Spline-based separable expansions for approximation, regression and classification

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IPAM Workshop I: Tensor Methods and their Applications in the Physical and Data Sciences, UCLA, United States, April 1, 2021

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What are we trying to accomplish?

Introduce a new technique for modeling functions in several variables:

- Regression tasks
- Classification tasks

Our recent submission to Frontiers:
Regression and classification with spline-based separable expansions.
N. Govindarajan, N. Vervliet, L. De Lathauwer.

The main challenge of approximating functions in high dimensions

Curse-of-dimensionality in approximation theory:

> *In general, to approximate a n-times differentiable function in D variables within ϵ-tolerance (measured in the uniform norm), one typically requires $M \gtrsim (\frac{1}{\epsilon})^{D/n}$ parameters*

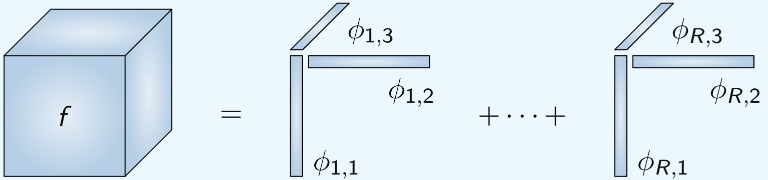
Optimal nonlinear approximation. DeVore et al., Manuscripta mathematica, 1989.

caveat:

> *Many high-dimensional functions in applications are inherently of "low complexity"*

Focus of this talk: exploiting low-rank structures through sums of separable functions

$$f(\boldsymbol{x}) = \sum_{r=1}^{R} \left(\prod_{d=1}^{D} \phi_{r,d}(x_d) \right)$$



Sums of separable functions = continuous analogs of polyadic decompositions

Revisiting this problem: are there any benefits of using splines over polynomials?

Past work (e.g., Mohlenkamp & Beylkin) mostly considered polynomials to approximate the component functions $\phi_{r,d}(\cdot)$,

why not use piece-wise polynomials a.k.a. splines?

What to expect next?

Spline basics and splines in higher dimensions: exploiting low-rank structures

Performing regression and classification

A Gauss–Newton algorithm exploiting sparsity

Numerical examples (regression)

Numerical examples (classification)

Key take-aways and future work

The knot set and B-spline basis terms

Let $\mathscr{T} = \{t_i\}_{i=0}^{N+M}$ denote the set of knots:

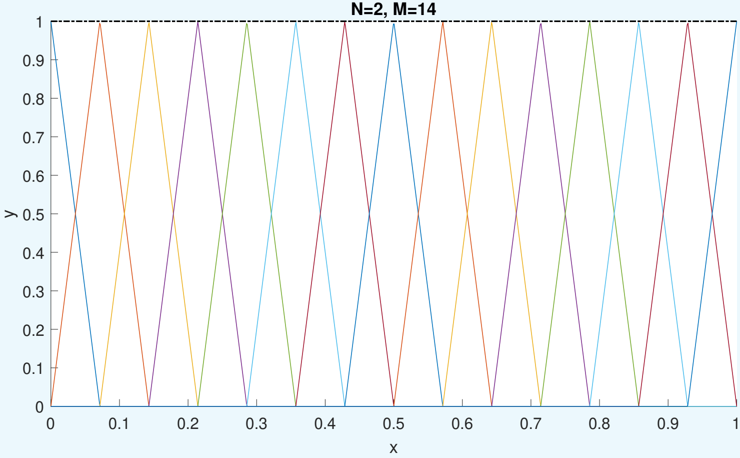
$$a = t_0 = \ldots = t_{N-1} \leq t_N \leq t_{N+1} \leq \ldots \leq t_{M+1} = \ldots = t_{M+N} = b.$$

The B-spline basis terms $\{B_{m,N}\}_{m=0}^{M}$ are defined through the recursion formula

$$B_{m,N}(x) := \frac{x - t_m}{t_{m+N} - t_m} B_{m,N-1}(x) + \frac{t_{m+N+1} - x}{t_{m+N+1} - t_{m+1}} B_{m+1,N-1}(x),$$

where $B_{m,0}(x) := \begin{cases} 1 & x \in [t_m, t_{m+1}) \\ 0 & \text{otherwise} \end{cases}.$

The B-spline basis elements $B_{m,N}(\cdot)$ are compactly supported!



