Intro to Reduced Basis Methods

Parametric Model Order Reduction

$$
\begin{tikzcd}
 & V_h \ni u_h(\mu) \arrow[dr, bend left, "s"] & \\
\mu \in \mathcal{P} \subset \mathbb{R}^p \arrow[ur, bend left, "\Phi"] \arrow[rr, "s \circ \Phi"] & & \mathbb{R}^m
\end{tikzcd}
$$

state space: V_h, $\dim V_h \in [10^4, 10^8]$

parameter domain: $\mathcal{P} \subset \mathbb{R}^p$

output space: $\mathbb{R}^m$, m = number of outputs

Assumption Φ can be evaluated, but expensive.
s can be evaluated.

Objectives a) compute $s \circ \Phi$ quickly for many $\mu \in \mathcal{P}$

b) compute $s \circ \Phi$ quickly for previously unknown $\mu \in \mathcal{P}$ after some preparation.

3 Ideas behind RB methods

1. approximate Φ by $\tilde{\Phi} : \mathcal{P} \longrightarrow V_N \subset V_h$ via (Petrov-)Galerkin projection, and $s \circ \Phi$ by $s \circ \tilde{\Phi}$ ($\dim V_N \in [1, 10^4]$)

2. build V_N from solution snapshots $\Phi(\mu_s)$:
$V_N := \operatorname{span}(\{\Phi(\mu_s) \mid 1 \leq s \leq S\})$

3. select μ_s using greedy search in $\mathcal{P}$ for worst-approx μ.

Today $\Phi(\mu) =: u_h(\mu)$ solution of elliptic PDE:

Elliptic FOM Let $\Phi(\mu) = u_h(\mu) \in V_h$ be given by

$$a(u_h(\mu), v_h; \mu) = \ell(v_h) \quad \forall v_h \in V_h,$$

where a is s.p.d. and $\ell \in V_h'$. Let $s \in V_h'$.
Denote by

$$\alpha(\mu) := \inf_{0 \neq v_h \in V_h} \frac{a(v_h, v_h; \mu)}{\|v_h\|^2} \qquad \gamma(\mu) := \sup_{0 \neq v_h, w_h \in V_h} \frac{a(v_h, w_h; \mu)}{\|v_h\| \|w_h\|}$$

the coercivity and norm constants of a.

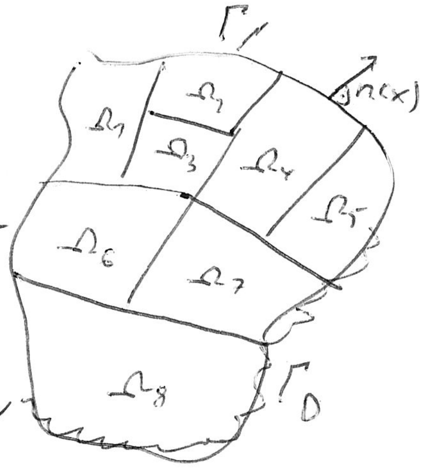
Example: Thermal Block Problem

Solve

$$\nabla \cdot [-\sigma(x;\mu) \nabla u(x,\mu)] = f(x) \qquad x \in \Omega$$

$$u(x,\mu) = 0 \qquad x \in \Gamma_D$$

$$\sigma(x,\mu) \nabla u(x,\mu) \cdot n(x) = g_\mu(x) \qquad x \in \Gamma_N$$



where

$$\sigma(x,\mu) \equiv \mu_p \qquad \text{for } x \in \Omega_p, \quad \mu \in (\mu_1, \ldots, \mu_P) \in \mathbb{R}^{P}_{>0}$$

Weak formulation:

$$\int_\Omega f(x)\varphi(x)\,dx = \int_\Omega \nabla \cdot [-\sigma(x,\mu) \nabla u(x,\mu)]\, \varphi(x)\,dx \qquad \left(\begin{aligned} &\nabla \cdot [-\sigma \nabla u\, \varphi] \\ &= (\nabla \cdot -\sigma \nabla u)\varphi + -\sigma \nabla u \nabla \varphi \end{aligned} \right)$$

$$= \int_{\partial\Omega} -\sigma(x,\mu) \nabla u(x,\mu) \cdot n(x)\,dx + \int_\Omega \sigma(x,\mu) \nabla u(x,\mu) \nabla \varphi(x)\,dx$$

$$= -\int_{\Gamma_N} g_\mu(x)\,dx$$

$\rightsquigarrow$ weak solution $u(x,\mu) \in H_0^1(\Omega)$ satisfies

$$\underbrace{\int_\Omega \sigma(x,\mu)\, \nabla u(x,\mu)\, \nabla v(x)\, dx}_{a(u,v)} = \underbrace{\int_\Omega f(x)\, v(x)\, dx + \int_{\Gamma_N} g_N(x)\, dx}_{\ell(v)} \qquad (*)$$

