

ANOVA approximation for control systems

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joint work with
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Motivation

Unknown function (control system):

$$H \colon \mathbb{R}^d \times \mathbb{R}^m \to \mathbb{R}^d,$$
 $H(\boldsymbol{x}, \boldsymbol{u}) \coloneqq F(\boldsymbol{x}) + G(\boldsymbol{x})\boldsymbol{u},$

with

- $F: \mathbb{R}^d \to \mathbb{R}^d, G: \mathbb{R}^d \to \mathbb{R}^{d \times m},$
- $d, m \in \mathbb{N}, m \ll d$.

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Given: samples $H(\boldsymbol{x}^i, \boldsymbol{u}^i)$ for $i=1,\dots,M$

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Goal: find $\tilde{H} \approx H$



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Example: Euler approximation of a controlled Duffing oscillator

$$H(\boldsymbol{x}, \boldsymbol{u}) = \boldsymbol{x} + \Delta t \begin{pmatrix} x_2 \\ x_1 - 3x_1^3 u \end{pmatrix}$$
$$= \begin{pmatrix} x_1 + \Delta t x_2 \\ x_2 + \Delta t x_1 \end{pmatrix} + \begin{pmatrix} 0 \\ -3\Delta t x_1^3 \end{pmatrix} u$$
$$= F(\boldsymbol{x}) + G(\boldsymbol{x})u$$

i. e.,

- d = 2,
- m = 1
- only 1D terms → low-dimensional

Overview

- ANOVA approximation for scalar-valued functions
- ANOVA approximation for control systems
- Numerical Example

ANOVA approximation



ANalysis **O**f **VA**riance (ANOVA) decomposition

[Caflish, Morokoff, Owen 97], [Rabitz, Alis 99], [Liu, Owen 06], [Kuo, Sloan, Wasilkowski, Wozniakowski 10], . . .

Decompose a d-dimensional function f into

$$f(\mathbf{x}) = f_{\varnothing}$$

$$+ f_{1}(x_{1}) + \dots + f_{d}(x_{d})$$

$$+ f_{1,2}(x_{1}, x_{2}) + f_{1,3}(x_{1}, x_{3}) + \dots + f_{d-1,d}(x_{d-1}, x_{d})$$

$$+ f_{1,2,3}(x_{1}, x_{2}, x_{3}) + \dots + f_{d-2,d-1,d}(x_{d-2}, x_{d-1}, x_{d})$$

$$\vdots$$

$$+ f_{[d]}(\mathbf{x})$$

constant one-dimensional terms two-dimensional terms three-dimensional terms

$$[d]\coloneqq\{1,\ldots,d\}$$

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$$[d]\coloneqq\{1,\ldots,d\}$$

- ightarrow in general multiple representations possible
- → conditions for uniqueness?



ANOVA approximation for control systems ANOVA approximation for scalar-valued functions

Definition

Let

$$\langle f, g \rangle_{L_2(\Omega, \omega)} \coloneqq \int_{\Omega} f(\boldsymbol{x}) \, g(\boldsymbol{x}) \, \omega(\boldsymbol{x}) \, d\boldsymbol{x}$$

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⇒ unique decomposition satisfying:

$$0=\langle f_{m v},f_{m z}
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Basis representation: For orthonormal basis $\{\varphi_k\}_{k\in\mathbb{N}_0^d}$ of $L_2(\Omega,\omega)$ we have

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{k} \in \mathbb{N}_0^d} c_{\boldsymbol{k}}(f) \, \varphi_{\boldsymbol{k}}(\boldsymbol{x}), \qquad c_{\boldsymbol{k}}(f) \coloneqq \langle f, \varphi_{\boldsymbol{k}} \rangle_{L_2(\Omega, \omega)}.$$

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[Potts, Schmischke 21]:

$$f_{\boldsymbol{v}}(\boldsymbol{x}_{\boldsymbol{v}}) = \sum_{\substack{\boldsymbol{k} \in \mathbb{N}_0^d \\ \text{supp } \boldsymbol{k} = \boldsymbol{v}}} c_{\boldsymbol{k}}(f) \, \varphi_{\boldsymbol{k}}(\boldsymbol{x}_{\boldsymbol{v}})$$

