Reduced basis methods and a posteriori error estimation for parametrized PDEs: Advances

ERROR BOUNDS

Gianluigi Rozza

Advanced Topics in Numerical Solution of PDEs: Reduced Basis Methods for Computational Mechanics

Advances

- **Advances: Elliptic Problems II, Parabolic Problems, Extensions**

  1. Elliptic Problems II
     (e) A Posteriori Error Estimation (elements)
     (f) General Outputs (non-compliant), Non-symmetric Forms (Dual Problem, A Posteriori Error Estimation)
  2. Parabolic Problems
     (a) Problem Statement, Truth Approximation
     (b) Reduced Basis Approximation
     (c) Offline-Online Computational Procedures
     (d) A Posteriori Error Estimation
     (e) POD - greedy sampling
  3. Possible Extensions
     - Stability Factors Approximation
     - Non-Coercive Problems

Last Episode...

Input and Output

- Input parameter $\boldsymbol{\mu} \in \boldsymbol{\mathcal{D}}$: geometry, material prop., B.C., sources
- Output of interest $s(\boldsymbol{\mu}) = \ell(u(\boldsymbol{\mu})) = f(u(\boldsymbol{\mu}))$: to be evaluated in real time or many-query contexts
- Field variable $u(\boldsymbol{\mu}) \in \boldsymbol{X}$: satisfies a $\boldsymbol{\mu}$-parametrized PDE

$$a(u(\boldsymbol{\mu}), v; \boldsymbol{\mu}) = f(v) \qquad \forall v \in \boldsymbol{X}$$

- Rapidly convergent global reduced basis (RB) approximations (Galerkin projection onto a space spanned by solution of governing PDE at N selected $\mu^1, \ldots, \mu^N$)
- Offline/Online computational procedures (very extensive and parameter independent Offline stage / inexpensive Online calculations for new I/O evaluation)

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A posteriori Error Estimation: Role

- Rapidly convergent global reduced basis (RB) approximations
- Offline/Online computational procedures
- **Rigorous a posteriori error estimation procedures**
  (inexpensive yet sharp bounds for the error in the RB field-variable and output approximations)

OFFLINE

Error bound permits "large" $\Xi_{\text{train}} \subset \mathcal{D}$,

$\Rightarrow$ rapidly convergent $W_N^{\mathcal{N}}$,

$\Rightarrow$ small $\partial t_{\text{comp}}(\mu \to s_N^{\mathcal{N}}(\mu))$; and

rigorous assessment $|s^{\mathcal{N}}(\mu) - s_N^{\mathcal{N}}(\mu)|$, $\forall\, \mu \in \mathcal{D}$.

ONLINE

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ONLINE

A posteriori Error Estimation: Preliminaries

Residual

Define $\boldsymbol{r}: \boldsymbol{\mathcal{D}} \rightarrow (\boldsymbol{X}^{\mathcal{N}})'$ and $\hat{e}: \boldsymbol{\mathcal{D}} \rightarrow \boldsymbol{X}^{\mathcal{N}}$,

$$\begin{aligned} r(v;\mu) &\equiv f(v) - a(u_N^{\mathcal{N}}(\mu), v; \mu) \ , \\ (\hat{e}(\mu), v)_X &= r(v;\mu), \ \forall v \in X^{\mathcal{N}} \ ; \end{aligned}$$

then dual norm given by

$$\begin{aligned} \|r(\,\cdot\,;\mu)\|_{(X^{\mathcal{N}})'} &= \sup_{v \in X^{\mathcal{N}}} \frac{r(v;\mu)}{\|v\|_X} \\ &= \|\hat{e}(\mu)\|_X \ . \end{aligned}$$

A posteriori Error Estimation: Preliminaries

Coercivity, Continuity Constants

Introduce coercivity "constants"

$$\alpha^{\mathrm{e}}(\mu) \equiv \inf_{w \in X^{\mathrm{e}}} \frac{a(w,w;\mu)}{\|w\|_X^2}, \quad \alpha^{\mathcal{N}}(\mu) \equiv \inf_{w \in X^{\mathcal{N}}} \frac{a(w,w;\mu)}{\|w\|_X^2} ;$$

for our *coercive* problems,

$$\alpha^{\mathcal{N}}(\mu) \geq \alpha^{\mathrm{e}}(\mu) \geq \alpha_0^{\mathrm{e}} > 0, \quad \forall\, \mu \in \mathcal{D} .$$

Also define continuity "constant,"

$$\gamma^{\mathrm{e}}(\mu) = \sup_{w \in X^{\mathrm{e}}} \sup_{v \in X^{\mathrm{e}}} \frac{a(w,v;\mu)}{\|w\|_X \, \|v\|_X} .$$

A posteriori Error Estimation: Preliminaries

Coercivity Lower Bound

Require

$$\alpha^{\mathcal{N}}_{\mathrm{LB}} : \mathcal{D} \to \mathbb{R}$$

such that

$$0 < \alpha^{\mathcal{N}}_{\mathrm{LB}}(\mu) \le \alpha^{\mathcal{N}}(\mu), \quad \forall\, \mu \in \mathcal{D}\ ,$$

and $\partial t_{\mathrm{comp}}(\mu \to \alpha^{\mathcal{N}}_{\mathrm{LB}}(\mu))$

is $[O(1)]$ independent of $\mathcal{N}$.

† A prescription can be found in [ARCME (Sec.10)].

A posteriori Error Estimators: Error Bounds

Error estimators:

$$\begin{aligned}\Delta_N^{\mathrm{en}}(\mu) &\equiv \|\hat{e}(\mu)\|_X / (\alpha_{\mathrm{LB}}^{\mathcal{N}}(\mu))^{1/2} ,\\ \Delta_N^{s}(\mu) &\equiv \|\hat{e}(\mu)\|_X^2 / \alpha_{\mathrm{LB}}^{\mathcal{N}}(\mu) ;\end{aligned}$$

Effectivities:

$$\begin{aligned}\eta_N^{\mathrm{en}}(\mu) &\equiv \Delta_N^{\mathrm{en}}(\mu) / |||u^{\mathcal{N}}(\mu) - u_N^{\mathcal{N}}(\mu)|||_\mu ,\\ \eta_N^{s}(\mu) &\equiv \Delta_N^{s}(\mu) / (s^{\mathcal{N}}(\mu) - s_N^{\mathcal{N}}(\mu)) .\end{aligned}$$

A posteriori Error Estimators: Error Bounds

Effectivity Results

Proposition 2

For $N = 1, \ldots$ †

$$\underset{\text{(rigor)}}{1} \quad \le \quad \eta_N^{\mathrm{en}} \quad \le \quad \underset{\text{(sharpness)}}{\sqrt{\frac{\gamma^{\mathrm{e}}(\mu)}{\alpha_{\mathrm{LB}}^{\mathcal{N}}(\mu)}}}, \quad \forall\, \mu \in \mathcal{D}\ ,$$

$$1 \quad \le \quad \eta_N^s(\mu) \quad \le \quad \frac{\gamma^{\mathrm{e}}(\mu)}{\alpha_{\mathrm{LB}}^{\mathcal{N}}(\mu)}, \quad \forall\, \mu \in \mathcal{D}\ ;$$

recall a is symmetric and s is “compliant” $(\ell = f)$. □

† Similar results obtain for $\Delta_N(\mu)$, the error bound in the X norm.