$\|u\| := \|\nabla u\|_{L^2(\Omega)}$, then

$$a(v,v;\mu) = \int_\Omega \sigma(x,\mu)\, |\nabla v(x)|^2\, dx$$

$$\geq \inf_x \sigma(x,\mu) \cdot \|v\|^2 \qquad \Rightarrow \alpha(\mu) \geq \inf_x \sigma(x,\mu)$$

$$a(u,v;\mu) = \int_\Omega \sigma(x,\mu)\, \nabla u(x) \cdot \nabla v(x)\, dx$$

$$\leq \cancel{\int_\Omega} \|\sigma(\cdot,\mu)\|_{L^\infty(\Omega)}\, \|\nabla u\|_{L^2(\Omega)} \cdot \|\nabla v\|_{L^2(\Omega)} \qquad \Rightarrow \gamma(\mu) \leq \|\sigma(\mu)\|_{L^\infty}$$

$+$ Finite element discretization

(choose $V_h \subset H_0^1(\Omega)$ and solve $(*)$ for $u_h(\mu), v_h \in V_h$)

<u>Elliptic ROM</u> Let $\tilde{\Phi}(\mu) =: u_N(\mu) \in V_N$ be given by

$$a(u_N(\mu), v_N; \mu) = \ell(v_N) \qquad \forall v_N \in V_N.$$

<u>Prop</u> $u_N(\mu)$ is well-defined.

<u>Proof</u> a is s.p.d. on $V_N \subset V_h$.

<u>A priori estimate</u> Let $e_N(\mu) := u_h(\mu) - u_N(\mu)$. We have

$$\alpha(\mu)\| e_N(\mu)\|^2 \leq a(e_N(\mu), e_N(\mu); \mu)$$

$$= \left(\inf_{v_N \in V_N}\right) a(e_N(\mu), u_h(\mu) - v_N; \mu)$$

$$\leq \left(\inf_{v_N \in V_N}\right) \gamma(\mu) \| e_N(\mu)\| \, \| u_h(\mu) - v_N\|$$

$$\boxed{\begin{aligned} &a(e_N(\mu), v_N) \\ &= \ell(v_N) - \ell(v_N) = 0 \\ &\text{Galerkin orthogonality} \end{aligned}}$$

$$\Longrightarrow \| e_N(\mu)\| \leq \frac{\gamma(\mu)}{\alpha(\mu)} \underbrace{\inf_{v_N \in V_N} \| u_h(\mu) - v_N\|}_{\text{best approx error}}$$

<u>Computing the Solution</u> Let $b_1, \ldots, b_N$ be basis of V_N,

$\mathbb{A}_{ij}(\mu) := a(b_j, b_i)$ $\quad \mathbb{L}_i := \ell(b_i)$ $\quad u_N(\mu) =: \sum_{i=1}^{N} \underline{u}_{N,i}(\mu) b_i$,

$\mathbb{S}_i := s(b_i)$

then

$$\mathbb{A}(\mu) \cdot \underline{u}_N(\mu) = \mathbb{L}_i, \qquad s(u_N(\mu)) = \mathbb{S} \cdot \underline{u}_N$$

<u>Problem</u> need to compute $\mathbb{A}(\mu)$ for each new μ.

Parameter Separability (affine decomposition) Assume that

$$a(v_h, w_h; \mu) = \sum_{q=1}^{Q} \Theta_q(\mu)\, a^q(v_h, w_h)$$

with bilinear forms a^q, $\Theta_q : \mathcal{P} \longrightarrow \mathbb{R}$.