$$B_{m,N}(x) = 0, \qquad x \in (-\infty, t_m) \cup [t_{m+N+1}, \infty).$$

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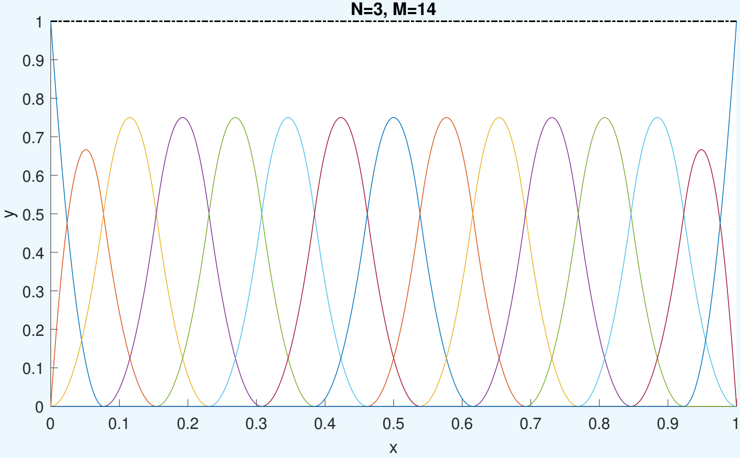

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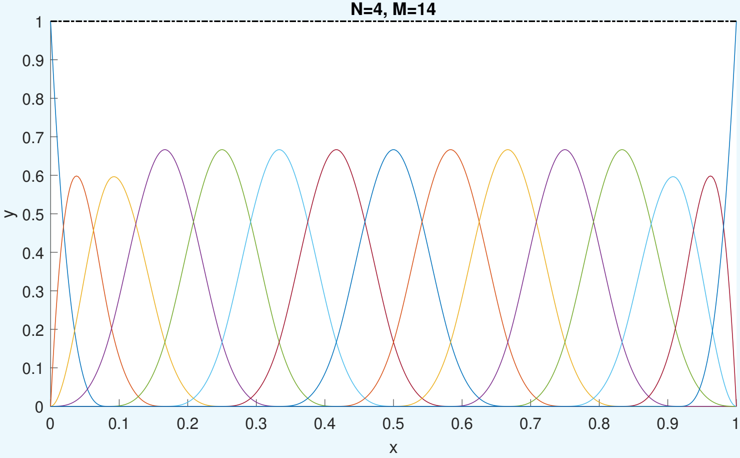

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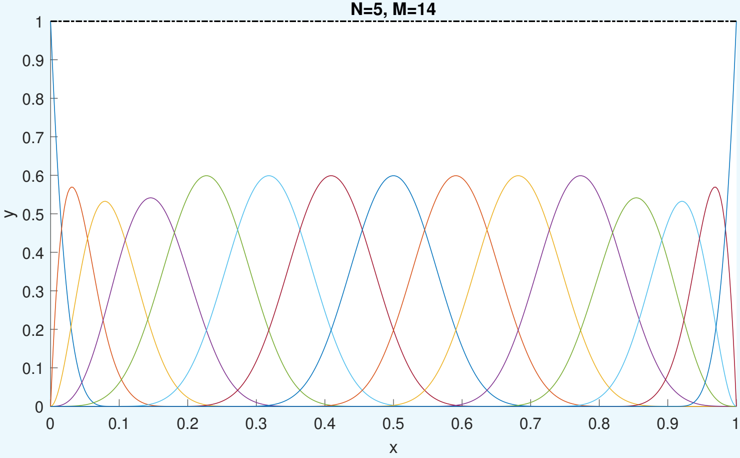


$$B_{m,N}(x) = 0, \qquad x \in (-\infty, t_m) \cup [t_{m+N+1}, \infty).$$

The B-spline function

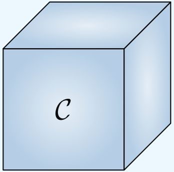
Any continuous function can be approximated arbitrarily well by

$$S(x) = \begin{bmatrix} B_{0,N}(x) & \cdots & B_{M,N}(x) \end{bmatrix} \begin{bmatrix} c_0 \\ \vdots \\ c_M \end{bmatrix} = B_{\mathscr{T},N}(x)\boldsymbol{c}.$$

through either *increasing* the knot density and order of the spline.

Taking direct tensor products of splines leads to exponential blow-up of coefficients...