A posteriori Error Estimators: Error Bounds

Proofs

It follows from $a(e(\mu), v; \mu) = (\hat{e}(\mu), v)_X$ for $v = e(\mu)$ and the Cauchy-Schwarz inequality that

$$|||e(\mu)|||_\mu^2 \leq \|\hat{e}(\mu)\|_X \, \|e(\mu)\|_X \ , \qquad (1)$$

but $(\alpha^{\mathcal{N}}(\mu))^{\frac{1}{2}} \, \|e(\mu)\|_X \leq a^{\frac{1}{2}}(e(\mu), e(\mu); \mu) \equiv |||e(\mu)|||_\mu$, and hence from (1) we obtain

$$(\alpha^{\mathcal{N}}(\mu))^{\frac{1}{2}} \frac{|||e(\mu)|||_\mu^2}{\|\hat{e}(\mu)\|_X} \leq |||e(\mu)|||_\mu$$

s.t. $|||e(\mu)|||_\mu \leq \Delta_N^{\mathrm{en}}(\mu)$ or $\eta_N^{\mathrm{en}}(\mu) \geq 1$.

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A posteriori Error Estimators: Error Bounds

Proofs: Again for $v = \hat{e}(\mu)$ in $a(e(\mu), v; \mu) = (\hat{e}(\mu), v)_X$ and the Cauchy-Schwarz inequality we have

$$\|\hat{e}(\mu)\|_X^2 \leq |||\hat{e}(\mu)|||_\mu \, |||e(\mu)|||_\mu \, . \qquad (2)$$

But from continuity $|||\hat{e}(\mu)|||_\mu \leq (\gamma^{\mathrm{e}}(\mu))^{\frac{1}{2}} \|\hat{e}(\mu)\|_X$, and hence from (2)

$$\eta_N^{\mathrm{en}} = \frac{\Delta_N^{\mathrm{en}}(\mu)}{|||e(\mu)|||_\mu} \equiv \frac{\alpha_{\mathrm{LB}}^{\mathcal{N}}(\mu))^{-\frac{1}{2}} \|\hat{e}(\mu)\|_X}{|||e(\mu)|||_\mu} \equiv$$

$$\frac{\alpha_{\mathrm{LB}}^{\mathcal{N}}(\mu))^{-\frac{1}{2}} \|\hat{e}(\mu)\|_X^2}{|||e(\mu)|||_\mu \|\hat{e}(\mu)\|_X} \leq \frac{\alpha_{\mathrm{LB}}^{\mathcal{N}}(\mu))^{-\frac{1}{2}} |||\hat{e}(\mu)|||_\mu \, |||e(\mu)|||_\mu}{|||e(\mu)|||_\mu \|\hat{e}(\mu)\|_X} \leq$$

$$(\alpha_{\mathrm{LB}}^{\mathcal{N}}(\mu))^{-\frac{1}{2}} (\gamma^{\mathrm{e}}(\mu))^{\frac{1}{2}}, \quad \text{or}$$

$$\eta_N^{\mathrm{en}}(\mu) \leq \sqrt{\frac{\gamma^{\mathrm{e}}(\mu)}{\alpha_{\mathrm{LB}}^{\mathcal{N}}(\mu)}}$$

A posteriori Error Estimators: Error Bounds

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$$\eta_N^{\mathrm{en}} = \frac{\Delta_N^{\mathrm{en}}(\mu)}{|||e(\mu)|||_\mu} \equiv \frac{\alpha_{\mathrm{LB}}^{\mathcal{N}}(\mu))^{-\frac{1}{2}}\|\hat{e}(\mu)\|_X}{|||e(\mu)|||_\mu} \equiv$$

$$\frac{\alpha_{\mathrm{LB}}^{\mathcal{N}}(\mu))^{-\frac{1}{2}}\|\hat{e}(\mu)\|_X^2}{|||e(\mu)|||_\mu\|\hat{e}(\mu)\|_X} \leq \frac{\alpha_{\mathrm{LB}}^{\mathcal{N}}(\mu))^{-\frac{1}{2}}|||\hat{e}(\mu)|||_\mu \, |||e(\mu)|||_\mu}{|||e(\mu)|||_\mu\|\hat{e}(\mu)\|_X} \leq$$

$$(\alpha_{\mathrm{LB}}^{\mathcal{N}}(\mu))^{-\frac{1}{2}}(\gamma^{\mathrm{e}}(\mu))^{\frac{1}{2}}, \quad \text{or}$$

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A posteriori Error Estimators: Error Bounds

Since $s^{\mathcal{N}}(\mu) - s_N^{\mathcal{N}}(\mu) = |||e(\mu)|||_\mu^2$, and hence since $\Delta_N^s(\mu) = \left(\Delta_N^{\text{en}}(\mu)\right)^2$

$$\eta_N^s(\mu) \equiv \frac{\Delta_N^s(\mu)}{s^{\mathcal{N}}(\mu) - s_N^{\mathcal{N}}(\mu)} = \frac{\left(\Delta_N^{\text{en}}(\mu)\right)^2}{|||e(\mu)|||_\mu^2} = \left(\eta_N^{\text{en}}(\mu)\right)^2. \quad (3)$$

Offline-Online: $||\hat{e}(\mu)||_X$

Ingredients: 1. Affine Parameter Dependence

$$
\begin{aligned}
r(v;\mu) &\equiv f(v) - a(u_N(\mu), v; \mu) \\
&= f(v) - a\Big(\sum_{n=1}^{N} u_{Nn}(\mu)\,\zeta^n, v; \mu\Big) \\
&= f(v) - \sum_{n=1}^{N} u_{Nn}(\mu)\, a(\zeta^n, v; \mu) \\
&= f(v) - \sum_{n=1}^{N} u_{Nn}(\mu) \sum_{q=1}^{Q} \Theta^q(\mu)\, a^q(\zeta^n, v)\ .
\end{aligned}
$$

Offline-Online: $||\hat{e}(\mu)||_X$

Ingredients: 2. Linear Superposition

$$(\hat{e}(\mu), v)_X = f(v) - \sum_{q=1}^{Q} \sum_{n=1}^{N} \Theta^q(\mu)\, u_{Nn}(\mu)\, a^q(\zeta^n, v),$$

$$\Rightarrow \quad \hat{e}(\mu) = \mathcal{C} + \sum_{q=1}^{Q} \sum_{n=1}^{N} \Theta^q(\mu)\, u_{Nn}(\mu)\, \mathcal{L}_n^q \;,$$

where
$$(\mathcal{C}, v)_X = f(v), \qquad \forall\, v \in X^{\mathcal{N}};$$
$$(\mathcal{L}_n^q, v)_X = -a^q(\zeta^n, v), \quad \forall\, v \in X^{\mathcal{N}},$$
$$1 \le n \le N,\ 1 \le q \le Q.$$

Offline-Online: $\|\hat{e}(\mu)\|_X$

Ingredients: 2. Linear Superposition

Thus $\|\hat{e}(\mu)\|_X^2$

$$= \left(\mathcal{C} + \sum_{q=1}^{Q} \sum_{n=1}^{N} \Theta^q(\mu)\, u_{N\,n}(\mu)\, \mathcal{L}_n^q\ , \bullet\right)_X$$

$$= (\mathcal{C}, \mathcal{C})_X + \sum_{q=1}^{Q} \sum_{n=1}^{N} \Theta^q(\mu)\, u_{N\,n}(\mu) \Big\{$$

$$2(\mathcal{C}, \mathcal{L}_n^q)_X + \sum_{q'=1}^{Q} \sum_{n'=1}^{N} \Theta^{q'}(\mu)\, u_{N\,n'}(\mu)\, (\mathcal{L}_n^q, \mathcal{L}_{n'}^{q'})_X \Big\}.$$

Offline-Online: $||\hat{e}(\mu)||_X$

Computational Procedure

Offline: once, parameter independent

Compute $\quad \mathcal{C},\ \mathcal{L}_n^q, \quad 1 \le n \le N_{\max},\ 1 \le q \le Q.$

Form/Store $\quad (\mathcal{C},\mathcal{C})_X,\ (\mathcal{C},\mathcal{L}_n^q)_X,\ (\mathcal{L}_n^q,\mathcal{L}_{n'}^{q'})_X,$

$$1 \le n, n' \le N_{\max},$$
$$1 \le q, q' \le Q.$$

Complexity depends on N, Q, *and* $\mathcal{N}$.

