GPS: Gaussian Process Subspace Regression for Model Reduction

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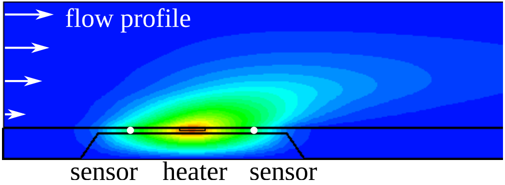
Motivation: Parametric Studies of Computational Models

Anemometer:

- flow-speed MEMS device
- calibration
- convection-diffusion PDE
- linear ODE ($n = 29{,}008$)



The MORwiki Community. Anemometer. Model Order Reduction Wiki, 2018.

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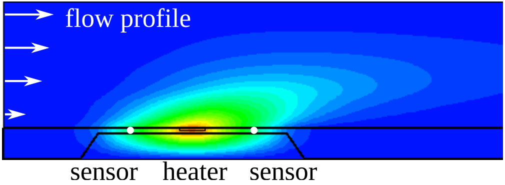
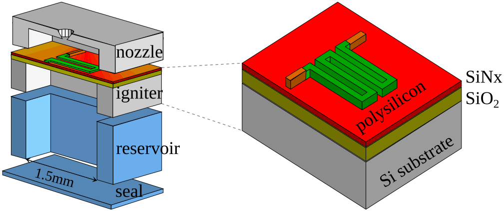


Microthruster:

- solid propellant micro-rocket
- design
- heat transfer PDE
- linear ODE ($n = 4{,}257$)



The MORwiki Community. Anemometer. Model Order Reduction Wiki, 2018.

Oberwolfach Benchmark Collection. Thermal model. Model Order Reduction Wiki, 2018.

Reduced Order Modeling via Projection to Subspaces

Physics

$$x(0), u(t)$$

$$\dot{x} = A x + B u$$
$$y = C x$$

$$y(t)$$

O(n) ~ O(n^2)
n > O(10^5)

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ROM

$x_r(0), u(t)$

$$\dot{x}_r = A_r x_r + B_r u$$
$$y_r = C_r x_r$$

$y_r(t)$

k = O(10)
Orders of magnitude faster!

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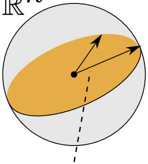

V

$$A_r = V^T A V$$
$$B_r = V^T B$$
$$C_r = C V$$

ROM

$x_r(0), u(t)$

$$\dot{x}_r = A_r x_r + B_r u$$
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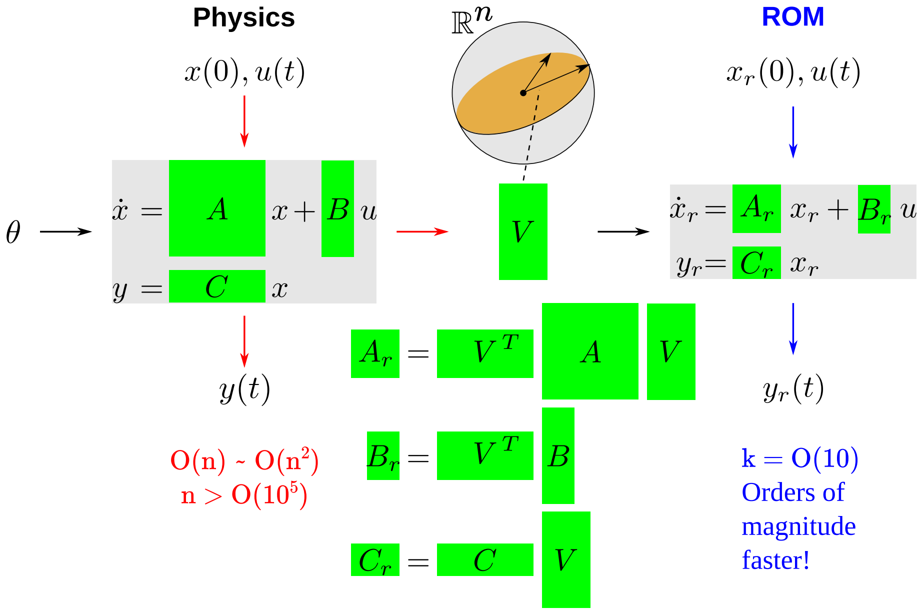