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[Potts, Schmischke 21]:

$$f_{\boldsymbol{v}}(\boldsymbol{x}_{\boldsymbol{v}}) = \sum_{\substack{\boldsymbol{k} \in \mathbb{N}_0^0 \\ \text{supp } \boldsymbol{k} = \boldsymbol{v}}} c_{\boldsymbol{k}}(f) \, \varphi_{\boldsymbol{k}}(\boldsymbol{x}_{\boldsymbol{v}})$$

$$k \in \mathbb{Z}^3$$
 $k = 0$ $|\sup k| = 1$ $|\sup k| = 2$ $|\sup k| = 3$

⇒ decomposition in the space of basis coefficients

[image credits: Laura Weidensager]

Numerical realization – ANOVA approximation

[Potts, Schmischke 21]

$$f = \sum_{\boldsymbol{v} \subseteq [d]} f_{\boldsymbol{v}}, \qquad f_{\boldsymbol{v}} = \sum_{\substack{\boldsymbol{k} \in \mathbb{Z}^d \\ \operatorname{supp} \boldsymbol{k} = \boldsymbol{v}}} c_{\boldsymbol{k}}(f) \, \varphi_{\boldsymbol{k}}$$

Numerical realization - ANOVA approximation

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Truncation

reduce number of ANOVA terms

$$\mathcal{T}_{V} f = \sum_{\substack{\mathbf{v} \subseteq [d] \\ \mathbf{v} \in V}} f_{\mathbf{v}}$$
$$f_{\mathbf{v}} = \sum_{\substack{\mathbf{k} \in \mathbb{Z}^{d} \\ \text{supp } \mathbf{k} = \mathbf{v}}} c_{\mathbf{k}}(f) \varphi_{\mathbf{k}}$$

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Projection

choose finite number of basis functions $\{\varphi_{k}\}_{k\in\mathbb{Z}^{d}}$

$$P_{N}f = \sum_{\substack{v \subseteq [d] \\ v \in V}} \tilde{f}_{v}$$
$$\tilde{f}_{v} = \sum_{k \in \mathcal{I}_{N}v} c_{k}(f) \varphi_{k}$$

Numerical realization – ANOVA approximation

[Potts, Schmischke 21]

$$f = \sum_{\boldsymbol{v} \subseteq [d]} f_{\boldsymbol{v}}, \qquad f_{\boldsymbol{v}} = \sum_{\substack{\boldsymbol{k} \in \mathbb{Z}^d \\ \text{supp } \boldsymbol{k} = \boldsymbol{v}}} c_{\boldsymbol{k}}(f) \, \varphi_{\boldsymbol{k}}$$

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Projection

choose finite number of basis functions $\{\varphi_{k}\}_{k\in\mathbb{Z}^{d}}$

$$\begin{split} P_{N}f &= \sum_{\substack{\boldsymbol{v} \subseteq [d] \\ \boldsymbol{v} \in V}} \tilde{f}_{\boldsymbol{v}} \\ \tilde{f}_{\boldsymbol{v}} &= \sum_{\boldsymbol{k} \in \mathcal{I}_{N}^{\boldsymbol{v}}} c_{\boldsymbol{k}}(f) \, \varphi_{\boldsymbol{k}} \end{split}$$

Regression

compute coefficients $c_{\pmb{k}}^\star$ from samples

$$f^{\star} = \sum_{\substack{v \subseteq [d] \\ v \in V}} f^{\star}_{v}$$
$$f^{\star}_{v} = \sum_{k \in \mathcal{I}_{N}v} c^{\star}_{k} \varphi_{k}$$

$$f(x) = f_\varnothing \qquad \text{constant} \\ + f_1(x_1) + f_2(x_2) + \ldots + f_d(x_d) \qquad \text{one-dimensional terms} \\ + f_{1,2}(x_1,x_2) + f_{1,3}(x_1,x_3) + \ldots + f_{d-1,d}(x_{d-1},x_d) \qquad \text{two-dimensional terms} \\ + f_{1,2,3}(x_1,x_2,x_3) + \ldots + f_{d-2,d-1,d}(x_{d-2},x_{d-1},x_d) \qquad \text{three-dimensional terms} \\ \vdots \\ + f_{[d]}(x) \qquad \qquad \text{d-dimensional term} \\ = \sum_{v \subseteq [d]} f_v(x_v)$$

$$f(\boldsymbol{x}) = f_\varnothing \qquad \text{constant}$$

$$+ f_1(x_1) + f_2(x_2) + \ldots + f_d(x_d) \qquad \text{one-dimensional terms}$$