Offline-Online: $\|\hat{e}(\mu)\|_X$

Computational Procedure

Online: many times, for each μ *deployed*

Evaluate $\|\hat{e}(\mu)\|_X^2 =$

$$\left[(\mathcal{C},\mathcal{C})_X + \sum_{q=1}^{Q}\sum_{n=1}^{N} \Theta^q(\mu)\, u_{Nn}(\mu) \Big\{ 2(\mathcal{C},\mathcal{L}_n^q)_X + \sum_{q'=1}^{Q}\sum_{n'=1}^{N} \Theta^{q'}(\mu)\, u_{Nn'}(\mu)\, (\mathcal{L}_n^q, \mathcal{L}_{n'}^{q'})_X \Big\} \right]$$

$$\text{— } O(Q^2N^2).$$

Complexity depends on N, Q, *but not* $\mathcal{N}$.

A Posteriori Error Estimation: Numerical Example

TBlock-$(\mathbf{3},\mathbf{3})$: Metrics

Define

$$\begin{aligned} \boldsymbol{\Delta}^s_{\max} &= \max_{\mu\in\Xi_{\text{test}}} \boldsymbol{\Delta}^s_N(\mu) \ , \\ \eta^s_{N,\ {\text{ave} \atop \max}} &= {\text{ave} \atop \max_{\mu\in\Xi_{\text{test}}}} \eta^s_N(\mu) \ ; \end{aligned}$$

recall from *Proposition 2* $\qquad \mu_r = 100$

$$1 \le \eta^s_{N,\max} \le \max_{\mu\in\Xi_{\text{test}}} \frac{\gamma^{\mathrm{e}}(\mu)}{\alpha_{\mathrm{LB}}(\mu)} \le 100 \ .^{\dagger}$$

† Result for $\overline{\mu} = (1,\ldots,1)$; improvement for "*multi*-inner product."

A Posteriori Error Estimation: Numerical Example

TBlock-$(3,3)$: Metrics

Effectivities †

N	$\Delta^s_{N,\max}$	$\eta^s_{N,\text{ave}}$	$\eta^s_{N,\max}$
10	$2.2036\text{E}+00$	6.7067	31.2850
20	$2.0020\text{E}-01$	7.5587	37.3024
30	$1.5100\text{E}-02$	12.1138	62.2537
40	$1.2000\text{E}-03$	14.4598	73.1151
50	$1.0000\text{E}-04$	10.2566	57.5113

† Note penalty for η^s_N "large" mitigated by rapid convergence $\Delta^s_N \to 0$.

Coercivity Lower Bound: Parametric Coercivity "$\boldsymbol{\Theta}$ Method"

If $\Theta^q(\mu) > 0$, $\forall \mu \in \mathcal{D}$ and $a^q(w,w) \geq 0$, $\forall w \in X^{\mathrm{e}}$, $1 \leq q \leq Q$, $a(\cdot,\cdot;\mu)$ is said to be *parametrically coercive*.

In this case:

$$a(w,w;\mu) = \sum_{q=1}^{Q} \Theta^q(\mu) a^q(w,w)$$

$$= \sum_{q=1}^{Q} \frac{\Theta^q(\mu)}{\Theta^q(\mu')} \Theta^q(\mu') a^q(w,w)$$

$$\geq \min_{q \in [1,Q]} \frac{\Theta^q(\mu)}{\Theta^q(\mu')} \sum_{q=1}^{Q} \Theta^q(\mu') a^q(w,w)$$

$$\geq \min_{q \in [1,Q]} \frac{\Theta^q(\mu)}{\Theta^q(\mu')} a(w,w;\mu') = \min_{q \in [1,Q]} \frac{\Theta^q(\mu)}{\Theta^q(\mu')} ||w||_X^2$$

so also

$$\alpha^{\mathcal{N}}(\mu) \equiv \inf_{w \in X^{\mathcal{N}}} \frac{a(w,w;\mu)}{||w||_X^2} \geq \min_{q \in [1,Q]} \frac{\Theta^q(\mu)}{\Theta^q(\mu')} = \alpha_{LB}^{\mathcal{N}}(\mu).$$

Reduced basis methods and a posteriori error estimation for parametrized PDEs: Advances

PRIMAL-DUAL PROBLEMS

Gianluigi Rozza

Course on Advanced Topics in Numerical Solution of PDEs: Reduced Basis Methods for Computational Mechanics

SISSA

MHPC Master in High Performance Computing

sissa mathLab innovating with mathematics

Problem Generalization: General Output

Consider $u \in X$

$$a(u, v; \mu) = f(v), \quad \forall v \in X,$$

and

$$s(\mu) = \ell(u(\mu))$$

If a is symmetric and $\ell = f$ we revert to compliant case. If not, with Primal only, we find $u_N \in W_N$ (Lagrange RB space)

$$a(u_N(\mu), v; \mu) = f(v), \quad \forall v \in W_N,$$

Then we need

$$s_N(\mu) = \ell(u_N(\mu)).$$

We can readily develop an a posteriori error bound for $s_N(\mu)$:

$$|s(\mu) - s_N(\mu)| \leq ||\ell||_{(X^{\mathcal{N}})'} \Delta_N(\mu)$$

where

$$||u(\mu) - u_N(\mu)||_X \leq \Delta_N(\mu) = \frac{||\hat{e}(\mu)||_X}{\alpha_{LB}(\mu)}.$$

Problem Generalization: General Output

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where

$$||u(\mu) - u_N(\mu)||_X \leq \Delta_N(\mu) = \frac{||\hat{e}(\mu)||_X}{\alpha_{LB}(\mu)}.$$

Problem Generalization: Output Error Bounds

Proof: First

$$\begin{aligned} a(e(\mu), v; \mu) =& r(v; \mu) = f(v) - a(u_N, v, \mu) \\ =& a(u, v, \mu) - a(u_N, v, \mu) = (\hat{e}(\mu), v)_X \end{aligned}$$

hence for $v = e$ $\quad \alpha_{LB}(\mu)||e(\mu)||_X^2 \leq ||\hat{e}(\mu)||_X ||e||_X$, or

$$||e(\mu)||_X \leq \frac{||\hat{e}(\mu)||}{\alpha_{LB}(\mu)}.$$

But then

$$\begin{aligned} |s(\mu) - s_N(\mu)| =& |\ell(u(\mu)) - \ell(u_N(\mu))| = |\ell(e(\mu))| \\ =& \frac{|\ell(e(\mu))|}{||e(\mu)||_X} ||e(\mu)||_X \leq \underbrace{\left(\sup_{v \in X^{\mathcal{N}}} \frac{\ell(v)}{||v||_X} \right)}_{||\ell||_{(X^{\mathcal{N}})'}} ||e(\mu)||_X \end{aligned}$$

$$\leq ||\ell||_{(X^{\mathcal{N}})'} \Delta_N(\mu) = \Delta_N^{s,nc}(\mu)$$

Problem Generalization: Primal-Dual

Dual Problem

Find $\boldsymbol{\Psi} \in \boldsymbol{X}$ such that

$$\boldsymbol{a(v, \Psi; \mu) = -\ell(v), \quad \forall v \in X.}$$

Note we no longer assume that $\boldsymbol{a}$ is symmetric, and hence $\boldsymbol{\Psi \neq -u}$ necessarily even if $\boldsymbol{\ell = f}$.