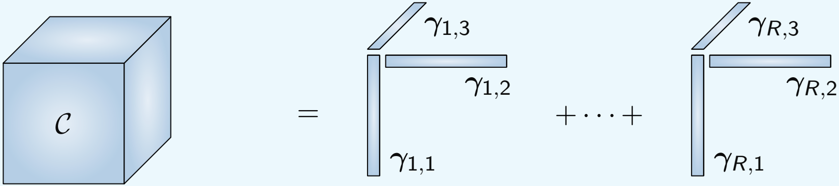
$$\hat{f}(x;\mathcal{C}) = \sum_{m_1=0}^{M_1} \cdots \sum_{m_D=0}^{M_D} c_{m_1 \cdots m_D} \prod_{d=1}^{D} B^{(d)}_{m_d, N^{(d)}}(x_d) = \mathcal{C} \bullet_1 B_d(x_1) \cdots \bullet_D B_D(x_D)$$



$\prod_{d=1}^{D}(M_d + 1)$ parameters

Exploit low-rank structure: $\mathcal{C}(\Gamma_1, \ldots, \Gamma_d) = [\![\Gamma_1, \ldots, \Gamma_D]\!]$, to alleviate this blow-up!

$$\hat{f}(x; \Gamma_1, \ldots, \Gamma_D) = \mathcal{C}(\Gamma_1, \ldots, \Gamma_D) \bullet_1 B_1(x_1) \cdots \bullet_D B_D(x_D) = \sum_{r=1}^{R} \prod_{d=1}^{D} B_d(x_d) \gamma_{r,d}$$



$\prod_{d=1}^{D}(M_d + 1)$ parameters

$R(\sum_{d=1}^{D} M_d + 1)$ parameters

Regression is performed by minimizing the quadratic objective function

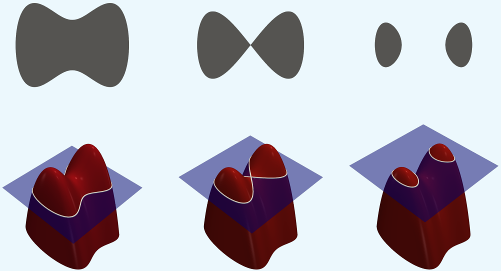
Given samples $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^{I} \subset [0,1]^D \times \mathbb{R}$ from a underlying target function $f \in C([0,1]^D)$, we minimize:

$$Q(\Gamma_1, \ldots, \Gamma_D) := \frac{1}{2} \sum_{i=1}^{I} \left(\hat{f}(x_i; \Gamma_1, \ldots, \Gamma_D) - y_i \right)^2 .$$

A level-set approach to modeling a binary classification function

Binary classification function $g : [0,1]^D \to \{0,1\}$ can be modeled by the function

$$g(x) = \begin{cases} 0 & f(x) \leq 0 \\ 1 & f(x) > 0 \end{cases}$$



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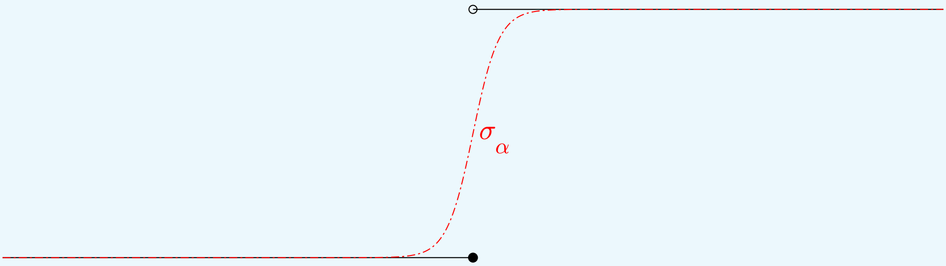
Replace step function with the logistic function $\sigma_\alpha : t \mapsto 1/(\exp(-\alpha t) + 1)$

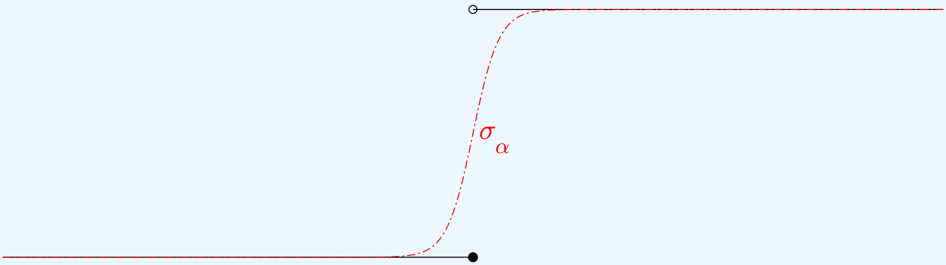


Replace g with

$$g_\alpha(x) \coloneqq (\sigma_\alpha \circ f)(x) = \sigma_\alpha(f(x)),$$

where $\alpha > 0$ controls sharpness of transition.

