Regionally Additive Models: Explainable-by-design models minimizing feature interactions

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Generalized Additive Models

Wikipedia says:

> *In statistics, a generalized additive model (GAM) is a generalized linear model in which the linear response variable depends linearly on unknown smooth functions of some predictor variables, and interest focuses on inference about these smooth functions.*

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$$y = f_1(x_1) + \ldots + f_D(x_D)$$

GAMs - Interpretability

GAMs are called explainable-by-design, why?

Output/target variable:

- $y_{\texttt{bike\_rentals}}$ the expected number of bike rentals

Input/covariates:

- $x_{\texttt{temperature}}$
- $x_{\texttt{humidity}}$
- $x_{\texttt{is\_weekday}}$

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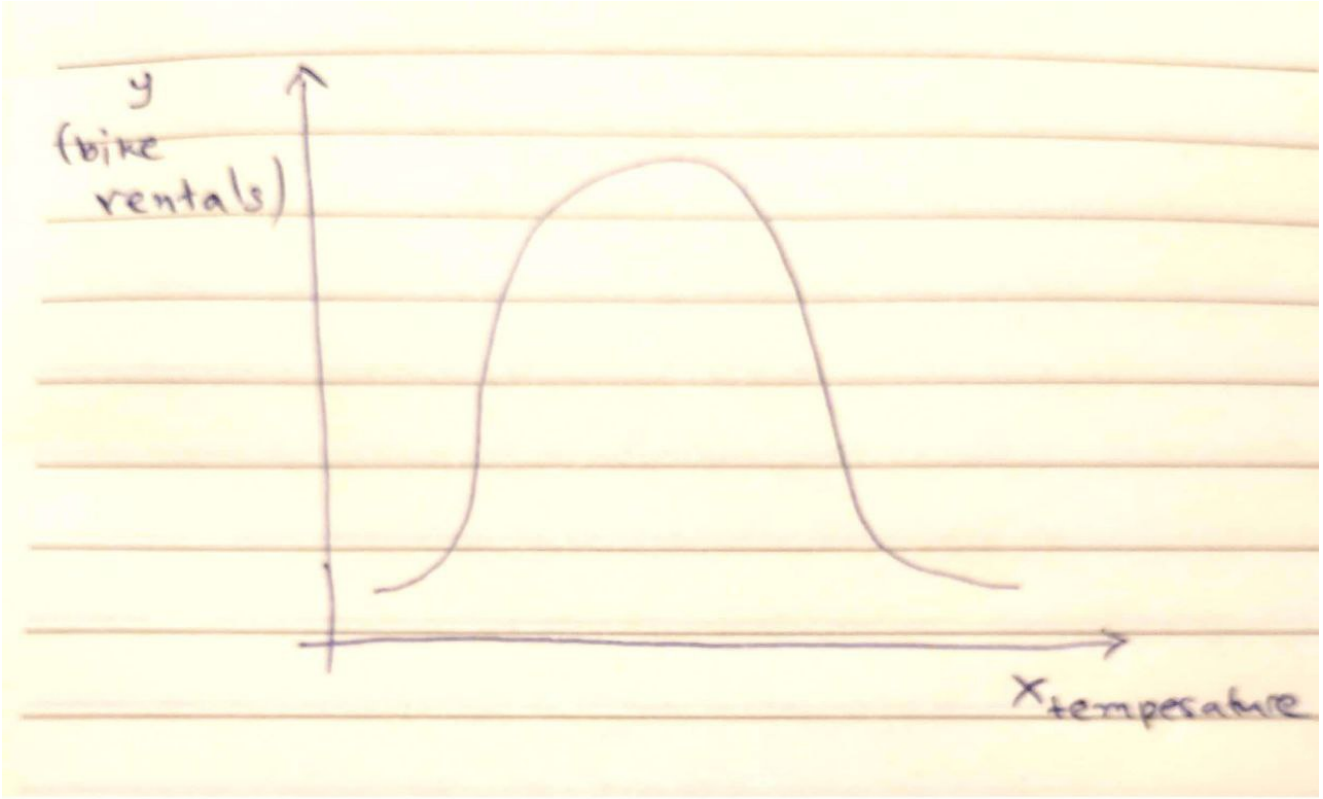