(We still assume that $\boldsymbol{a}$ is coercive and affine, but this case considers transport-advection-convection terms.)

Problem Generalization: Primal-Dual

RB Approach Galerkin

Introduce

$$W^{pr}_{N_{pr}} = span\left\{u(\mu^k_{pr}) \equiv \zeta^k, 1 \leq k \leq N_{pr}\right\},$$
$$W^{du}_{N_{du}} = span\left\{\Psi(\mu^k_{du}), 1 \leq k \leq N_{du}\right\},$$
$$1 \leq N_{pr} \leq N_{pr,max}, \qquad 1 \leq N_{du} \leq N_{du,max}$$

Then $u_{N_{pr}} \in W^{pr}_{N_{pr}}, \Psi_{N_{du}} \in W^{du}_{N_{du}}$ satisfy

$$a(u_{N_{pr}}(\mu), v; \mu) = f(v), \quad \forall v \in W^{pr}_{N_{pr}},$$
$$a(v, \Psi_{N_{du}}(\mu); \mu) = -\ell(v), \quad \forall v \in W^{du}_{N_{du}},$$

Problem Generalization: Primal-Dual

And [Patera & Ronquist, Giles & Pierce]

$$s_{N_{pr},N_{du}}(\mu) = \ell(u_{N_{pr}}) - r^{pr}(\Psi_{N_{du}};\mu)$$

where

$$r^{pr}(v;\mu) = f(v) - a(u_{N_{pr}}, v;\mu)$$
$$r^{du}(v;\mu) = -\ell(v) - a(v, \Psi_{N_{du}};\mu)$$

Offline-Online is similar to Primal-only, but now we need to do everything both for Primal and Dual (see following Sampling).

Problem Generalization: Primal-Dual

A Priori Theory

It is standard that

$$|s - s_{N_{pr},N_{du}}| \leq$$

$$C \left(\inf_{w^{pr} \in W^{pr}_{N_{pr}}} ||u - w^{pr}||_X \right) \left(\inf_{w^{du} \in W^{du}_{N_{du}}} ||\Psi - w^{du}||_X \right)$$

Proof:

$$|s - s_{N_{pr},N_{du}}| = \underbrace{\ell(u - u_{N_{pr}})}_{e^{pr}} + r^{pr}(\Psi_{N_{du}}; \mu)$$

$$= -a(e^{pr}, \Psi; \mu) + a(e^{pr}, \Psi_{N_{du}}; \mu)$$

$$= -a(e^{pr}, e^{du}; \mu).$$

Then apply continuity and Galerkin optimality to Primal and Dual.

Problem Generalization: A Posteriori Output Bounds

We can readily derive that

$$|s^{\mathcal{N}} - s^{\mathcal{N}}_{N_{pr},N_{du}}| \leq \Delta_N^{s(,nc)} \qquad \text{“}N \equiv N_{pr}, N_{du}\text{”}$$

where

$$\Delta_N^s(\mu) = ||r_N^{du}(\cdot;\mu)||_{(X^{\mathcal{N}})'} \Delta_N(\mu).$$

Proof: we know that

$$\begin{aligned} s - s_{N_{pr},N_{du}} &= \ell(u - u_{N_{pr}}) + r^{pr}(\Psi_{N_{du}};\mu) \\ &= \ell(e^{pr}) + a(e^{pr}, \Psi_{N_{du}};\mu) = -r^{du}(e^{pr};\mu) \end{aligned}$$

So

$$\begin{aligned} |s - s_{N_{pr},N_{du}}| &\leq ||r^{du}(\cdot;\mu)||_{(X^{\mathcal{N}})'} ||e^{pr}||_X \\ &\leq ||r^{du}(\cdot;\mu)||_{(X^{\mathcal{N}})'} \Delta_N(\mu) \end{aligned}$$

where recall that $||e^{pr}||_X \leq \Delta_N(\mu)$.

Problem Generalization: A Posteriori Output Bounds

We can readily derive that

$$|s^{\mathcal{N}} - s^{\mathcal{N}}_{N_{pr},N_{du}}| \le \Delta_N^{s(,nc)} \qquad \text{“}N \equiv N_{pr}, N_{du}\text{”}$$

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where recall that $||e^{pr}||_X \le \Delta_N(\mu)$.

Problem Generalization: Sampling

The Offline-Online procedure is very similar to before, but now we evaluate both a Primal and a Dual residual dual norm. We have

$$|s - s_{N_{pr},N_{du}}| \leq \left(\frac{||r^{du}(\cdot;\mu)||_{(X^{\mathcal{N}})'}}{\alpha_{LB}^{1/2}(\mu)} \right) \left(\frac{||r^{pr}(\cdot;\mu)||_{(X^{\mathcal{N}})'}}{\alpha_{LB}^{1/2}(\mu)} \right)$$

Hence if ϵ_{max}^{s} is the smallest output error desired, we perform a Primal greedy until ($\Rightarrow N_{pr,max}$)

$$\frac{||r^{pr}(\cdot;\mu)||_{(X^{\mathcal{N}})'}}{\alpha_{LB}^{1/2}(\mu)} \leq \sqrt{\epsilon_{max}^{s}}, \quad \text{over } \Xi_{train}^{pr}.$$

and a Dual greedy until ($\Rightarrow N_{du,max}$)

$$\frac{||r^{du}(\cdot;\mu)||_{(X^{\mathcal{N}})'}}{\alpha_{LB}^{1/2}(\mu)} \leq \sqrt{\epsilon_{max}^{s}}, \quad \text{over } \Xi_{train}^{du}.$$

If (say) the Dual converges much more quickly than the Primal, it would be more efficient to choose "$N_{pr,max} = 0$" and let the Dual do all the work.

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Reduced basis methods and a posteriori error estimation for parametrized PDEs: Advances

TIME DEPENDENT PROBLEMS

Gianluigi Rozza

Course on Advanced Topics in Numerical Solution of PDEs: Reduced Basis Methods for Computational Mechanics

ma per seguir virtute e canoscenza

SISSA

MHPC Master in High Performance Computing

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Parabolic Problems

Given $\boldsymbol{\mu} \in \mathcal{D} \subset \mathbb{R}^P$, $\quad t \in (0, t_f]$

evaluate $s^{\mathrm{e}}(t;\boldsymbol{\mu}) = \ell(u^{\mathrm{e}}(t;\boldsymbol{\mu});\boldsymbol{\mu})$

where $u^{\mathrm{e}}(t;\boldsymbol{\mu}) \in X^{\mathrm{e}}(\Omega)$ satisfies[1]

$$m\left(\frac{\partial u^{\mathrm{e}}}{\partial t}(t;\boldsymbol{\mu}), v;\boldsymbol{\mu}\right) + a(u^{\mathrm{e}}(t;\boldsymbol{\mu}), v;\boldsymbol{\mu}) = g(t)\ f(v;\boldsymbol{\mu}), \quad \forall\, v \in X^{\mathrm{e}}\ .$$

[1] We assume for simplicity that $u^{\mathrm{e}}(0;\boldsymbol{\mu}) = u_0^{\mathrm{e}} = \mathbf{0}$.

Parabolic Problems: Hypotheses

$a(\cdot,\cdot;\mu)$: bilinear, affine in μ,
X^e-continuous,
X^e-coercive,† $\quad \forall \mu \in \mathcal{D}$

$m(\cdot,\cdot;\mu)$: bilinear, affine in μ,
$L^2(\Omega)$-continuous,
$L^2(\Omega)$-coercive, $\quad \forall \mu \in \mathcal{D}$

$f(\cdot;\mu)$: linear, affine in μ,
$L^2(\Omega)$-bounded, $\quad \forall \mu \in \mathcal{D}$

$g(\cdot)$: $L^2(0,t_f)$ "control"

$\ell(\cdot;\mu)$: linear, affine in μ,
$L^2(\Omega)$-bounded,† $\quad \forall \mu \in \mathcal{D}$

† In fact, a may satisfy a weak coercivity condition.

