

ANOVA meets control

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joint work with

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Research Seminar Numerics

Motivation

Unknown function (control system):

$$H: \mathbb{R}^d \times \mathbb{R}^m \rightarrow \mathbb{R}^d,$$

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

with

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

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Example: Euler approximation of a controlled Duffing oscillator

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

$$= \begin{pmatrix} x_1 + \Delta t x_2 \\ x_2 + \Delta t x_1 \end{pmatrix} + \begin{pmatrix} 0 \\ -3\Delta t x_1^3 \end{pmatrix} u$$

$$= F(\mathbf{x}) + G(\mathbf{x})u$$

i. e.,

- $d = 2,$
- $m = 1,$
- only 1D terms \rightsquigarrow low-dimensional

Overview

- 1 ANOVA approximation for scalar-valued functions
- 2 ANOVA approximation for control systems
- 3 Numerical Example

ANOVA approximation

ANalysis Of VAriance (ANOVA) decomposition

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

Decompose a d -dimensional function f into

$$\begin{aligned}
 f(\mathbf{x}) = & f_{\emptyset} && \text{constant} \\
 & + f_1(x_1) + \dots + f_d(x_d) && \text{one-dimensional terms} \\
 & + f_{1,2}(x_1, x_2) + f_{1,3}(x_1, x_3) + \dots + f_{d-1,d}(x_{d-1}, x_d) && \text{two-dimensional terms} \\
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 & + f_{[d]}(\mathbf{x}) && d\text{-dimensional term}
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$$[d] := \{1, \dots, d\}$$

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- in general multiple representations possible
- conditions for uniqueness?

Definition

Let

$$\langle f, g \rangle_{L_2(\Omega, \omega)} := \int_{\Omega} f(\mathbf{x}) g(\mathbf{x}) \omega(\mathbf{x}) \, d\mathbf{x}$$

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Basis representation: For orthonormal basis $\{\varphi_{\mathbf{k}}\}_{\mathbf{k} \in \mathbb{N}_0^d}$ of $L_2(\Omega, \omega)$ we have

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[Potts, Schmiscke 21]:

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

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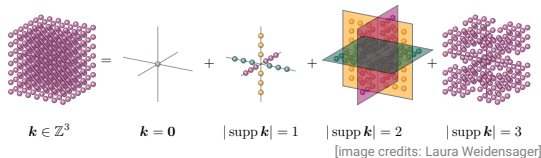
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\Rightarrow decomposition in the space of basis coefficients

Numerical realization – ANOVA approximation

[Potts, Schmischke 21]

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

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Truncation

reduce number of ANOVA terms

$$\mathcal{T}_V f = \sum_{\substack{\mathbf{v} \subseteq [d] \\ \mathbf{v} \in V}} f_{\mathbf{v}}$$

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Numerical realization – ANOVA approximation

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$$f = \sum_{v \subseteq [d]} f_v, \quad f_v = \sum_{\substack{k \in \mathbb{Z}^d \\ \text{supp } k = v}} c_k(f) \varphi_k$$

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Projection

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

$$P_N f = \sum_{\substack{v \subseteq [d] \\ v \in V}} \tilde{f}_v$$

$$\tilde{f}_v = \sum_{k \in \mathcal{I}_N v} c_k(f) \varphi_k$$

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Regression

compute coefficients c_k^* from samples

$$f^* = \sum_{\substack{v \subseteq [d] \\ v \in V}} f_v^*$$

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

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

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constant

one-dimensional terms

two-dimensional terms

~~three-dimensional terms~~

~~d-dimensional term~~

$$\approx \sum_{\substack{\mathbf{v} \subseteq [d] \\ \mathbf{v} \in V}} f_{\mathbf{v}}(\mathbf{x}_{\mathbf{v}}) = \mathcal{T}_V f$$

set V according to sparsity

Projection

Recap: reduced the number of ANOVA terms

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

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\rightsquigarrow data-driven approximation

Regression

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

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

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↪ minimize $\|\mathbf{A}\mathbf{c} - \mathbf{f}\|_2^2$

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- ▷ at points $\{\mathbf{x}^1, \dots, \mathbf{x}^M\}$ i.i.d. random according to the density ω ,

i. e.,

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

- least squares solution $\mathbf{c}^* = (\mathbf{A}^\top \mathbf{A})^{-1} \mathbf{A}^\top \mathbf{f}$
 - [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

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

- ▷ from samples of the function f
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- final approximation

$$f^*(\mathbf{x}) := \sum_{\mathbf{k} \in \mathcal{I}_N} c_{\mathbf{k}}^* \varphi_{\mathbf{k}}(\mathbf{x})$$

ANOVA approximation for control systems

Setting

Unknown function:

$$H: \mathbb{R}^d \times \mathbb{R}^m \rightarrow \mathbb{R}^d,$$
$$H(\mathbf{x}, \mathbf{u}) := F(\mathbf{x}) + G(\mathbf{x})\mathbf{u},$$

with

- $F: \mathbb{R}^d \rightarrow \mathbb{R}^d$,
- $G: \mathbb{R}^d \rightarrow \mathbb{R}^{d \times m}$,
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Assumption: F and G of low-dimensional structure

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Given:

- sampling points $(\mathbf{x}^i, \mathbf{u}^i)$, $i = 1, \dots, M$
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Goal: find $\tilde{H} \approx H$

Assumption: F and G of low-dimensional structure

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Approach: ANOVA approximation

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

Approach: ANOVA approximation

Problem: F and G cannot be sampled separately

Setting

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Approach: ANOVA approximation

Problem: F and G cannot be sampled separately
 \rightsquigarrow individual approximation not possible