Offline - Online Decomposition Precompute

$$\mathbb{A}^q_{ij} := a^q(b_j, b_i),$$

then

$$\mathbb{A}(\mu) = \sum_{q=1}^{Q} \Theta_q(\mu)\, \mathbb{A}^q$$

Effort for solution

$$\underbrace{\mathcal{O}(Q \cdot N^2)}_{\text{assembly}} + \underbrace{\mathcal{O}(N^3)}_{\substack{\text{solution}\\ \text{(dense!)}}} + \underbrace{\mathcal{O}(N)}_{\text{output}}$$

A posteriori estimate

$$\alpha(\mu)\, \| e_N(\mu) \|^2 \leq a(e_N(\mu), e_N(\mu); \mu)$$

$$= \ell(e_N(\mu)) - a(u_N(\mu), e_N(\mu); \mu)$$

$$=: \mathcal{R}_N(e_N(\mu); \mu)$$

$$\leq \underbrace{\sup_{0 \neq v_h \in V_h} \frac{\mathcal{R}_N(v_h; \mu)}{\| v_h \|}}_{\| \mathcal{R}_N \|_{V_h'}} \cdot \| e_N(\mu) \|$$

$$\Longrightarrow \quad \| e_N(\mu) \| \leq \frac{1}{\alpha(\mu)} \cdot \| \mathcal{R}_N(\mu) \|_{V_h'} =: \Delta_N(\mu)$$

Efficiency of $\Delta_N(\mu)$

$$\mathcal{R}_N(v_h;\mu) = l(v_h) - a(u_N(\mu), v_h; \mu)$$
$$= a(e_N(\mu), v_h; \mu)$$
$$\leq \gamma(\mu) \, \| e_N(\mu) \| \, \| v_h \|$$

$$\Rightarrow \quad \| \mathcal{R}_N(\mu) \|_{V_h'} \leq \gamma(\mu) \, \| e_N(\mu) \|$$

$$\Rightarrow \quad \Delta_N(\mu) \leq \frac{\gamma(\mu)}{\alpha(\mu)} \, \| e_N(\mu) \|$$

Weak Greedy Basis Generation

Input: $\Xi_{train} \subset \mathcal{P}$, ε

$V_0 \leftarrow \{0\}$, $\quad N \leftarrow 0$ — need offline-online decomp. of Δ_N

while $\max\limits_{\mu \in \Xi_{train}} \Delta_N(\mu) > \varepsilon$:

$\quad \mu_{N+1} \leftarrow \operatorname{argmax}\limits_{\mu \in \Xi_{train}} \Delta_N(\mu)$

$\quad V_{N+1} \leftarrow \operatorname{span} V_N \cup \{ u_h(\mu_{N+1}) \}$

$\quad N \leftarrow N+1$

Output: V_N

Decomposition of Δ_N

Let for $f \in V_h'$ be $r_f \in V_h$ s.t.

$$(r_f, v_h) = f(v_h) \quad \forall v_h \in V_h \qquad \text{(Riesz representative of } f\text{)}$$

Then:

$$\| \mathcal{R}_N(\mu) \|_{V_h'}^2 = \left(r_{\mathcal{R}_N(\mu)}, r_{\mathcal{R}_N(\mu)} \right)$$

$$= 2\sum_{i=1}^{N} (r_\ell, r_{a(b_i,\cdot;\mu)})\, u_{N,i}(\mu)$$

$$+ \sum_{i,j=1}^{N} (r_{a(b_i,\cdot;\mu)}, r_{a(b_j,\cdot;\mu)})\, u_{N,i}(\mu)\, u_{N,j}(\mu)$$

$$\longrightarrow \quad \sum_{q=1}^{N} r_{a^q(b_i,\cdot;\mu)}$$

effort to evaluate Δ_N online: $\mathcal{O}(Q^2 N^2)$

Kolmogorov N-width

$$d_N := \inf_{\substack{V_N \subset V_h \\ \dim V_N \le N}} \sup_{\mu \in \mathcal{P}} \underbrace{\inf_{v_N \in V_N} \| u_h(\mu) - v_N \|}_{\text{error in a priori estimate}}$$

<u>Thm</u> For affinely decomp. elliptic problems we have

$$d_N \le C e^{-cN^{1/Q}}$$

<u>Proof</u> e.g. Ohlberger, Rave, '16

1. $u_h(\mu)$ depends ~~holomorphically~~ analytically on $\Theta_1(\mu), \ldots, \Theta_Q(\mu)$
2. power series expansion