$$+ f_{1,2}(x_1, x_2) + f_{1,3}(x_1, x_3) + \ldots + f_{d-1,d}(x_{d-1}, x_d) \qquad \text{two-dimensional terms}$$

$$+ f_{1,2,3}(x_1, x_2, x_3) + \ldots + f_{d-2,d-1,d}(x_{d-2}, x_{d-1}, x_d) \qquad \text{three-dimensional terms}$$

$$\vdots$$

$$+ f_{[d]}(x) \qquad \text{d-dimensional term}$$

$$= \sum_{\boldsymbol{x} \in [d]} f_{\boldsymbol{v}}(\boldsymbol{x}_{\boldsymbol{v}})$$

Problem: 2^d many terms (curse of dimensionality)

$$f(x) = f_\varnothing \qquad \qquad \text{constant} \\ + f_1(x_1) + f_2(x_2) + \ldots + f_d(x_d) \qquad \qquad \text{one-dimensional terms} \\ + f_{1,2}(x_1, x_2) + f_{1,3}(x_1, x_3) + \ldots + f_{d-1,d}(x_{d-1}, x_d) \qquad \qquad \text{two-dimensional terms} \\ + f_{1,2,3}(x_1, x_2, x_3) + \ldots + f_{d-2,d-1,d}(x_{d-2}, x_{d-1}, x_d) \qquad \qquad \text{three-dimensional terms} \\ \vdots \\ + f_{[d]}(x) \qquad \qquad \otimes \sum_{\substack{v \subseteq [d] \\ |v| = [d]}} f_v(x_v) \\ \otimes \sum_{\substack{v \subseteq [d] \\ |v| = [d]}} f_v(x_v)$$

Problem: 2^d many terms (curse of dimensionality)

 \Rightarrow introduce $q \in \mathbb{N}, q < d$ (superposition dimension)

$$f(x) = f_{\varnothing}$$

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$$\vdots$$

$$+ f_{[a]}(x)$$

$$\approx \sum_{v \subseteq [d]} f_{v}(x_{v}) = \mathcal{T}_{V} f$$
set V according to sparsity

constant one-dimensional terms two-dimensional terms

three-dimensional terms



ANOVA approximation for control systems ANOVA approximation for scalar-valued functions

Projection

Recap: reduced the number of ANOVA terms

$$f_{m{v}}(m{x}_{m{v}}) = \sum_{\substack{m{k} \in \mathbb{Z}^d \ \mathrm{supp} \ m{k} = m{v}}} c_{m{k}}(f) \, arphi_{m{k}}(m{x}_{m{v}})$$

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Problem: infinitely many coefficients needed ⇒ impossible in practice



Recap: reduced the number of ANOVA terms

$$f_{\boldsymbol{v}}(\boldsymbol{x}_{\boldsymbol{v}}) = \sum_{\substack{\boldsymbol{k} \in \mathbb{Z}^d \\ \text{supp } \boldsymbol{k} = \boldsymbol{v}}} c_{\boldsymbol{k}}(f) \, \varphi_{\boldsymbol{k}}(\boldsymbol{x}_{\boldsymbol{v}})$$

Problem: infinitely many coefficients needed ⇒ impossible in practice

 \leadsto introduce finite index sets \mathcal{I}_{N^v} and approximate by

$$f_{\boldsymbol{v}}(\boldsymbol{x}_{\boldsymbol{v}}) \approx \sum_{\boldsymbol{k} \in \mathcal{I}_{N^{\boldsymbol{v}}}} c_{\boldsymbol{k}}(f) \, \varphi_{\boldsymbol{k}}(\boldsymbol{x}_{\boldsymbol{v}}), \quad \boldsymbol{v} \subseteq [d]$$

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and thus

$$f(\boldsymbol{x}) pprox \sum_{\boldsymbol{k} \in \mathcal{I}_{\boldsymbol{N}}} c_{\boldsymbol{k}}(f) \, \varphi_{\boldsymbol{k}}(\boldsymbol{x}), \qquad \mathcal{I}_{\boldsymbol{N}} \coloneqq \bigcup_{|\boldsymbol{v}| \leq q} \mathcal{I}_{\boldsymbol{N}^{\boldsymbol{v}}}$$