Replace step function with the logistic function $\sigma_\alpha : t \mapsto 1/(\exp(-\alpha t) + 1)$



g_α is further replaced by the approximant

$$\hat{g}_\alpha(x; \Gamma_1, \ldots, \Gamma_D) := \sigma_\alpha \circ \hat{f}(x; \Gamma_1, \ldots, \Gamma_D),$$

Classification is performed by minimizing the Logistic objective function

Given a collection of labeled data $\{(x_i, y_i)\}_{i=1}^{I} \subset [0,1]^D \times \{0,1\}$, the performance of $\hat{g}_\alpha$ is optimized when both

$$\prod_{y_i=0} (1 - \hat{g}_\alpha(x_i; \Gamma_1, \ldots, \Gamma_D)) \quad \text{and} \quad \prod_{y_i=1} \hat{g}_\alpha(x_i; \Gamma_1, \ldots, \Gamma_D)$$

is maximized as much as possible.

Classification is performed by minimizing the Logistic objective function

This is equivalent to minimizing the objective function

$$L_\alpha(\Gamma_1, \dots, \Gamma_D) := -\sum_{i=1}^{I} y_i \log \hat{g}_\alpha(x_i; \Gamma_1, \dots, \Gamma_D) + (1 - y_i) \log \left(1 - \hat{g}_\alpha(x_i; \Gamma_1, \dots, \Gamma_D)\right).$$

Minimization of objective functions is effectively done with Gauss-Newton dogleg algorithm

- Exploit multi-linear structure of the objective functions, see:
  - *Optimization-based algorithms for tensor decompositions: Canonical polyadic decomposition, decomposition in rank-$(L_r, L_r, 1)$ terms, and a new generalization.* Sorber et al., SIAM J. Optim., 2013.
  - *Numerical optimization-based algorithms for data fusion.* Vervliet et al., Data Handling in Science and Technology, 2019.
- Main computational burden:

  evaluating gradients and Grammian-vector products.

Benefit of compactly supported B-splines: significant speed-ups in Grammian and gradient by exploiting sparsity!

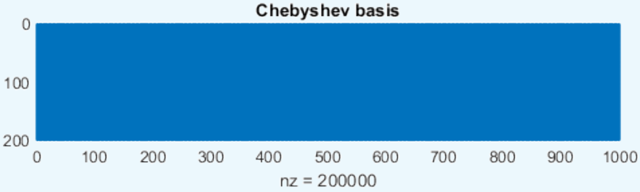
Gradient:

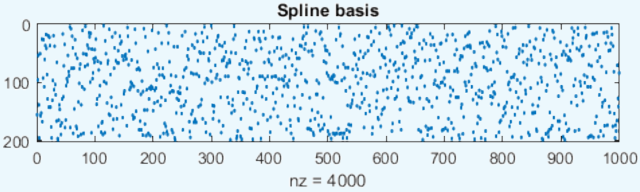
$$g_{r,d} = A_d \left(\left(\mathop{\Huge *}_{k=1, k \neq d}^{D} A_k^\top \gamma_{r,k} \right) * \boldsymbol{\eta} \right).$$

Grammian (of the Jacobian) vector product

$$w_{r,d} = A_d \left(\left(\mathop{\Huge *}_{k=1, k \neq d}^{D} A_k^\top \gamma_{r,k} \right) * \boldsymbol{\xi} * \left(\sum_{\tilde{d}=1}^{D} \sum_{\tilde{r}=1}^{R} \left(\mathop{\Huge *}_{k=1, k \neq d}^{D} A_k^\top \gamma_{\tilde{r},k} \right) * A_{\tilde{d}}^\top z_{\tilde{r},\tilde{d}} \right) \right).$$

Benefit of compactly supported B-splines: significant speed-ups in Grammian and gradient by exploiting sparsity!

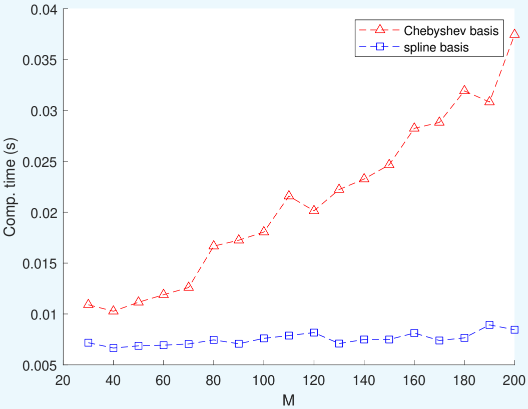




If the order of the B-spline is kept low:

$$\mathcal{O}\left(DIMR\right) \quad \rightarrow \quad \mathcal{O}\left(DIR\right) \text{ flops}$$

Benefit of compactly supported B-splines: significant speed-ups in Grammian and gradient by exploiting sparsity!



average required computation time to pass through one cycle of the GN algorithm.