<u>Thm</u> The V_N generated by the weak greedy algorithm (for $S_{train} = \mathcal{P}$) satisfy

$$\sup_{\mu\in\mathcal{P}} \inf_{v_N \in V_N} \| u_h(\mu) - v_N \| \le \sqrt{2C}\, \eta\, e^{-c' N^{1/Q}},$$

where $c' = 2^{-1-2Q} c$ and $\eta = \sup_{\mu \in \mathcal{P}} \frac{\gamma(\mu)}{\alpha(\mu)}$. <u>Proof</u> DeVore, Petrova, Wojtaszczyk '13

<u>Output error bound</u> We have

$$|s(u_h(\mu)) - s(u_N(\mu))| = |s(e_N(\mu))|$$
$$\leq \|s\|_{V_h'} \cdot \|e_N(\mu)\| \leq \|s\|_{V_h'} \, \Delta_N(\mu)$$

<u>Output error bound - compliant case</u> Assume

$$s = \ell,$$

then

$$\underline{s(e_N(\mu))} = \ell(e_N(\mu))$$
$$= a(u_h(\mu), e_N(\mu); \mu)$$
$$\overset{\text{symmetry}}{=} a(e_N(\mu), u_h(\mu); \mu)$$
$$\overset{\text{Gal. orth}}{=} \underline{a(e_N(\mu), e_N(\mu); \mu)} \geq 0$$

$$= \mathcal{R}(e_N(\mu); \mu) \leq \|\mathcal{R}_N(\mu)\|_{V_h'} \cdot \|e_N(\mu)\| \leq \frac{1}{\alpha(\mu)} \|\mathcal{R}_N(\mu)\|^2$$

Moreover

$$\mathcal{R}_N(v_{N,\mu})^2 = a(e_N, v_{N,\mu})^2$$
$$\overset{\text{C.S.}}{\leq} a(e_N, e_{N,\mu}) \cdot a(v_N, v_N; \mu)$$
$$\leq s(e_N(\mu)) \cdot \gamma(\mu) \|v_N\|^2$$

$$\Rightarrow \quad \frac{1}{\alpha(\mu)} \|\mathcal{R}_N(\mu)\|^2_{V_h'} \leq \frac{\gamma(\mu)}{\alpha(\mu)} \, s(e_N(\mu))$$

Output error bound - primal dual approach

For general $s \neq \ell$ let $V_N^{du} \subset V_h$ be RB space for the dual problem

$$a(v_h, u_h^{du}(\mu); \mu) = -s(v_h) \qquad \forall v_h \in V_h$$

and let $u_N^{du}(\mu) \in V_N^{du}$ solve

$$a(v_N, u_N^{du}(\mu); \mu) = -s(v_N) \qquad \forall v_N \in V_N.$$

Then for the corrected output

$$s(u_N(\mu)) - R(u_N^{du}(\mu); \mu)$$

we have

$$\left| s(u_h(\mu)) - \left(s(u_N(\mu)) - R(u_N^{du}(\mu); \mu) \right) \right|$$

$$= \left| s(e_N(\mu)) + a(e_N(\mu), u_N^{du}(\mu); \mu) \right|$$

$$= \left| -a(e_N(\mu), u_h^{du}(\mu); \mu) + a(e_N(\mu), u_N^{du}(\mu); \mu) \right|$$

$$= \left| a(e_N(\mu), e_N^{du}(\mu); \mu) \right|$$

$$\leq \| \mathcal{R}_N(\mu) \|_{V_h'} \cdot \| e_N^{du}(\mu) \| \leq \frac{1}{\alpha(\mu)} \| \mathcal{R}_N(\mu) \|_{V_h'} \| \mathcal{R}_N^{du}(\mu) \|_{V_h'}$$

Generate V_N^{du} using weak greedy with same error tolerance

<u>Note</u> Except for compliant case, symmetry is never used.

