^{\text{global}} = \lambda^{\text{interval}} = \lambda^{\text{length}} = 0$, with benchmarks:

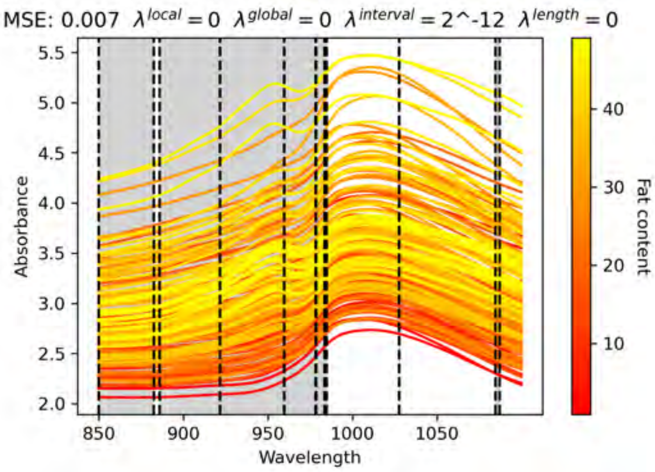
- Random Forest in Breiman [2001]
- SVR-FD in Blanquero et al. [2020]

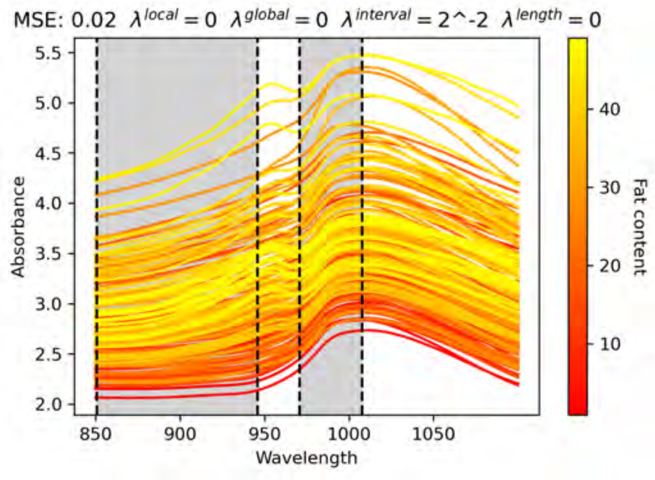
Table: Results for ORRT with $D = 1$ and $\lambda^{\text{local}} = \lambda^{\text{global}} = \lambda^{\text{interval}} = \lambda^{\text{length}} = 0$.

K	Out-of-sample average SSR		
	RF	ORRT $D = 1$	SVR-FD
	2.13		
1		4.74	0.25
2		0.54	0.23
3		0.22	0.24
4		0.18	0.29
5		0.19	0.41
6		0.17	0.40
7		0.13	0.45
8		0.18	0.45
9		0.19	0.49
10		0.19	0.50

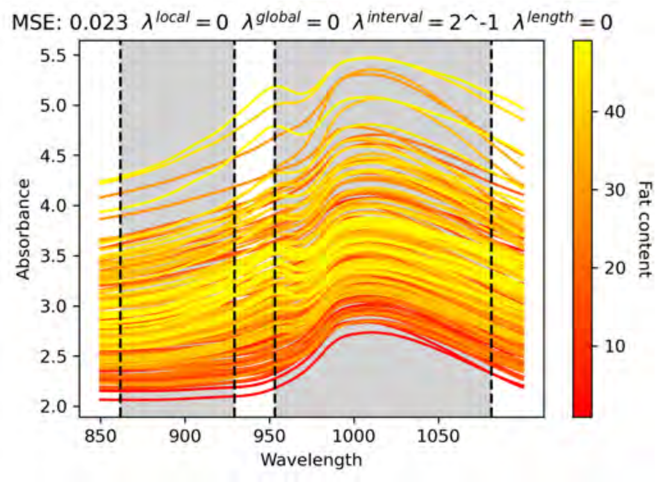
Controlling the number of critical intervals


MSE: 0.007 $\lambda^{local} = 0$ $\lambda^{global} = 0$ $\lambda^{interval} = 0$ $\lambda^{length} = 0$
Absorbance
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
850
900
950
1000
1050
Wavelength
Fat content
40
30
20
10