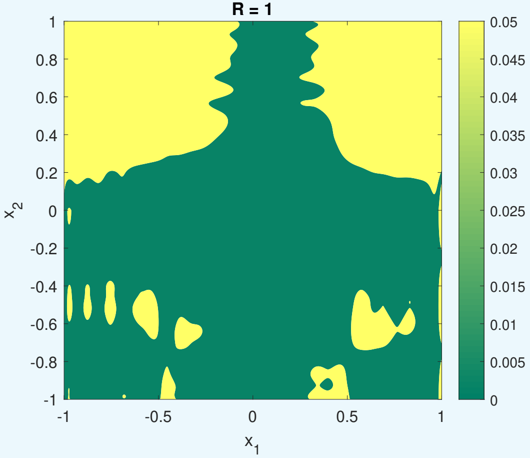
$N = 4,\ R = 3,\ I = 1000.$

A $R = 3$ separable function

Consider the following example

$$f(\boldsymbol{x}) = \underbrace{|x_1||x_2|}_{\text{non-smooth term}} + \sin(2\pi x_1)\cos(2\pi x_2) + x_1^2 x_2, \quad \boldsymbol{x} \in [-1,1] \times [-1,1].$$

As expected... an $R = 3$ is sufficient for a good approximation



Absolute error

(Knots are uniformly distributed on the approximation domain)

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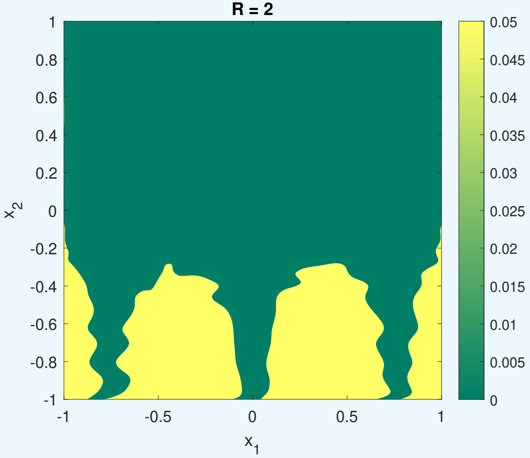

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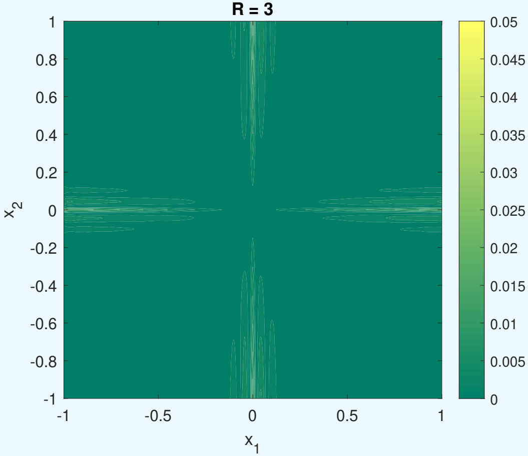

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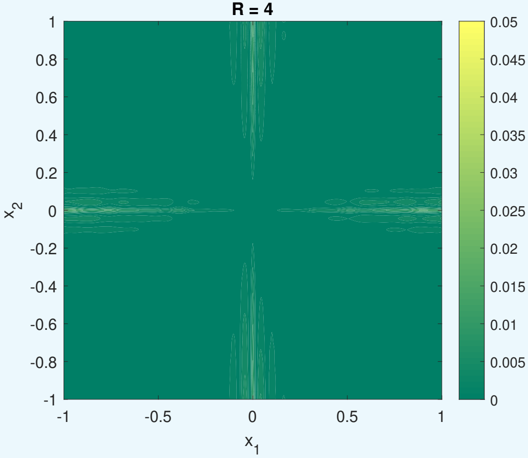