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 $\hat{=} \text{ projection using a finite dictionary } \{\varphi_{\pmb{k}}\}_{\pmb{k}\in\mathcal{I}_{\pmb{N}}}\subset\{\varphi_{\pmb{k}}\}_{\pmb{k}\in\mathbb{N}_0^d}$

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Still: computation of the integrals $c_{k}(f) = \langle f, \varphi_{k} \rangle_{L_{2}(\Omega, \omega)}, k \in \mathcal{I}_{N}$

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Projection

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→ data-driven approximation

Goal: approximate coefficients $c_{m k}(f)$ in $f({m x}) pprox \sum_{{m k} \in {\mathcal I}_{m N}} c_{m k}(f) \, \varphi_{m k}({m x})$

- $\, \triangleright \text{ from samples of the function } f$
- riangleright at points $\{m{x}^1,\dots,m{x}^M\}$ i.i.d. random according to the density ω



Goal: approximate coefficients $c_{k}(f)$ in $f(x) \approx \sum_{k \in \mathcal{I}_{N}} c_{k}(f) \varphi_{k}(x)$

- $\, \triangleright \text{ from samples of the function } f$
- \triangleright at points $\{ m{x}^1, \dots, m{x}^M \}$ i.i.d. random according to the density $\omega,$

i. e.,

$$\underbrace{\begin{pmatrix} \varphi_{\boldsymbol{k}_1}(\boldsymbol{x}^1) & \cdots & \varphi_{\boldsymbol{k}_N}(\boldsymbol{x}^1) \\ \vdots & & \vdots \\ \varphi_{\boldsymbol{k}_1}(\boldsymbol{x}^M) & \cdots & \varphi_{\boldsymbol{k}_N}(\boldsymbol{x}^M) \end{pmatrix}}_{\boldsymbol{A} \in \mathbb{R}^{M \times |\mathcal{I}_{\boldsymbol{N}}|}} \underbrace{\begin{pmatrix} c_{\boldsymbol{k}_1} \\ \vdots \\ c_{\boldsymbol{k}_N} \end{pmatrix}}_{\boldsymbol{c}} \approx \underbrace{\begin{pmatrix} f(\boldsymbol{x}^1) \\ \vdots \\ f(\boldsymbol{x}^M) \end{pmatrix}}_{\boldsymbol{f}}$$

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- \triangleright from samples of the function f
- \triangleright at points $\{x^1, \dots, x^M\}$ i.i.d. random according to the density ω ,

i. e..

$$\underbrace{\begin{pmatrix} \varphi_{\boldsymbol{k}_1}(\boldsymbol{x}^1) & \cdots & \varphi_{\boldsymbol{k}_N}(\boldsymbol{x}^1) \\ \vdots & & \vdots \\ \varphi_{\boldsymbol{k}_1}(\boldsymbol{x}^M) & \cdots & \varphi_{\boldsymbol{k}_N}(\boldsymbol{x}^M) \end{pmatrix}}_{\boldsymbol{A} \in \mathbb{R}^{M \times |\mathcal{I}_{\boldsymbol{N}}|}} \underbrace{\begin{pmatrix} c_{\boldsymbol{k}_1} \\ \vdots \\ c_{\boldsymbol{k}_N} \end{pmatrix}}_{\boldsymbol{c}} \approx \underbrace{\begin{pmatrix} f(\boldsymbol{x}^1) \\ \vdots \\ f(\boldsymbol{x}^M) \end{pmatrix}}_{\boldsymbol{f}} \qquad \qquad \sim \text{minimize } \|\boldsymbol{A}\boldsymbol{c} - \boldsymbol{f}\|_2^2$$



Goal: approximate coefficients $c_k(f)$ in $f(x) \approx \sum_{k \in \mathcal{T}_N} c_k(f) \varphi_k(x)$

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- least squares solution $c^* = (A^T A)^{-1} A^T f$
 - [Kämmerer, Ullrich, Volkmer 21]: good condition number with high probability, if $|\mathcal{I}_N| < \frac{M}{\log M}$
 - [Bartel, Potts, Schmischke 22]: can be computed efficiently (LSQR + fast multiplication)

Regression

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$$f^{\star}(\boldsymbol{x}) \coloneqq \sum_{\boldsymbol{k} \in \mathcal{I}_{N}} c_{\boldsymbol{k}}^{\star} \, \varphi_{\boldsymbol{k}}(\boldsymbol{x})$$