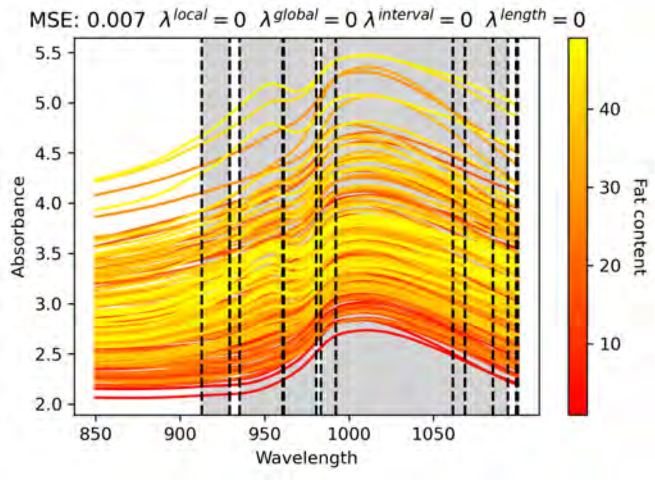

MSE: 0.007 λ^local = 0 λ^global = 0 λ^interval = 2^-12 λ^length = 0
Absorbance
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
850
900
950
1000
1050
Wavelength
Fat content
40
30
20
10

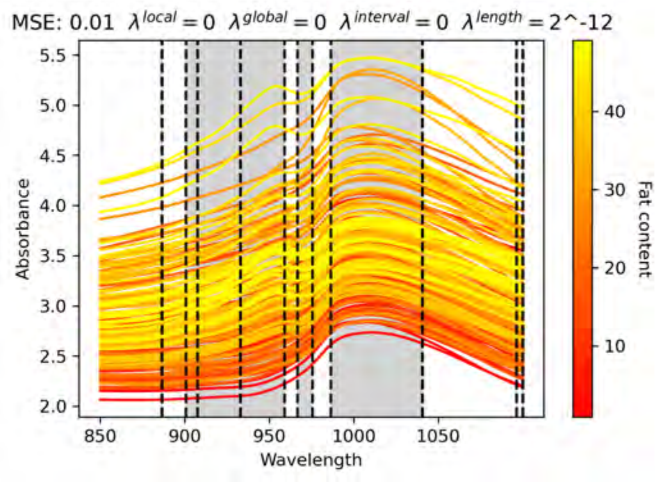


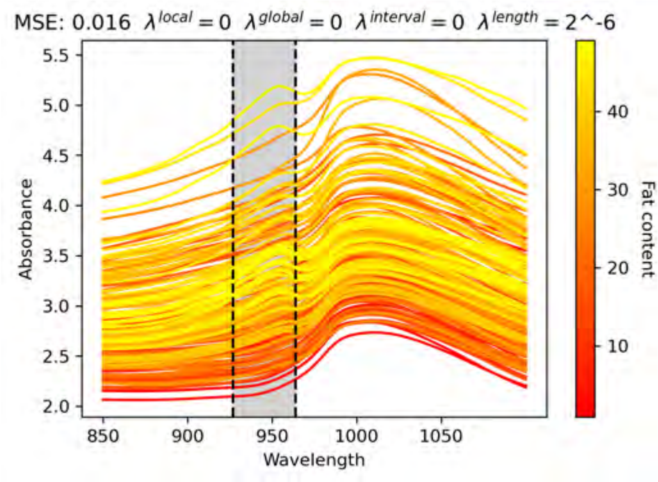
MSE: 0.02 $\lambda^{local} = 0$ $\lambda^{global} = 0$ $\lambda^{interval} = 2$^-2 $\lambda^{length} = 0$
Absorbance
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
850
900
950
1000
1050
Wavelength
40
30
20
10
Fat content


MSE: 0.023 λ^local = 0 λ^global = 0 λ^interval = 2^-1 λ^length = 0
Absorbance
Wavelength
Fat content
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
850
900
950
1000
1050
40
30
20
10

Controlling the proportion of curve


MSE: 0.007 $\lambda^{local} = 0$ $\lambda^{global} = 0$ $\lambda^{interval} = 0$ $\lambda^{length} = 0$
Absorbance
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
850
900
950
1000
1050
Wavelength
Fat content
40
30
20
10


MSE: 0.01 λ^local = 0 λ^global = 0 λ^interval = 0 λ^length = 2^-12
Absorbance
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
850
900
950
1000
1050
Wavelength
40
30
20
10
Fat content


MSE: 0.016 λ^local = 0 λ^global = 0 λ^interval = 0 λ^length = 2^-6
Absorbance
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
850
900
950
1000
1050
Wavelength
40
30
20
10
Fat content

Conclusions

- Optimal Randomized Classification and Regression Trees, a *continuous optimization* approach to build trees with *probabilistic* cuts, has been adapted to handle *functional data*.
- *Critical intervals* for prediction are detected simultaneously.
- The *proportion of the curves* to be used, as well as the *number of critical intervals* can be controlled.
- Preliminary results indicate that our approach is *competitive to benchmark methods, including RF.*

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Future research

- Adapt our approach to deal with other complex data, for instance, *text data* or *network data*.
- Embed our approach in *bagging* (as RF) or *boosting ensembles*.

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Thank you for your attention!

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