$\Longrightarrow$ everything works for non-symmetric coercive problems

Instationary Problems

$$
\begin{tikzcd}
 & X([0,T];V_h) \arrow[dr, bend left, "\mathrm{id}_{[0,T]} \otimes s"] & \\
 & X([0,T];V_N) \arrow[u, hook] & \\
\mathcal{P} \arrow[uur, bend left, "\Phi"] \arrow[ur, bend left, "\tilde{\Phi}"] \arrow[rr, "s \circ \Phi"] & & L^\infty([0,T])^n
\end{tikzcd}
$$

Default (there are also space-time approaches)

<u>Note</u> Weak greedy in $\mathcal{P}$ + time does not work well (same (μ, t) can be selected twice)

<u>POD</u> Given (snapshot) vectors $v_{h,1}, \dots, v_{h,S} \in V_h$, and with $e_1, \dots, e_S$ the canonical basis of $\mathbb{R}^S$, let $\Lambda : \mathbb{R}^S \to V_h$ be the linear map given by

$$\Lambda(e_s) = v_{h,s} \qquad s = 1, \dots, S,$$

then

$$\mathrm{POD}(\{v_{h,1}, \dots, v_{h,S}\}, N)$$

is the set of the first N left-singular vectors of Λ.

<u>Thm</u> Let $V_N := \mathrm{span}(\mathrm{POD}(\{v_{h,1}, \dots, v_{h,S}\}, N))$ $\quad \underbrace{\begin{pmatrix} v_{h,1} & \cdots & v_{h,S} \end{pmatrix}}_{X}$,

then

$$\sum_{s=1}^{S} \inf_{v_N \in V_N} \| v_{h,s} - v_N \|^2 = \sum_{s=N+1}^{S} \sigma_s^2 = \min_{\substack{W_N \subset V_h \\ \dim W_N = N}} \sum_{s=1}^{S} \inf_{w_N \in W_N} \| v_{h,s} - w_N \|^2$$

σ_s: s-th singular value of Λ

POD-Greedy algorithm

Input: $S_{train} \subset \mathcal{P}$, ε, M

$V_0 \leftarrow \{0\}$, $N \leftarrow 0$

while $\max_{\mu \in S_{train}} \Delta_N(\mu) > \varepsilon$:

$\mu^*_{N+1} \leftarrow \operatorname{argmax}_{\mu \in S_{train}} \Delta_N(\mu)$

~~$V_{N+M} \leftarrow \operatorname{span} V_N \cup POD(\{u_h(t_0;\mu), \dots, u_h(t_K;\mu$~~

$\leftarrow$ orth. proj. onto V_N

$V_{N+M} \longleftarrow \operatorname{span} V_N \cup POD(u_h(t_0;\mu) - P_{V_N} u_h(t_0;\mu), \dots,$
$u_h(t_K;\mu) - P_{V_N} u_h(t_K;\mu), M)$

$N \leftarrow N+M$

Offline-online decomposition of nonlinear operators using the discrete empirical interpolation method (DEIM)

$\mathcal{A}(\mu): V_h \longrightarrow V_h'$ nonlinear operator

1. Compute set of vectors $\mathcal{M}$ approximating ~~an~~ $\mathcal{A}(v;\mu)$ for all $\mu \in \mathcal{P}$ an $v \in V_h$ of interest (e.g. evaluate $\mathcal{A}$ on solution snapshots $u_h(\mu)$).
2. Compute interpolation basis $c_1, \dots, c_M$ as $POD(\mathcal{M}, M)$.
3. Compute interpolation DoFs $i_1, \dots, i_M$ using EI-Greedy algorithm:

EI - Greedy

Input: $c_1, \dots, c_M$

for $k \leftarrow 1$ to M:

Let $\tilde{I}_{k-1}(c_k)$ be given by

$$\tilde{I}_{k-1}(c_k) \in \operatorname{span}\{c_1, \dots, c_{k-1}\} \wedge \tilde{I}_{k-1}(c_k)_{i_\ell} = (c_k)_{i_\ell} \quad 1 \le \ell <$$

$$i_k \leftarrow \operatorname*{argmax}_{1 \le i \le \dim V_h} |c_k - \tilde{I}_{k-1}(c_k)|$$

Then approximate

$$\mathcal{A}(v_h; \mu) \sim \tilde{I}_M \mathcal{A}(v_h; \mu)$$

For given RB $b_1, \dots, b_N$, $u_N = \sum_{i=1}^{N} u_{N,i} b_i$, we have

$$\langle I_M \mathcal{A}(\cancel{u_N}; \mu), b_j \rangle$$

$$= \langle \sum_{i=1}^{M} \lambda_i c_i, b_j \rangle = \sum_{i=1}^{M} \lambda_i \langle c_i, b_j \rangle$$

need to know u_N at $C \cdot M$ dofs in case of FEM/FV op. $\rightsquigarrow$ store these dofs of $b_1, \dots, b_N$.