ANOVA approximation for control systems

Unknown function:

$$H \colon \mathbb{R}^d \times \mathbb{R}^m \to \mathbb{R}^d,$$

 $H(\boldsymbol{x}, \boldsymbol{u}) \coloneqq F(\boldsymbol{x}) + G(\boldsymbol{x})\boldsymbol{u},$

with

- $F: \mathbb{R}^d \to \mathbb{R}^d$,
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Given:

- sampling points $({m x}^i, {m u}^i), i=1,\ldots,M$
- $\bullet \ \ \mathsf{samples} \ H(\boldsymbol{x}^i, \boldsymbol{u}^i)$

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Important: avoid ANOVA approximation of H in $oldsymbol{z} = (oldsymbol{x}, oldsymbol{u})$

for m>1 introduces many additional terms – nonexistent interactions of the components of ${m u}$

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ightsquigarrow exploit linearity in $oldsymbol{u}$ instead



ANOVA approximation for control systems ANOVA approximation for control systems

Unit vectors as control

Simplest approach: $\mathbb{U}=\{m{0},m{e}_1,\dots,m{e}_m\}$ with $\{m{e}_\ell\}_{\ell=1}^m$ unit vectors of \mathbb{R}^m

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 $hd samples ig(H_j(oldsymbol{x}^i,oldsymbol{0})ig)_{i=1}^M ext{ for } ilde F_j$

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→ proceed rowwise:

$$H_j({m x},{m u}) = F_j({m x}) + \sum_{\ell=1}^m G_{j\ell}({m x})\,u_\ell, \quad j=1,\ldots,d$$

- riangleright samples $\left(H_j(oldsymbol{x}^i, oldsymbol{0})
 ight)_{i=1}^M$ for $ilde{F}_j$
- ho samples $\left(H_j(m{x}^i,m{e}_\ell)-H_j(m{x}^i,m{0})
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 \checkmark preserves structure (linearity in u)

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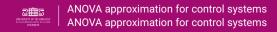
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- \triangleright samples $(H_i(\boldsymbol{x}^i, \boldsymbol{e}_\ell) H_i(\boldsymbol{x}^i, \boldsymbol{0}))_{i=1}^M$, for $\tilde{G}_{i\ell}$
 - \checkmark preserves structure (linearity in u)
- $m{X} \quad M(m+1)$ function evaluations necessary at each unit vector all x^i

 - non-flexible



 $\ensuremath{\mathbf{Aim}}\xspace$ preserve structure + use only one set of samples of H

 $\ensuremath{ \mbox{Aim:}}$ preserve structure + use only one set of samples of H

Observation: ANOVA approximation separately for F and G would mean

$$H_j(\boldsymbol{x}, \boldsymbol{u}) = F_j(\boldsymbol{x}) + \sum_{\ell=1}^m G_{j\ell}(\boldsymbol{x}) u_\ell$$
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$$H_j(\boldsymbol{x}, \boldsymbol{u}) = F_j(\boldsymbol{x}) + \sum_{\ell=1}^m G_{j\ell}(\boldsymbol{x}) u_\ell \approx \sum_{\boldsymbol{k} \in \mathcal{I}(V_1)} c_{\boldsymbol{k}}^1 \varphi_{\boldsymbol{k}}^1(\boldsymbol{x}) +$$
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 \Rightarrow for $(\boldsymbol{x}^i, \boldsymbol{u}^i)$ i.i.d. random:

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ight)_{i=1,\,oldsymbol{k}\in\mathcal{I}(V_\ell)}^M, \quad oldsymbol{U}_\ell \coloneqq \mathrm{diag}(u_\ell^1,\ldots,u_\ell^M)$$

 ${\bf Aim:}$ preserve structure + use only one set of samples of H

Observation: ANOVA approximation separately for F and G would mean

$$H_j(\boldsymbol{x}, \boldsymbol{u}) = F_j(\boldsymbol{x}) + \sum_{\ell=1}^m G_{j\ell}(\boldsymbol{x}) u_\ell \approx \sum_{\boldsymbol{k} \in \mathcal{I}(V_1)} c_{\boldsymbol{k}}^1 \varphi_{\boldsymbol{k}}^1(\boldsymbol{x}) + \sum_{\ell=1}^m \left(\sum_{\boldsymbol{s} \in \mathcal{I}(V_{\ell+1})} c_{\boldsymbol{s}}^{\ell+1} \varphi_{\boldsymbol{s}}^{\ell+1}(\boldsymbol{x}) \right) u_\ell, \quad j = 1, \dots, d$$