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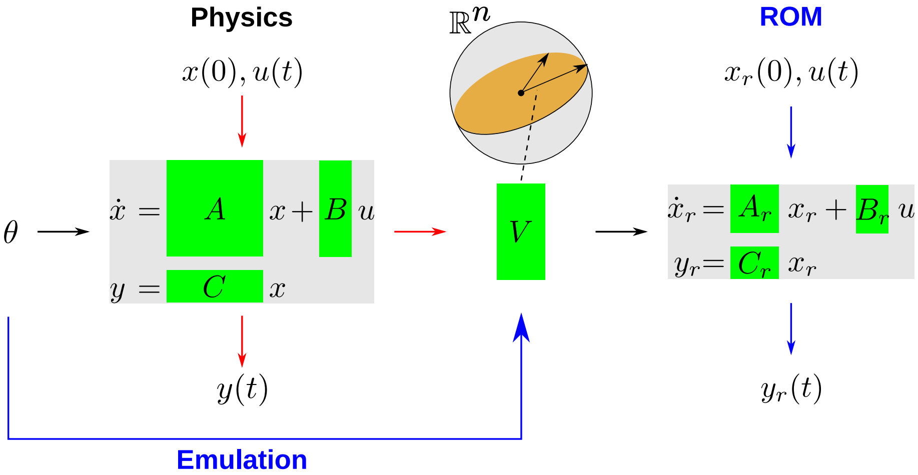
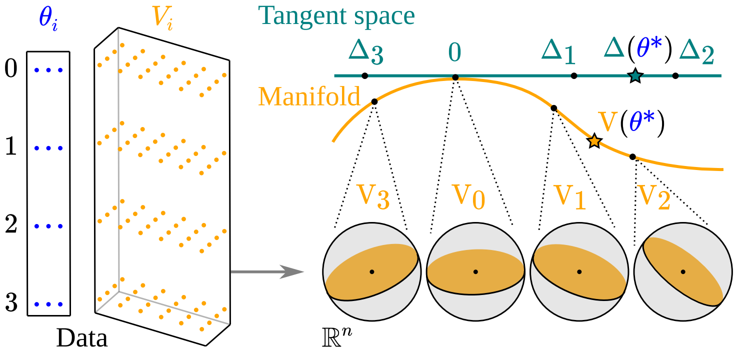


Emulator + ROM ⇒ Parametric ROM

Problem: Emulating Subspace-valued Functions

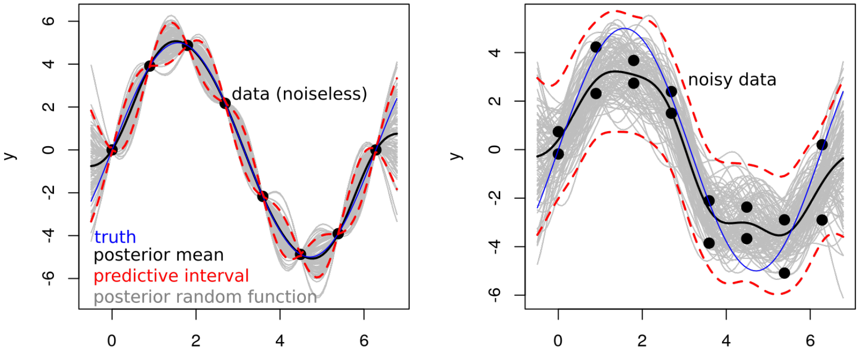
- Old idea: interpolate on tangent spaces.
- Pros: ↗ 7–45 times speedup than direct ROM.
- Cons: ↘ inflexible, ↘ extrinsic, ↘ no UQ.