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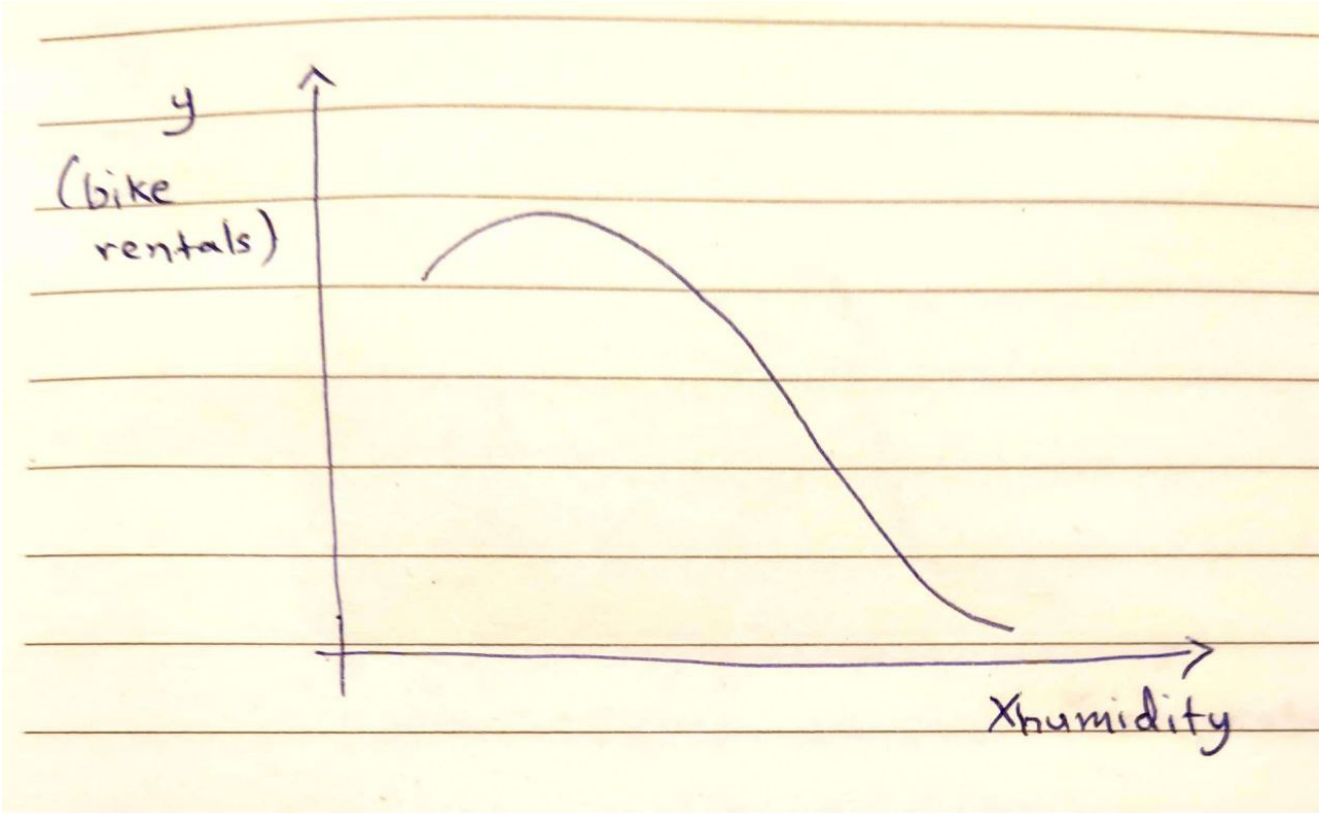