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

Approach: ANOVA approximation

Problem: F and G cannot be sampled separately

- ↪ individual approximation not possible
- ↪ coupled reconstruction

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

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

↪ unnecessary costs + error

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- sampling points $(\mathbf{x}^i, \mathbf{u}^i)$, $i = 1, \dots, M$
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Approach: ANOVA approximation

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

Approach: ANOVA approximation

Problem: F and G cannot be sampled separately

↪ individual approximation not possible

↪ coupled reconstruction

↪ exploit linearity in \mathbf{u} instead

Unit vectors as control

Simplest approach: $\mathbb{U} = \{0, e_1, \dots, e_m\}$ with $\{e_\ell\}_{\ell=1}^m$ unit vectors of \mathbb{R}^m

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\Rightarrow may produce samples of F and G artificially

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\rightsquigarrow proceed rowwise:

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

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✓ preserves structure (linearity in \mathbf{u})

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- ▷ samples $(H_j(\mathbf{x}^i, \mathbf{e}_\ell) - H_j(\mathbf{x}^i, \mathbf{0}))_{i=1}^M$ for $\tilde{G}_{j\ell}$

- ✓ preserves structure (linearity in \mathbf{u})
- ✗ $M(m+1)$ function evaluations necessary
 - at each unit vector all \mathbf{x}^i
 - non-flexible

Matrix approach

Aim: preserve structure + use only one set of samples of H

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Observation: ANOVA approximation separately for F and G would mean

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

Matrix approach

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Observation: ANOVA approximation separately for F and G would mean

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

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

$$\mathbf{c}^\ell := \left(c_{\mathbf{k}}^\ell \right)_{\mathbf{k} \in \mathcal{I}(V_\ell)}, \quad \mathbf{A}_\ell := \left(\varphi_{\mathbf{k}}^\ell(\mathbf{x}^i) \right)_{i=1, \mathbf{k} \in \mathcal{I}(V_\ell)}^M, \quad \mathbf{U}_\ell := \text{diag}(u_\ell^1, \dots, u_\ell^M)$$

Matrix approach

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

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$$\mathbf{c}^\ell := \left(c_{\mathbf{k}}^\ell \right)_{\mathbf{k} \in \mathcal{I}(V_\ell)}, \quad \mathbf{A}_\ell := \left(\varphi_{\mathbf{k}}^\ell(\mathbf{x}^i) \right)_{i=1, \mathbf{k} \in \mathcal{I}(V_\ell)}^M, \quad \mathbf{U}_\ell := \text{diag}(u_\ell^1, \dots, u_\ell^M)$$

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$$\left(H_j(\mathbf{x}^i, \mathbf{u}^i) \right)_{i=1}^M \approx \begin{pmatrix} \mathbf{A}_1 & \mathbf{U}_1 \mathbf{A}_2 & \dots & \mathbf{U}_m \mathbf{A}_{m+1} \end{pmatrix} \begin{pmatrix} \mathbf{c}^1 \\ \vdots \\ \mathbf{c}^{m+1} \end{pmatrix}$$

Matrix approach

Aim: preserve structure + use only one set of samples of H

Observation: ANOVA approximation separately for F and G would mean

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\Rightarrow find least squares solution

Efficient implementation

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

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

Recap – ANOVA approximation:

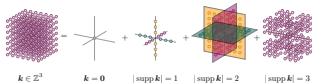
Truncation

$$\begin{aligned} f(\mathbf{x}) &= f_0 \\ &+ f_1(x_1) + f_2(x_2) + \dots + f_d(x_d) \\ &+ f_{1,2}(x_1, x_2) + f_{1,3}(x_1, x_3) + \dots + f_{d-1,d}(x_{d-1}, x_d) \\ &+ f_{1,2,3}(x_1, x_2, x_3) + \dots + f_{d-2,d-1,d}(x_{d-2}, x_{d-1}, x_d) \\ &\vdots \\ &+ f_{[d]}(\mathbf{x}) \\ &\approx \sum_{\substack{v \subseteq [d] \\ v \in V}} f_v(\mathbf{x}_v) = \mathcal{T}_V f \end{aligned}$$

reduce number of ANOVA terms

Projection

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



Regression

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

\rightsquigarrow minimize $\|\mathbf{A}\mathbf{c} - \mathbf{f}\|_2^2$

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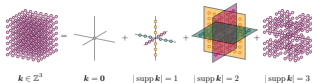
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↪ set V without interactions between the u_{ℓ}

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

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⇒ exact reconstruction of
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⇒ minimize $\|\mathbf{A}\mathbf{c} - \mathbf{f}\|_2^2$

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

Numerical Example

Toy example

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

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

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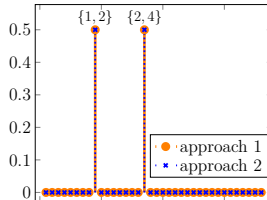
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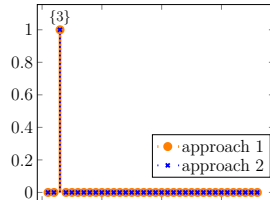
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\Rightarrow correctly identified

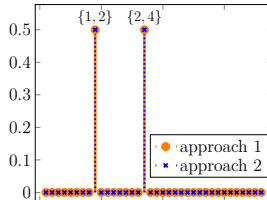
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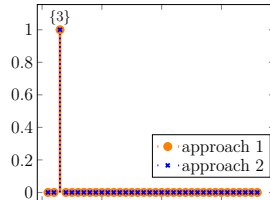
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2 error results \rightsquigarrow same order of magnitude 10^{-10}

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