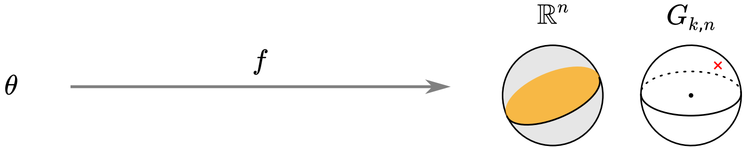
D. Amsallem, C. Farhat. Interpolation method for adapting ROMs and application to aeroelasticity. *AIAA Journal*, 46(7):1803–1813, July 2008. (587 cites; 78 in 2020.)

Gaussian Process (GP) Models: Basics

- Unknown function: $f : \Theta \mapsto \mathbb{R}$, real-valued.
- GP prior process: $f \sim \mathcal{GP}(\mu(x), k(x, x'; \psi))$, hyper-parameters ψ.
- Likelihood: $p(y \mid f) \sim N(f, \sigma^2)$, non-singular Gaussian.
- Posterior: $p(f \mid y, x) \propto p(f \mid x)\ p(y \mid f)$.
- Noiseless data $\Rightarrow$ conditional, $p(f_* \mid f, x_*, x)$.
- Noisy data $\Rightarrow p(f_* \mid y, x_*, x) = \int p(f_* \mid f, x_*, x)\ p(f \mid y, x)\ df$.



Gaussian Process Subspace (GPS) Model



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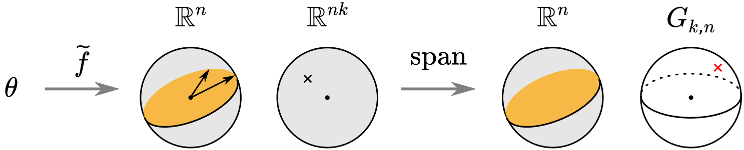

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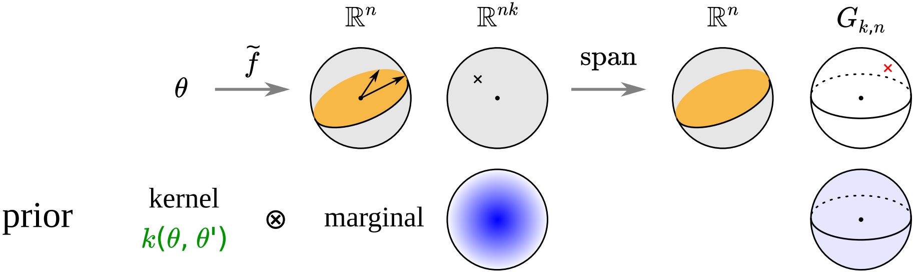