Absolute error

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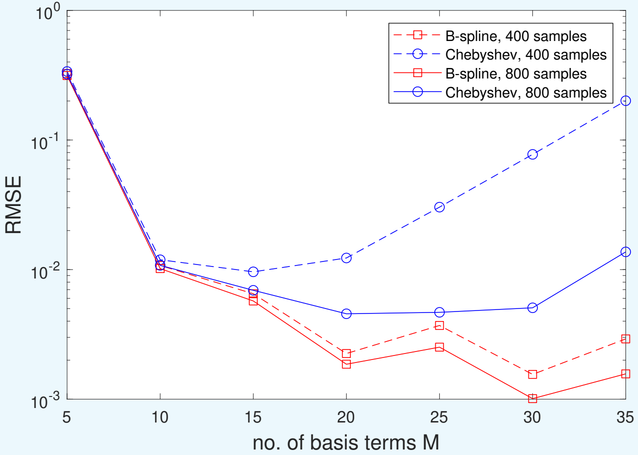
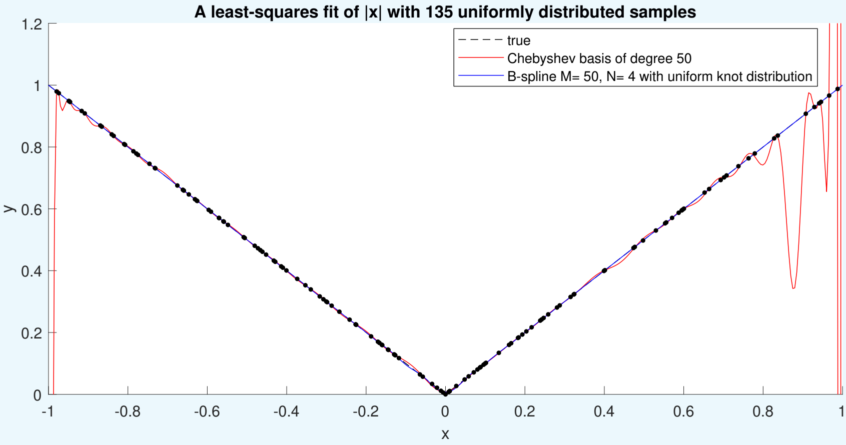
Unlike for splines, Runge's phenomenon can adversely affect quality of approximation



No of separable terms $R = 3$.

(Knots are uniformly distributed on the approximation domain)

Taming Runge's phenomenon with splines: *keep order low and increase knots*



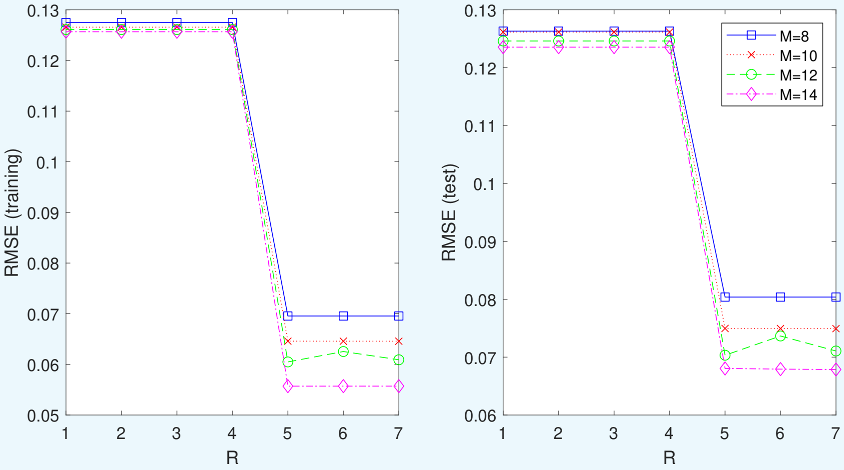
Runge's phenomenon can adversely contribute to the overfitting problem

Low-rank structures in real life datasets - an example

NASA dataset from the UCI machine learning repository:

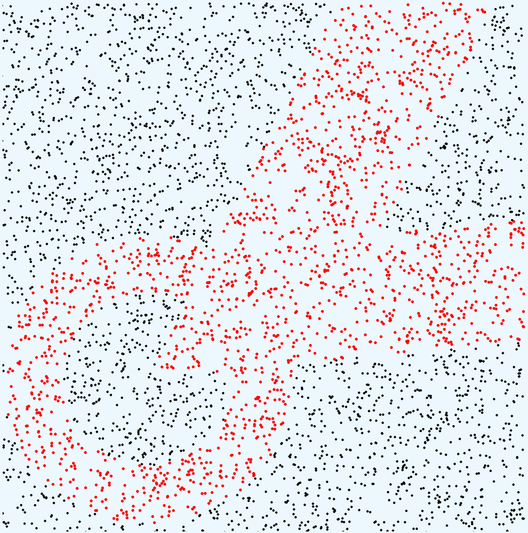
- independent variables:
  - *frequency*,
  - *angle of attack*,
  - *chord length*,
  - *free-stream velocity*,
  - *suction-side displacement thickness*.
- dependent variable: *self-noise generated by airfoil*.
- randomly split data into a training (1202 samples) and a test (301 samples) sets.