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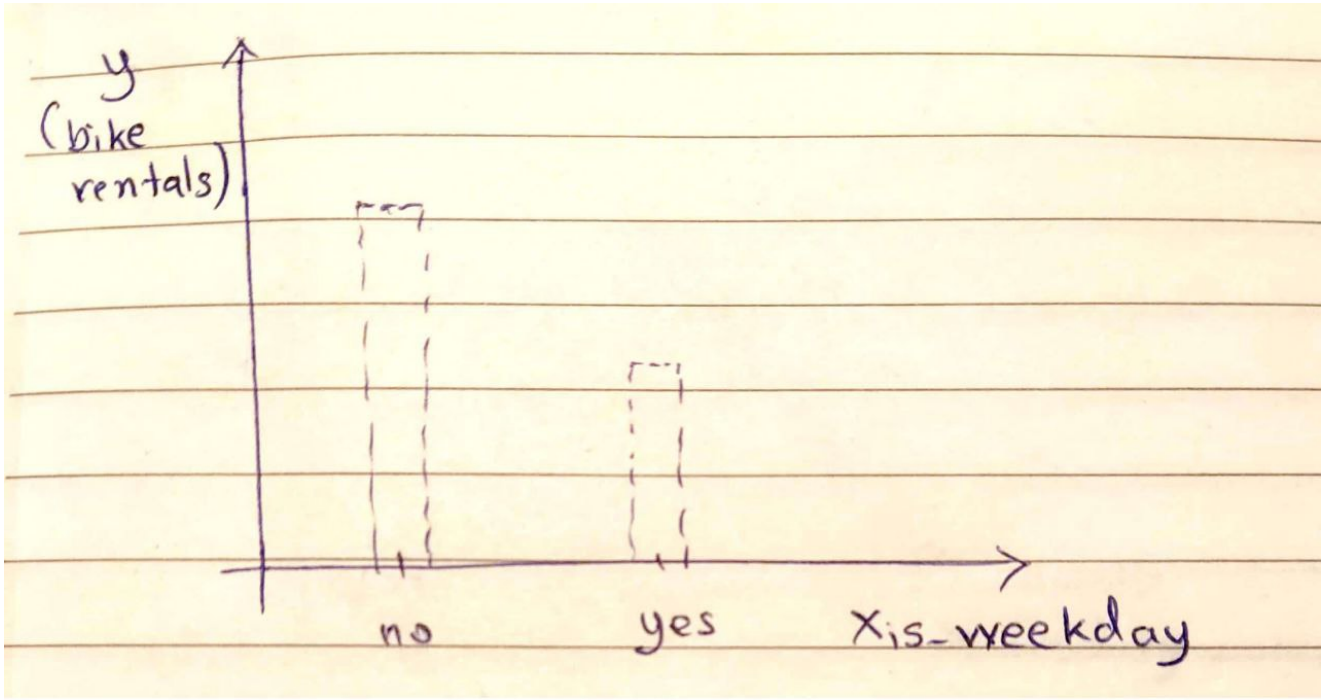
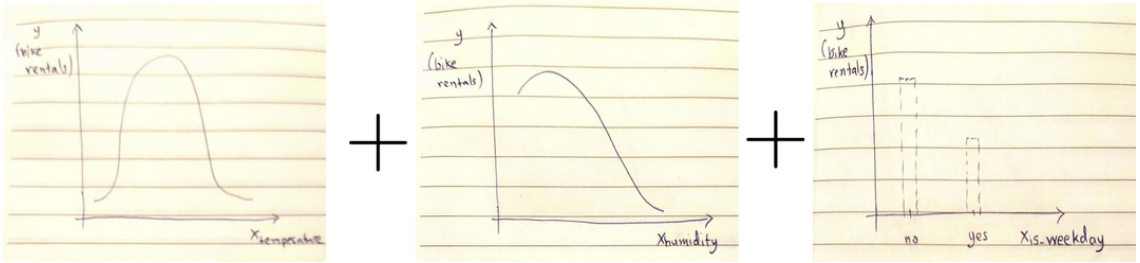


GAMs - Interpretability

GAMs are explainable-by-design, why?

$$y = f_1(x_{\texttt{temperature}}) + f_2(x_{\texttt{humidity}}) + f_3(x_{\texttt{is\_weekday}})$$



GAMs - Limitations

What if:

- temperature has different effect on week-days vs weekends

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- Solution 1: GA^2M
- Solution 2: RAM

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What if:

- Have you ever rided a bike with cold and humidity?