Parabolic Problems:FD-FE Approximation - Discretization

FD in time: EB (Euler Backward) or CN (Crank-Nicholson)

$$\Delta t = t_f / K \;\; \Rightarrow$$

$$\begin{aligned} t^k &= \; k\Delta t, \; 0 \leq k \; \leq K \;, \text{ or} \\ \mathbb{I} &= \; \{t^0, t^1, \ldots, t^K\} \; ; \\ \mathbb{K} &= \; \{1, 2, \ldots, K\} \; . \end{aligned}$$

FE in space: $X^{\mathcal{N}} \in X^{\mathrm{e}}$.

Parabolic Problems:FD-FE Approximation - EB-Galerkin

Given $\mu \in \mathcal{D}$, $\forall\, k \in \mathbb{K}$

evaluate $s^{\mathcal{N}\,k}(\mu) = \ell(u^{\mathcal{N}\,k}(\mu);\mu)$

where $u^{\mathcal{N}\,k}(\mu) \in X^{\mathcal{N}}$ satisfies

$$m\left(\frac{u^{\mathcal{N}\,k}(\mu) - u^{\mathcal{N}\,k-1}(\mu)}{\Delta t}, v\right) + a(u^{\mathcal{N}\,k}(\mu), v;\mu) = g(t^k)\, f(v;\mu), \qquad \forall\, v \in X^{\mathcal{N}}\ .$$

TRUTH: $s^{\mathcal{N}\,k}(\mu) \approx s^{\mathrm{e}}(t^k;\mu)$, $u^{\mathcal{N}\,k}(\mu) \approx u^{\mathrm{e}}(t^k;\mu)$.

Parabolic RB: Rapid Convergence

A reduced basis approximation $\forall\, k \in \mathbb{K}$

$$s_N^{\mathcal{N}\,k} \in \mathbb{R} \text{ and } u_N^{\mathcal{N}\,k}(\mu) \in X_N^{\mathcal{N}} \subset X^{\mathcal{N}}:$$

for all $\mu \in \mathcal{D}$,

$$s_N^{\mathcal{N}\,k}(\mu) \to s^{\mathcal{N}\,k}(\mu) \text{ and } u_N^{\mathcal{N}\,k}(\mu) \to u^{\mathcal{N}\,k}(\mu)$$

rapidly as $N = \dim(X_N^{\mathcal{N}}) \to \infty (= 10\text{–}200)$.[2]

[2] The reduced basis inherits the *fixed* truth temporal discretization.

Parabolic RB: Rigor & Certainty

A posteriori error bounds $\Delta_N^k(\mu)$ and $\Delta_N^{s\,k}(\mu)$:

$$1 \text{ (rigor)} \leq \frac{\Delta_N^k(\mu)}{\|u^{\mathcal{N}\,k}(\mu) - u_N^{\mathcal{N}\,k}(\mu)\|} \leq C \text{ (sharpness)}$$

and $$\|\cdot\| \equiv \|\cdot\|_{L^2(\Omega)}$$

$$1 \text{ (rigor)} \leq \frac{\Delta_N^{s\,k}(\mu)}{|s^{\mathcal{N}\,k}(\mu) - s_N^{\mathcal{N}\,k}(\mu)|} \leq C \text{ (sharpness)}$$

for all $N \in \mathbb{N}$ and all $k \in \mathbb{K}$, $\mu \in \mathcal{D}$.

Parabolic RB: Computational Efficiency

Offline-Online computational strategies: $\forall\, k \in \mathbb{K}$

$$t_{\text{comp}}^{\text{Offline}} \gg \text{cost}\left\{\mu \to s^{\mathcal{N}\,k}(\mu)\right\}\,;$$

BUT

$$\partial t_{\text{comp}} \equiv \textit{marginal}\ \text{cost}\left\{\mu \overset{\text{Online}}{\longrightarrow} s_N^{\mathcal{N}\,k}(\mu), \Delta_N^{s\,k}(\mu)\right\}$$

depends only on Q and N *and* K — but *not* on $\mathcal{N}$.[3]

[3] We may choose our truth FE discretization very conservatively.

Parabolic RB: Relevance

Real-Time Context: $\forall\, k \in \mathbb{K}$

$$\mu \qquad \rightarrow \qquad s_N^{\mathcal{N}\,k}(\mu), \Delta_N^{s\,k}(\mu)$$

$$t_0 \qquad\qquad t_0 + \partial t_{\text{comp}}$$

Many-Query Context: $\forall\, k \in \mathbb{K}$

$$\{\mu_j \qquad \rightarrow \qquad s_N^{\mathcal{N}\,k}(\mu_j), \Delta_N^{s\,k}(\mu_j)\}_{j=1,\ldots,J^{\text{ev}}}\ (\rightarrow\infty)$$

$$t_0 \qquad\qquad t_0 + \partial t_{\text{comp}} J^{\text{ev}}$$

Parabolic RB: Crucial Ingredients

Affine Parameter Dependence

Smooth $(P+1)$-*Dimensional* Manifold $\mathcal{M}^{\mathcal{N}\,K}$

Galerkin Projection

POD(t)-Greedy(μ) Sampling Procedures

[Haasdonk, Ohlberger, M2AN, 2008 and NRP, Calcolo, 2009]

Stability Factor Estimates, and
A Posteriori Error Bounds

Offline-Online Computational Procedures

Parabolic RB: Affine Parameter Dependence

Definition: $f(v;\mu),\ \ell(v;\mu)$

$$z(w,v;\mu) = \sum_{q=1}^{Q_z} \Theta_z^q(\mu)\, z^q(w,v)$$

where for $q = 1,\ldots,Q_z$ $\qquad z:\ m$ or a

$$\begin{array}{llll} \Theta_z^q: & \mathcal{D} \to \mathbb{R}, & & \mu\text{-}\textit{dependent} \text{ functions ;} \\ z^q: & X^{\mathrm{e}} \times X^{\mathrm{e}} \to \mathbb{R}, & & \mu\text{-}\textit{independent} \text{ forms .} \end{array}$$

[3] In fact, *broadly applicable* to many instances of property *and* geometry parametric variation.

Parabolic RB: $\mathbb{T}$-$\mathcal{D}$ Manifold $\mathcal{M}^{\mathcal{N}\,\mathcal{K}}$

We assume

the form a is *stable*; and

the $\Theta^q_{m,a}(\mu)$, $1 \le q \le Q_{m,a}$, are *smooth*;