An $R = 5$ separable function is sufficient to model the NASA dataset



The separable rank can be increased to account for complexity of the classification sets

Consider the labeled dataset:



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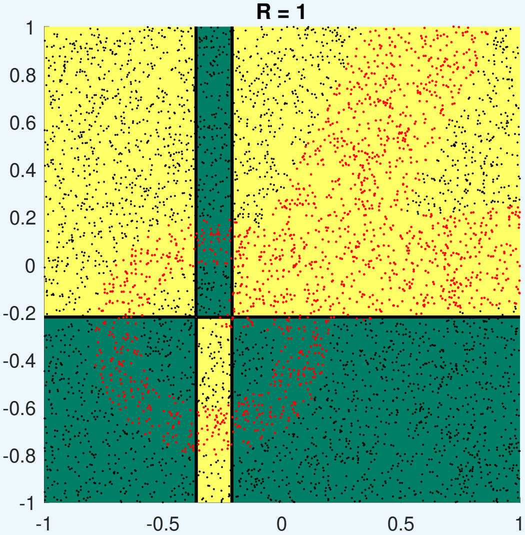

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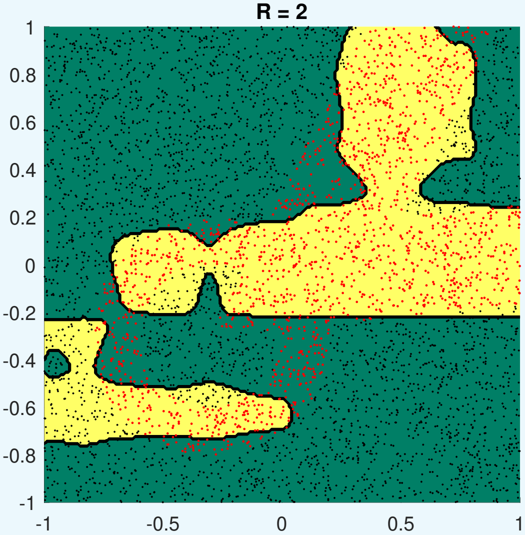

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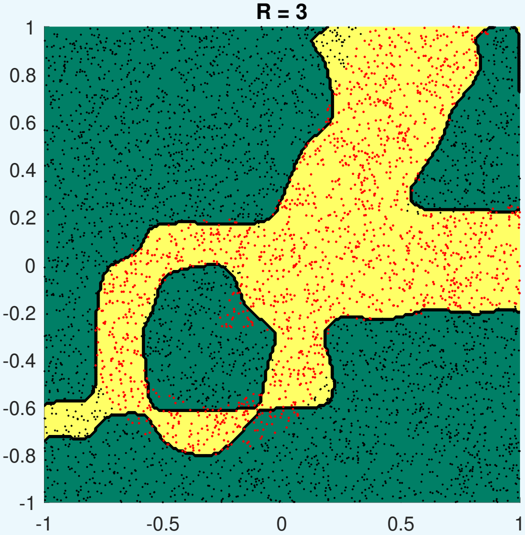

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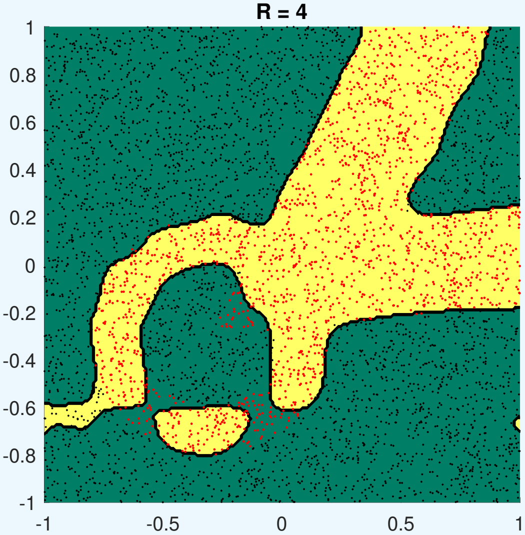