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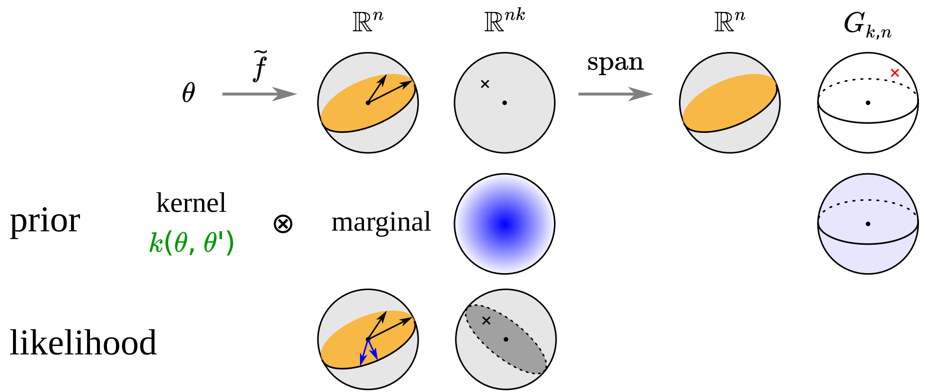
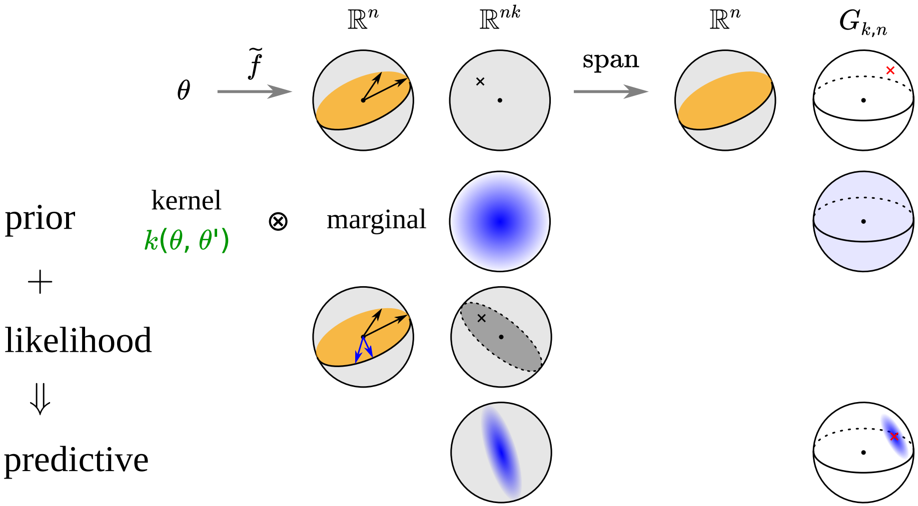


Gaussian Process Subspace (GPS) Model



The GPS Model

Prior process: $\tilde{f} \sim \mathscr{GP}(0, k \otimes \mathbf{I}_{nk})$.

$$(\mathbf{m}_*, \mathbf{m}) \sim N_{nk(l+1)}(0, \mathbf{K}_{l+1} \otimes \mathbf{I}_{nk})$$

Equal likelihood to all bases of a subspace:

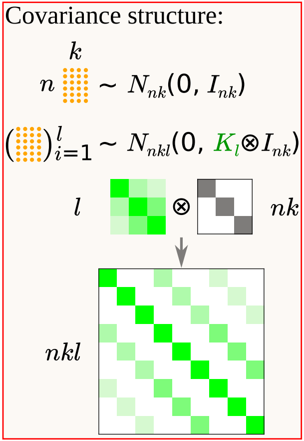
$$L(\mathbf{m}_i | \mathfrak{X}_i) = 1(\mathbf{m}_i \in [\mathbf{x}_i])$$

$$[\mathbf{x}_i] = \{\mathrm{vec}(\mathbf{X}_i \mathbf{A}) : \mathbf{A} \in \mathrm{GL}_k\}$$

Predictive distribution has an analytical form:

$$\mathbf{m}_* | \mathfrak{X} \sim N_{nk}(0, \mathbf{I}_k \otimes \mathbf{\Sigma})$$

$$\mathbf{\Sigma}(\boldsymbol{\theta}) = \varepsilon^2 \mathbf{I}_n + \mathbf{X}[\mathbb{X}^T(\tilde{\mathbf{K}}_l \otimes \mathbf{I}_n)\mathbb{X}]^{-1}\mathbf{X}^T$$