then

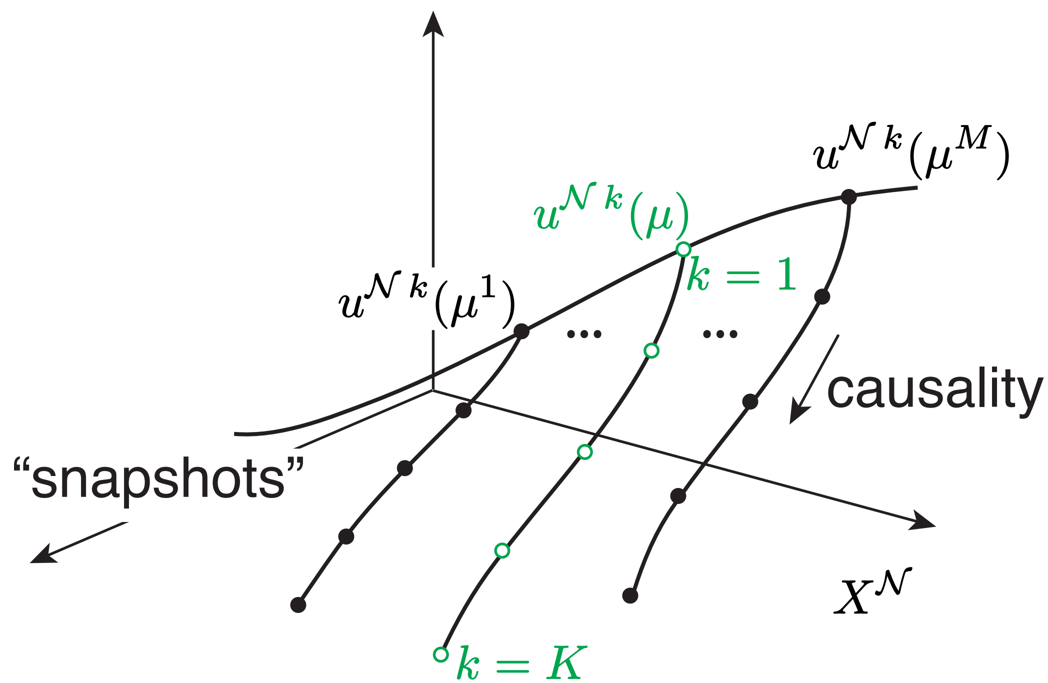
$$\mathcal{M}^{\mathcal{N}\,K} \equiv \{u^{\mathcal{N}\,k}(\mu) \,|\, \forall\, k \in \mathbb{K},\ \forall\, \mu \in \mathcal{D}\}$$

lies on a *smooth* $(P+1)$-dimensional manifold in $X^{\mathcal{N}}$.

Parabolic RB

$\mathbb{T}$-$\mathcal{D}$ Manifold $\mathcal{M}^{\mathcal{N}\,K}$

Reduced Basis Space



$$X_N^{\mathcal{N}} \subset \mathrm{span}\{u^{\mathcal{N}\,k}(\mu^m),\ 1 \le k \le K,\ 1 \le m \le M\}$$

Parabolic RB: Galerkin Projection

Given $\mu \in \mathcal{D}$, $\forall\, k \in \mathbb{K}$

evaluate $s_N^{\mathcal{N}\,k}(\mu) = \ell(u_N^{\mathcal{N}\,k}(\mu); \mu)$

where $u_N^{\mathcal{N}\,k}(\mu) \in X_N^{\mathcal{N}}$ satisfies

$$m\left(\frac{u_N^{\mathcal{N}\,k}(\mu) - u_N^{\mathcal{N}\,k-1}(\mu)}{\Delta t}, v\right) + a(u_N^{\mathcal{N}\,k}(\mu), v; \mu) = g(t^k)\, f(v; \mu), \qquad \forall\, v \in X_N^{\mathcal{N}} .$$

[3] The reduced basis inherits the *fixed* truth temporal discretization.

Parabolic RB: POD-Greedy Sampling

Set $\mathcal{Z} = \emptyset, S_* = \{\mu_*\}$; [HO]

While $N \leq N_{\max,0}$

$\{\chi_m,\ 1 \leq m \leq M_1\} = \mathrm{POD}(\{u^{\mathcal{N}}(t^k, \mu_*),\ \forall\, k \in \mathbb{K}\}, M_1)$;

$\mathcal{Z} \leftarrow \{\mathcal{Z}, \{\chi_m,\ 1 \leq m \leq M_1\}\}$;

$N \leftarrow N + M_2$;

$\{\zeta_n,\ 1 \leq n \leq N\} = \mathrm{POD}(\mathcal{Z}, \mathcal{N})$;

$X_N = \mathrm{span}\{\zeta_n,\ 1 \leq n \leq N\}$;

$\mu_* = \arg\max_{\mu \in \Xi_{\mathrm{train}}} \Delta_N^K(\mu)$ t^f

$S_* \leftarrow \{S_*, \mu_*\}$;

end.

Set $X_N = \mathrm{span}\{\zeta_n,\ 1 \leq n \leq N\},\ 1 \leq N \leq N_{\max}$.

Parabolic RB: Greedy Sampling - Advantage

Combines optimality/causality features of

(*small*) POD in time, $\mathbb{T}$

with optimality/high-dimensionality features of

(*exhaustive*) Greedy in parameter, $\boldsymbol{\mathcal{D}}$;

complexity remains $\boldsymbol{O(\mathcal{N}) + O(n_{\text{train}})}$

— *not* $\boldsymbol{O(\mathcal{N} n_{\text{train}})}$.

CRB: Crucial Ingredients - Stability Factor Estimates

Calculation of $\alpha^{\mathrm{LB}}(\mu)$: $\mathcal{D} \to \mathbb{R}_+$. We introduce

$$\sigma^{\mathcal{N}}(\mu) = \inf_{v \in X^{\mathcal{N}}} \frac{m(v,v;\mu)}{||v||^2}, \forall \mu \in \mathcal{D}$$

$$0 < \alpha^{\mathrm{LB}}(\mu) \leq \alpha^{\mathcal{N}}(\mu), \qquad \text{(coercivity constant)}$$

$$0 < \sigma^{\mathrm{LB}}(\mu) \leq \sigma^{\mathcal{N}}(\mu), \qquad \text{(stability factor)}$$

by

Successive Constraint Method (SCM)

Huynh, Rozza, Sen, Patera, *A successive constraint linear optimization method for lower bounds of parametric coercivity and inf-sup stability constants.* Comptes Rendus Mathematique. 2007, Vol 345, Pages 473-478.

exactly as in elliptic case.

CRB: Crucial Ingredients - A Posteriori Error Bounds Formulation

Introduce residual

$$
\begin{aligned}
r^k(v;\mu) = g(t^k)\, f(v) - m\left(\frac{u_N^{\mathcal{N}\,k}(\mu) - u_N^{\mathcal{N}\,k-1}(\mu)}{\Delta t}, v; \mu\right) \\
- a(u_N^{\mathcal{N}\,k}(\mu), v; \mu), \quad \forall\, v \in X^{\mathcal{N}},\ \forall\, k \in \mathbb{K}\ ;
\end{aligned}
$$

and recall $\alpha^{\mathrm{LB}}(\mu) \colon \mathcal{D} \to \mathbb{R}_+$ such that $\forall\, \mu \in \mathcal{D}$,

$$0 < \alpha^{\mathrm{LB}}(\mu) \leq \alpha^{\mathcal{N}}(\mu) \text{ (coercivity constant).}$$

CRB: Crucial Ingredients - A Posteriori Error Bounds Formulation

Define

$$\Delta_N^k(\mu) \equiv \sqrt{\frac{\Delta t}{\alpha^{\mathrm{LB}}(\mu)\sigma^{\mathrm{LB}}(\mu)} \sum_{k'=1}^{k} \left(\varepsilon_N^2(t^{k'};\mu)\right)} \;,$$

$$\Delta_N^{s\,k}(\mu) \equiv \left(\sup_{v\in X^{\mathcal{N}}} \frac{\ell(v)}{\|v\|}\right) \Delta_N^k(\mu) \;,$$

where $\varepsilon_N(t^k;\mu) \equiv \|r^k(\,\cdot\,;\mu)\|_{(X^{\mathcal{N}})'}$.

Then

$$\|u^{\mathcal{N}\,k}(\mu) - u_N^{\mathcal{N}\,k}(\mu)\|_{L^2(\Omega)} \leq \Delta_N^k(\mu)^{\dagger} \;,$$

$$|s^{\mathcal{N}\,k}(\mu) - s_N^{\mathcal{N}\,k}(\mu)| \leq \Delta_N^{s\,k}(\mu)^{\ddagger} \;,$$

for all $N \in \mathbb{N}$ and all $k \in \mathbb{K}$, $\mu \in \mathcal{D}$.