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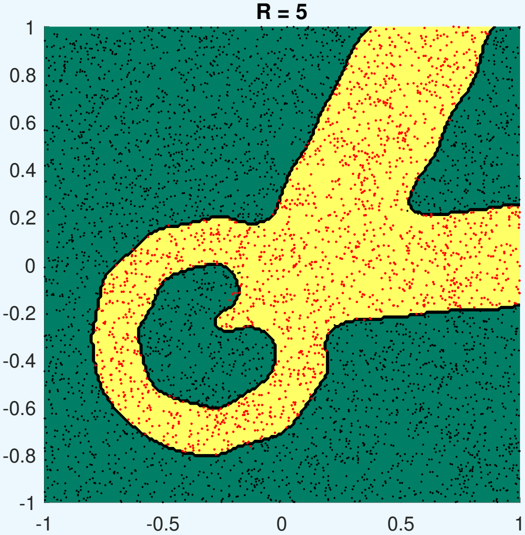
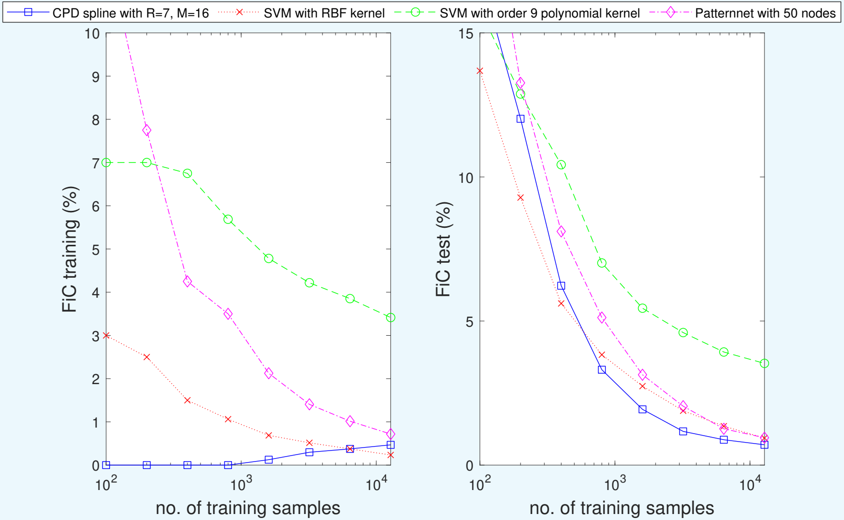
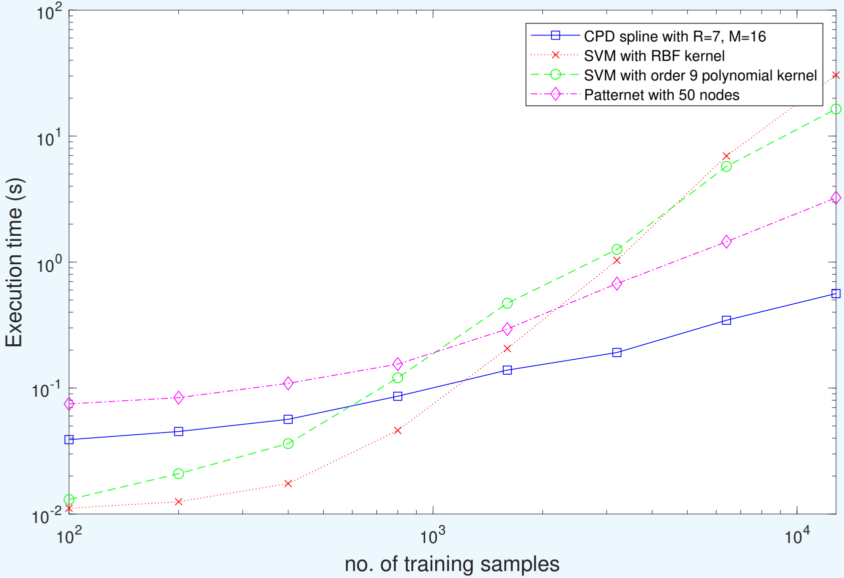


Our method compared with well-established techniques for classification



CPU time for training grows more moderately with dataset size



Key take-aways and future work

Important take-aways:

- With B-splines, sparsity can be exploited to further accelerate GN algorithm
- Runge phenomenon effects are easily suppressed by keeping order of the spline low
- Low-rank structures do appear in practice!
- A new promising technique for (binary) classification

Future work:

- Extend to other decompositions, e.g., Hierarchical Tucker, Tensor Train,
- multi-class classification,
- knot optimization

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