Solutions:

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Solutions:

- $f(x_{\texttt{temperature}}, x_{\texttt{humidity}} | x_{\texttt{is\_weekday}})$ RA^2M

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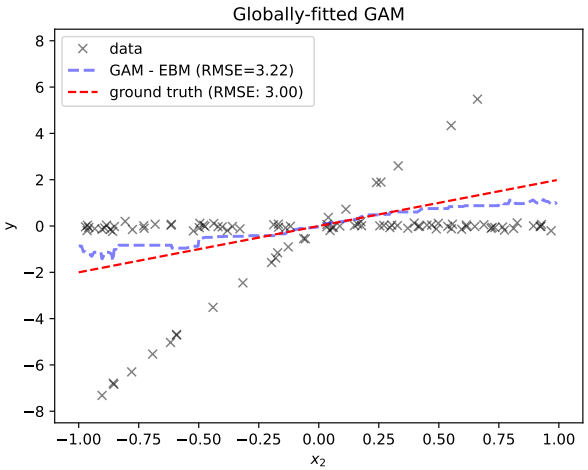
Solutions:

- $f(x_{\texttt{temperature}}, x_{\texttt{humidity}} | x_{\texttt{is\_weekday}})$ RA^2M
- $f(x_{\texttt{temperature}} | x_{\texttt{humidity}} = \{high, low\}, x_{\texttt{is\_weekday}})$ RAM with two conditions

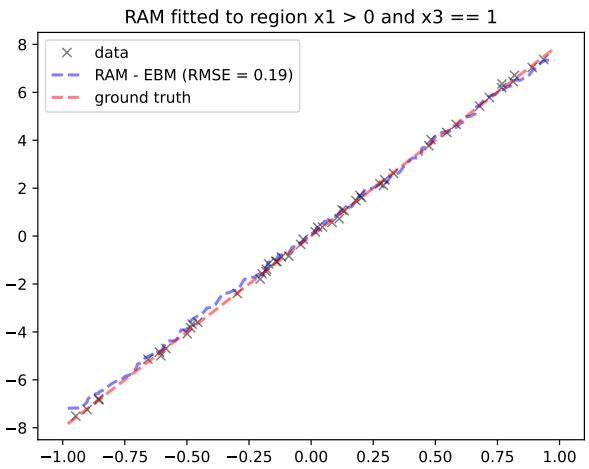
RAM on toy example

$$f(\boldsymbol{x}) = 8x_2\mathbb{1}_{x_1>0}\mathbb{1}_{x_3=0}$$

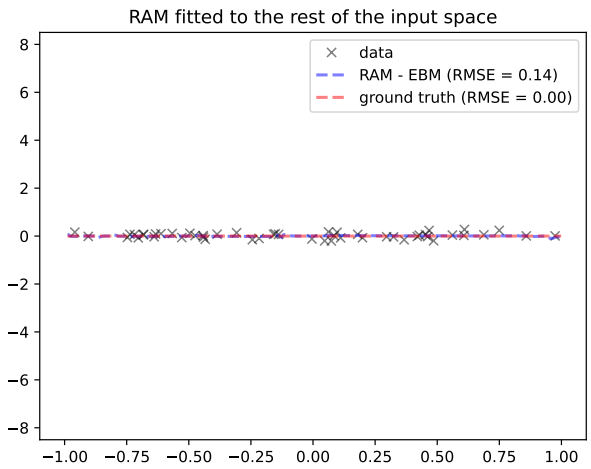
$$x_1, x_2 \sim \mathcal{U}(-1,1), x_3 \sim \mathit{Bernoulli}(0,1)$$



(a) $f_2(x_2)$



(b) $f_2(x_2)\mathbb{1}_{x_1>0 \text{ and } x_3=1}$



(c) $f_2(x_2)\mathbb{1}_{x_1\leq 0 \text{ or } x_3\neq 1}$

Figure: (Left) GAM, (Middle and Right) RAM

How RAM works (1)

3-step approach:

- Fit a Black-box model to capture all complex structures
  - it should be differentiable
  - neural network
- Use a Regional Effect method to find important interactions
  - RHALE - Gkolemis et. al
  - Feature Interactions - Herbinger et. al
- Fit a univariate function on each detected subregion

Step 1

- Fit a Black-box model to capture all complex structures
  - it should be differentiable
  - A neural network is a good option

Step 2

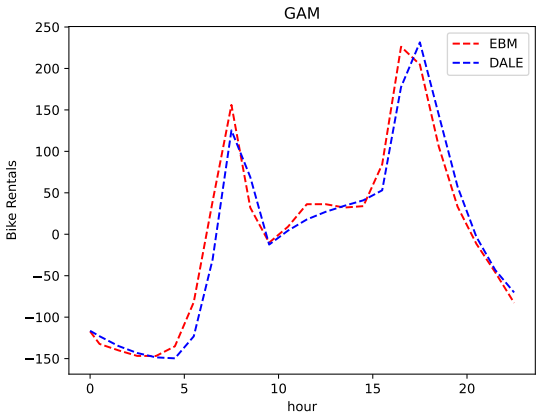
- Use a Regional Effect method to find important interactions
  - RHALE - Gkolemis et. al
  - Feature Interactions - Herbinger et. al

Step 3

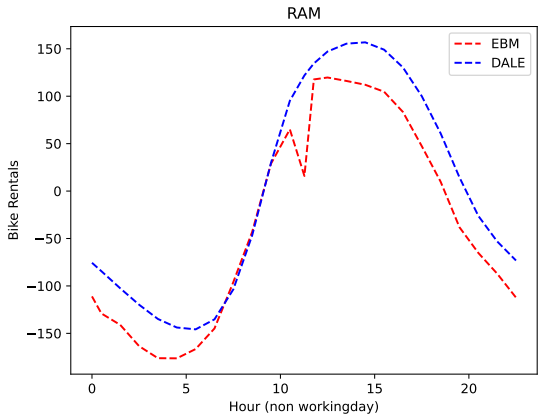
- Fit a univariate function on each detected subregion
  -

Bike Sharing dataset

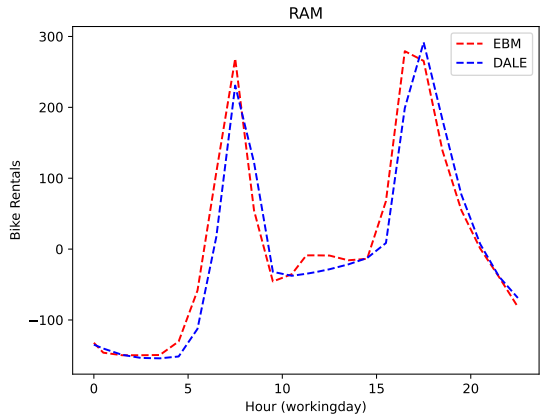
Predict bike-rentals (on daily basis) given some features of the day



(a) $f(X_{\texttt{hour}})$



(b) $f(X_{\texttt{hour}})\mathbb{1}_{X_{\texttt{workingday}}\neq 1}$



(c) $f(X_{\texttt{hour}})\mathbb{1}_{X_{\texttt{workingday}}=1}$

Experimental Results

	Black-box	**x-by-design**			
	all orders	1^{st} order		2^{nd} order	
	DNN	**GAM**	**RAM**	**GA^{2}M**	**RA^{2}M**
Bike (MAE)	0.254	0.549	0.430	0.298	0.278
Bike (RMSE)	0.389	0.734	0.563	0.438	0.412
Housing (MAE)	0.373	0.600	0.553	0.554	0.533
Housing (RMSE)	0.533	0.819	0.754	0.774	0.739

What next?

A lot has to be done!

- Results are only preliminary
  - Experiment with more datasets
  - Sometimes wide bins are needed
- Can we learn uncertain RAMs?
  - How do we model uncertainty?

Thank you for the attention

- For more discussion or future ideas on RAM, contact me:
  - vgkolemis@athenarc.gr
  - gkolemis@hua.gr
- Questions?