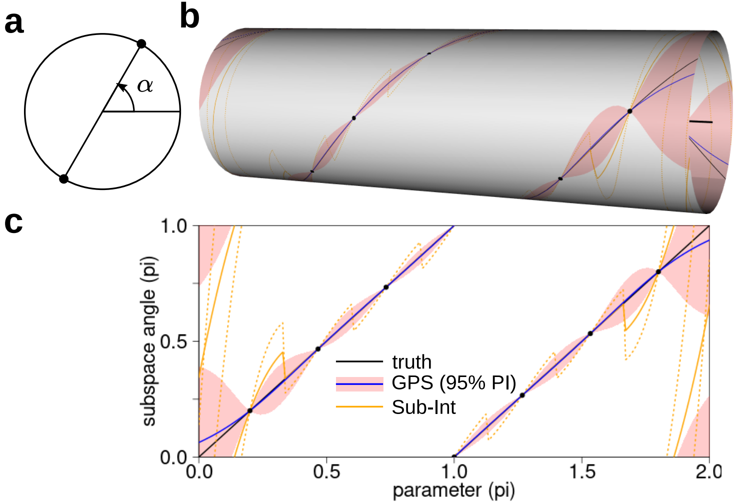


Theorem (Zhang, Mak, Dunson, 2021+)

Subspace prediction by the GPS has a matrix angular central Gaussian distribution $\mathfrak{M}_* | \mathfrak{X} \sim MACG(\mathbf{\Sigma})$, which admits easy sampling and inference.

Visualization of the GPS posterior process

- Target function $f : \mathbb{R} \mapsto G_{1,2}$
- Constant-speed rotation of lines in the plane.



Computational Complexity of GPS

Table: Interpolatory PROM methods: floating point operations.

	predict subspace	compute ROM
GPS	$k^3 l^3$	$2k^3 l^2$
Subspace-Int	$8nk^2$	$2nk^2$
Matrix-Int[1]	-	$2k^2 l$
Manifold-Int[2]	-	$\mathcal{O}(k^3 l)$

- *Subspace-Int*: most used; ↘ scale with $n > \mathcal{O}(10^5)$.
- *Matrix-/Manifold-Int*: ↗ faster online computation; ↘ less accurate.

[1] H. Panzer, J. Mohring, R. Eid, B. Lohmann. Parametric model order reduction by matrix interpolation. *at - Automatisierungstechnik*, 58 (8): 475–484, Aug. 2010.

[2] D. Amsallem, C. Farhat. An online method for interpolating linear parametric reduced-order models. *SIAM Journal on Scientific Computing*, 33 (5): 2169–2198, Jan. 2011.

Prediction Accuracy of GPS: Anemometer

Setup:

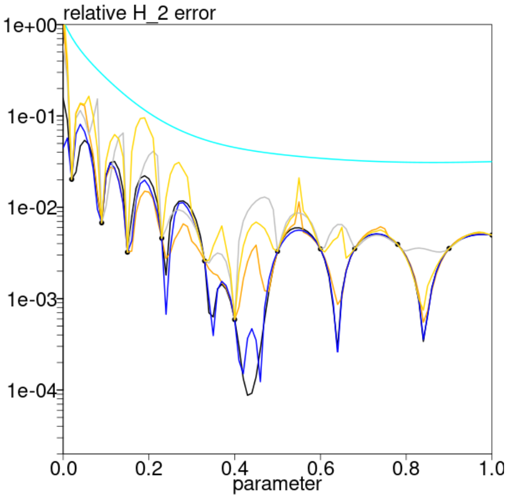
- subspace dim: $k = 20$
- sample size: $l = 12$

References: (lower is better)

- local bases (lower bound)
- global basis (upper bound)

Methods:

- GPS (rel. speedup: 6.7)
- Subspace interpolation
- Manifold interpolation
- Matrix interpolation



Prediction Accuracy of GPS: Anemometer

Setup:

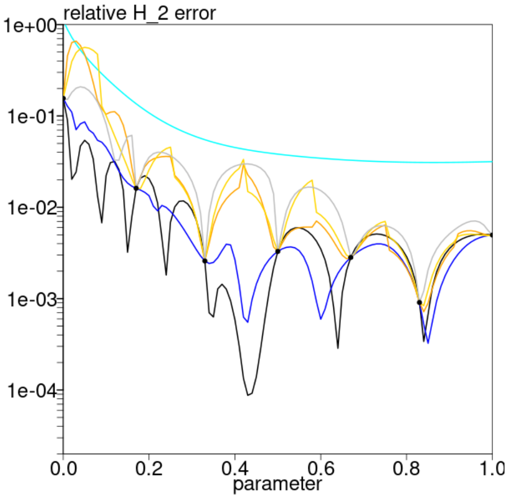
- subspace dim: $k = 20$
- sample size: $l =$ 7