In practice we may also consider $^{\dagger}L^2(0,t_f;X)$ norms, and ‡primal-dual techniques.

CRB: Crucial Ingredients - Offline-Online Procedures

Evaluation $\mu \to$ $\forall\, k \in \mathbb{K}$

$$\left(\; u_N^{\mathcal{N}\,k}(\mu) \; \right), \quad s_N^{\mathcal{N}\,k}(\mu) \;,$$

and $\Delta_N^k(\mu)$

$$\left(\; \|r^k(\,\cdot\,;\mu)\|_{(X^{\mathcal{N}})'}, \; \alpha^{\mathrm{LB}}(\mu) - \mathsf{SCM} \; \right), \quad \Delta_N^{s\,k}(\mu) \;,$$

very similar to $(\approx K\times)$ elliptic case.

Adavances

- **Advances: Elliptic Problems II, Parabolic Problems**
  1. Elliptic Problems II
     (e) A Posteriori Error Estimation (elements)
     (f) General Outputs (non-compliant), Non-symmetric Forms (Dual Problem, A Posteriori Error Estimation)
  2. Parabolic Problems
     (a) Problem Statement, Truth Approximation
     (b) Reduced Basis Approximation
     (c) Offline-Online Computational Procedures
     (d) A Posteriori Error Estimation
     (e) POD - greedy sampling
  3. Possible Extensions
     (a) **SCM-Successive Constraint Method**
     Review paper: RHP[Sec. 10] Ar.Comp.Meth.Eng. Vol. 15, 229–275, 2008
     Paper HRSP C.R. Acad.Sci.Paris Vol. 345, 473–478, 2007

Reduced basis methods and a posteriori error estimation for parametrized PDEs

STABILITY FACTORS: SCM

Gianluigi Rozza

Course on Advanced Topics in Numerical Solution of PDEs: Reduced Basis Methods for Computational Mechanics

Coercivity Lower Bound†: Objective

Require $\alpha_{\mathrm{LB}}^{\mathcal{N}} : \mathcal{D} \rightarrow \mathbb{R}$ such that

$$0 < \alpha_{\mathrm{LB}}^{\mathcal{N}}(\mu) \le \alpha^{\mathcal{N}}(\mu), \quad \forall\, \mu \in \mathcal{D} \ ,$$
$$\partial t_{\mathrm{comp}}(\mu \rightarrow \alpha_{\mathrm{LB}}^{\mathcal{N}}(\mu)) \text{ is } O(1) \ ,$$

where

$$\alpha^{\mathcal{N}}(\mu) = \inf_{w \in X^{\mathcal{N}}} \frac{a(w, w; \mu)}{\|w\|_X^2} \quad (\ge \alpha_0^{\mathrm{e}},\ \forall\, \mu \in \mathcal{D}) \ .^{\dagger}$$

† We consider symmetric a; extension to non-symmetric a is simple.

Coercivity Lower Bound: Reformulation - Affine Parameter Dependence

Recall

$$a(w, w; \mu) = \sum_{q=1}^{Q} \Theta^q(\mu)\, a^q(w, w)\ ;$$

hence

$$\alpha^{\mathcal{N}}(\mu) = \inf_{w \in X^{\mathcal{N}}} \mathcal{J}^{\text{obj}}(\mu; w)$$

where

$$\mathcal{J}^{\text{obj}}(\mu; w) \equiv \sum_{q=1}^{Q} \Theta^q(\mu)\, \frac{a^q(w, w)}{\|w\|_X^2}\ .$$

Coercivity Lower Bound: Reformulation - "Pseudo" - Linear Form

Express

$$\alpha^{\mathcal{N}}(\mu) = \inf_{y \in \mathcal{Y}} \mathcal{J}^{\mathrm{obj}}(\mu; y)$$

where

$$\mathcal{J}^{\mathrm{obj}}(\mu; y) \equiv \sum_{q=1}^{Q} \Theta^q(\mu)\, y_q$$

$$\mathcal{Y} = \Big\{ y \in \mathbb{R}^Q \;\Big|\; \exists\, w_y \in X^{\mathcal{N}} \text{ s.t. }$$

$$y_q = \frac{a^q(w_y, w_y)}{\|w_y\|_X^2},\; 1 \le q \le Q \Big\}.$$

Coercivity Lower Bound: Bounds - Set $\mathcal{Y}_{\mathrm{LB}}$ ...

Introduce

$$\begin{aligned}\mathcal{B} &= \Pi_{q=1}^{Q}\left[\inf_{w\in X^{\mathcal{N}}}\frac{a^q(w,w)}{\|w\|_X^2}, \sup_{w\in X^{\mathcal{N}}}\frac{a^q(w,w)}{\|w\|_X^2}\right]\\ \mathcal{C}_J &= \{\mu_{\mathrm{SCM}}^1\in\mathcal{D},\ldots,\mu_{\mathrm{SCM}}^J\in\mathcal{D}\}\end{aligned}$$

and, given $\mu\in\mathcal{D}$,

$$\mathcal{C}_J^{M,\mu} = \{M \text{ points in } \mathcal{C}_J \text{ closest to } \mu\}\ .$$

---

†We consider the Successive Constraint Method (SCM). [HRSP]

Coercivity Lower Bound: Bounds - . . . Set $\mathcal{Y}_{\mathrm{LB}}$ . . .

Define $\mathcal{Y}_{\mathrm{LB}}(\mu; \mathcal{C}_J, M)$:

$$\mathcal{Y}_{\mathrm{LB}}(\mu) \equiv \Big\{ y \in \mathbb{R}^Q \;\Big|\; \text{(I)} \quad y \in \mathcal{B} \text{ , and}$$

$$\text{(II)} \; \sum_{q=1}^{Q} \Theta^q(\mu')\, y_q > \alpha^{\mathcal{N}}(\mu'),\; \forall\, \mu' \in \mathcal{C}_J^{M,\mu} \Big\}.$$

Lemma 3.1. Given $\mathcal{C}_J \subset \mathcal{D},\;\; M \in \mathbb{N}$,

$$\mathcal{Y} \subset \mathcal{Y}_{\mathrm{LB}}(\mu; \mathcal{C}_J, M),\; \forall\, \mu \in \mathcal{D} \;.$$

Coercivity Lower Bound: Bounds† - . . . Set $\mathcal{Y}_{\mathrm{LB}}$

Proof: For any $y \in \mathcal{Y}$, $\exists\, w_y \in X^{\mathcal{N}}$ such that

$$y_q = \frac{a^q(w_y,w_y)}{\|w_y\|_X^2}, \quad 1 \le q \le Q :$$

$$\inf_{w \in X^{\mathcal{N}}} \frac{a^q(w,w)}{\|w\|_X^2} \le \underbrace{\frac{a^q(w_y,w_y)}{\|w_y\|_X^2}}_{y_q} \le \sup_{w \in X^{\mathcal{N}}} \frac{a^q(w,w)}{\|w\|_X^2} \quad ; \quad \mathbf{(I)}$$

$$\sum_{q=1}^{Q} \Theta^q(\mu) \underbrace{\frac{a^q(w_y,w_y)}{\|w_y\|_X^2}}_{y_q} = \frac{a(w_y,w_y;\mu)}{\|w_y\|_X^2}$$

$$\ge \alpha^{\mathcal{N}}(\mu), \quad \forall\, \mu \in \mathcal{D}\,. \quad \mathbf{(II)}$$

Coercivity Lower Bound: Bounds - Lower Bound

Let

$$\alpha^{\mathcal{N}}_{\mathrm{LB}}(\mu;\mathcal{C}_J,M) = \min_{y\in\mathcal{Y}_{\mathrm{LB}}(\mu;\mathcal{C}_J,M)} \mathcal{J}^{\mathrm{obj}}(\mu;y)\ ;$$

a *linear optimization* problem (LP).