 \Rightarrow for $(\boldsymbol{x}^i, \boldsymbol{u}^i)$ i.i.d. random:

$$oldsymbol{c}^\ell \coloneqq \left(c_{oldsymbol{k}}^\ell
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yields

$$\left(H_j(oldsymbol{x}^i,oldsymbol{u}^i)
ight)_{i=1}^Mpprox \left(oldsymbol{A}_1 \quad oldsymbol{U}_1oldsymbol{A}_2 \quad \dots \quad oldsymbol{U}_moldsymbol{A}_{m+1}
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⇒ find least squares solution

[https://github.com/NFFT/ANOVAapprox.jl]

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Recap - ANOVA approximation:

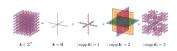




reduce number of ANOVA terms

Projection

choose finite number of basis functions $\{\varphi_{k}\}_{k\in\mathbb{Z}^{d}}$



Regression

$$\underbrace{\begin{pmatrix} \varphi_{k_1}(x^1) & \cdots & \varphi_{k_N}(x^1) \\ \vdots & & \vdots \\ \varphi_{k_1}(x^M) & \cdots & \varphi_{k_N}(x^M) \end{pmatrix}}_{\boldsymbol{A} \in \mathbb{R}^{M \times |\mathcal{I}_N|}} \underbrace{\begin{pmatrix} c_{k_1} \\ \vdots \\ c_{k_N} \end{pmatrix}}_{\boldsymbol{c}} \approx \underbrace{\begin{pmatrix} f(x^1) \\ \vdots \\ f(x^M) \end{pmatrix}}_{\boldsymbol{f}}$$

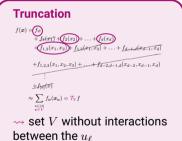
$$\Rightarrow \text{ minimize } \|\boldsymbol{A}\boldsymbol{c} - \boldsymbol{f}\|_2^2$$

$$\leadsto$$
 minimize $\|\boldsymbol{A}\boldsymbol{c}-\boldsymbol{f}\|_2^2$

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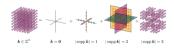
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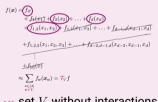
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Recap – ANOVA approximation:

Truncation



 \rightsquigarrow set V without interactions between the u_{ℓ}

Projection

use the Chebyshev basis

$$\{\varphi_k^{\text{cheb}}\}_{k\in\mathbb{N}_0} = \{1, \sqrt{2}x, \dots\}$$

choose only one basis function for all u_ℓ

⇒ exact reconstruction of all u_{ℓ}

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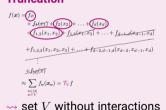
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$$H_j({m x},{m u}) = F_j({m x}) + \sum_{\ell=1}^m G_{j\ell}({m x})\,u_\ell, \quad j=1,\ldots,d$$

Recap - ANOVA approximation:

Truncation

between the u_{ℓ}



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 \leadsto minimize $\|\boldsymbol{A}\boldsymbol{c}-\boldsymbol{f}\|_2^2$

 \Rightarrow only need suitable preprocessing step (adjust the index sets V and \mathcal{I}_{N^v} appropriately)

Numerical Example

- d = 8 and m = 1
- · consider only one component

$$H_j(\boldsymbol{x}, u) = \underbrace{(x_4 - x_1) x_2}_{F(\boldsymbol{x})} - \underbrace{x_3}_{G(\boldsymbol{x})} u$$

maximum two-dimensional terms

$$\rightsquigarrow q = 2$$

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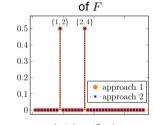
- maximum two-dimensional terms $\Rightarrow q = 2$
- Chebyshev basis for both approaches
 - ▷ approach 1 unit vectors
 - □ proach 2 − matrix approach

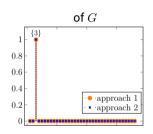
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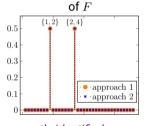
 \Rightarrow correctly identified

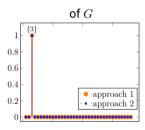
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- \Rightarrow correctly identified
- **2** error results \rightsquigarrow same order of magnitude 10^{-10}

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