References: (lower is better)

- local bases (lower bound)
- global basis (upper bound)

Methods:

- GPS (rel. speedup: 34)
- Subspace interpolation
- Manifold interpolation
- Matrix interpolation



Prediction Accuracy of GPS: Anemometer

Setup:

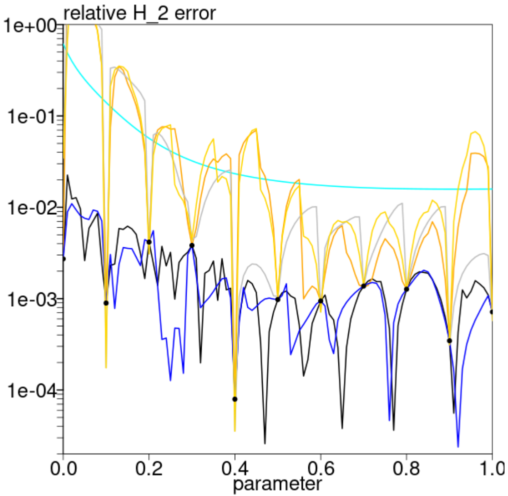
- subspace dim: $k =$ 40
- sample size: $l =$ 11

References: (lower is better)

- local bases (lower bound)
- global basis (upper bound)

Methods:

- GPS (rel. speedup: 4.4)
- Subspace interpolation
- Manifold interpolation
- Matrix interpolation



GPS retains accuracy of local reduced bases!

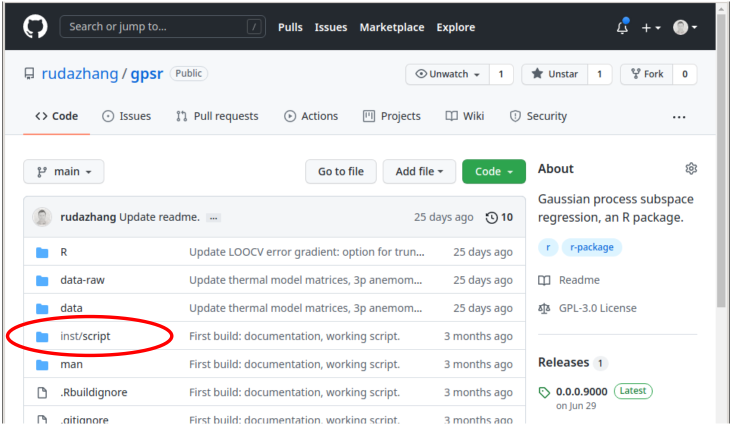
Summary

- Problem: approximate subspace-valued functions
- Use: parametric reduced order modeling (PROM)
- State of the art: interpolate on tangent spaces
  - ↘ inflexible, extrinsic, deterministic
  - ↘ slow for large-scale systems, $n \gg 1$
- New idea: GP for subspace prediction
  - high-dim ($> 10^5$), non-vector output
  - ↗ accurate (small sample, high dim) + UQ $\Leftarrow$ Bayesian nonparametric
  - ↗ fast: suitable for online computation
  - data-driven (GP) + physics-based (ROM) method for surrogate modeling of engineering systems.
  - future directions: prior, kernel, etc.

RZ, S. Mak, D. Dunson. Gaussian Process Subspace Regression for Model Reduction. arXiv, 2021. https://arxiv.org/abs/2107.04668.

Software

R package for GPS: https://github.com/rudazhang/gpsr



Scripts for replicating the numerical examples in paper.