Proposition 3.2. Given $\mathcal{C}_J \subset \mathcal{D}$, $M \in \mathbb{N}$,

$$\alpha^{\mathcal{N}}_{\mathrm{LB}}(\mu) \le \alpha^{\mathcal{N}}(\mu),\ \forall\, \mu \in \mathcal{D}\ .$$

Proof:

$$\begin{aligned} \alpha^{\mathcal{N}}_{\mathrm{LB}}(\mu) &= \min_{y\in\mathcal{Y}_{\mathrm{LB}}(\mu)} \mathcal{J}^{\mathrm{obj}}(\mu;y) \\ &\le \min_{y\in\mathcal{Y}} \mathcal{J}^{\mathrm{obj}}(\mu;y) \qquad \text{Lemma 3.1: } \mathcal{Y} \subset \mathcal{Y}_{\mathrm{LB}} \\ &= \alpha^{\mathcal{N}}(\mu)\ . \end{aligned}$$

Coercivity Lower Bound: Bounds - Set $\mathcal{Y}_{\mathrm{UB}}$

Define

$$\mathcal{Y}_{\mathrm{UB}}(\mu; \mathcal{C}_J, M) = \{y^\star(\mu') \mid \mu' \in \mathcal{C}_J^{M,\mu}\}$$

where

$$y^\star(\mu) = \arg\inf_{y \in \mathcal{Y}} \mathcal{J}^{\mathrm{obj}}(\mu; y) \; ;$$

clearly $\mathcal{Y}_{\mathrm{UB}} \subset \mathcal{Y}$.

Coercivity Lower Bound: Bounds - Upper Bound

Let

$$\alpha_{\mathrm{UB}}^{\mathcal{N}}(\mu; \mathcal{C}_J, M) = \min_{y \in \mathcal{Y}_{\mathrm{UB}}(\mu; \mathcal{C}_J, M)} \mathcal{J}^{\mathrm{obj}}(\mu; y) \ ;$$

a simple *enumeration* exercise.

Proposition 3.3. Given $\mathcal{C}_J \subset \mathcal{D}$, $M \in \mathbb{N}$,

$$\alpha_{\mathrm{UB}}^{\mathcal{N}}(\mu) \geq \alpha^{\mathcal{N}}(\mu), \ \forall \, \mu \in \mathcal{D} \ .$$

Coercivity Lower Bound: Greedy Selection: $\mathcal{C}_J$ Procedure

Given $\Xi_{\text{train}}(\text{SCM})$, $\varepsilon_{\text{SCM}} \in [0,1]$, M

$$
\begin{aligned}
&\texttt{While} \ \max_{\mu\in\Xi_{\text{train}}} \left[\frac{\alpha^{\mathcal{N}}_{\text{UB}}(\mu;\mathcal{C}_J)-\alpha^{\mathcal{N}}_{\text{LB}}(\mu;\mathcal{C}_J)}{\alpha^{\mathcal{N}}_{\text{UB}}(\mu;\mathcal{C}_J)}\right] > \varepsilon_{\text{SCM}}: \\
&\qquad \mu^{J+1}_{\text{SCM}} = \arg\max_{\mu\in\Xi_{\text{train}}} \left[\frac{\alpha^{\mathcal{N}}_{\text{UB}}(\mu;\mathcal{C}_J)-\alpha^{\mathcal{N}}_{\text{LB}}(\mu;\mathcal{C}_J)}{\alpha^{\mathcal{N}}_{\text{UB}}(\mu;\mathcal{C}_J)}\right]; \\
&\qquad \mathcal{C}_{J+1} = \mathcal{C}_J \cup \mu^{J+1}_{\text{SCM}}; \\
&\qquad J \leftarrow J+1; \\
&\texttt{end.} \quad \texttt{Set } J_{\max} = J.
\end{aligned}
$$

Coercivity Lower Bound: Greedy Selection: $\mathcal{C}_J$ Convergence

If a is *parametrically* coercive,

$$\begin{aligned} \Theta^q(\mu) &> 0, \ \ \forall\, \mu \in \mathcal{D}\ , \\ a^q(w,w) &\geq 0, \ \ \forall\, w \in X,\ 1 \leq q \leq Q\ , \end{aligned}$$

$J = 1$ suffices to ensure $\alpha_{\mathrm{LB}}^{\mathcal{N}}(\mu) > 0,\ \forall\, \mu \in \mathcal{D}$.

Generally, continuity of $\Theta^{\cdot}$ ensures finite $J_{\max}$ such that tolerance is satisfied: but $J_{\max}(P)$?

Coercivity Lower Bound: Offline-Online Procedure - Offline

In Greedy, perform

$$J_{\max}\, \mathrm{LP}(Q, M) \Rightarrow \mathcal{C}_{J_{\max}} \;;$$

$$2Q + J_{\max} \text{ eigenproblems}^{\dagger} \text{ over } X^{\mathcal{N}}$$
$$\Rightarrow \text{(I) } \mathcal{B} \text{ and (II) } \{\alpha^{\mathcal{N}}(\mu') \mid \mu' \subset \mathcal{C}_{J_{\max}}\} \Rightarrow \mathcal{Y}_{\mathrm{LB}} \;;$$

$$J_{\max}\, Q \text{ inner products over } X^{\mathcal{N}} \Rightarrow \mathcal{Y}_{\mathrm{UB}} \;.$$

† Eigenproblems efficiently treated by Lanczos method.

Coercivity Lower Bound: Offline-Online Procedure - Online

Given $\mu \in \mathcal{D}$, perform

sort over $\mathcal{C}_{J_{\max}} \Rightarrow \mathcal{C}^{M,\mu}_{J_{\max}}$;

$(M+1)\,Q$ evaluations $\mu' \to \Theta^{\cdot}(\mu')$;

M *look-ups* $\mu' \to \alpha^{\mathcal{N}}(\mu')$;

$\mathbf{LP}\,(Q, M) \qquad \to \alpha^{\mathcal{N}}_{\mathbf{LB}}(\mu)$.

Cost *independent* of $\mathcal{N}$.

Advances

- **Advances: Elliptic Problems II, Parabolic Problems**

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   (a) Stability Factors
   (b) **Non-Coercive Problems**

Reduced basis methods and a posteriori error estimation for parametrized PDEs: Advances

NON-COERCIVE PROBLEMS

Gianluigi Rozza

Course on Advanced Topics in Numerical Solution of PDEs: Reduced Basis Methods for Computational Mechanics

Noncoercive Problems: Inf-Sup Elements - Supremizer

We are given a bilinear form $a : X^1 \times X^2 \to \mathbb{R}$. Then

$$\beta_{\text{inf-sup}} = \inf_{w \in X^1} \sup_{v \in X^2} \frac{a(w,v)}{||w||_{X^1} ||v||_{X^2}};$$

we can also say that for any $w \in X^1$ there exists a v^* in X^2 (the inner supremizer) such that

$$a(w, v^*(w)) \geq \beta ||w||_{X^1} ||v^*||_{X^2}.$$

Note that $\beta \geq 0$ (if β is negative, just switch sign of v), however it is not necessarily true that $\beta > 0$.

Noncoercive Problems: Inf-Sup Elements - Supremizer

We introduce the inner supremizing operator $T : X^1 \to X^2$ as the following linear operator:

$$(Tw, v)_{X^2} = a(w, v), \qquad \forall v \in X^2;$$

why is $v = Tw$ the supremizer of $a(w,v)/||v||_{X^2}$? Note

$$a(w, Tw) = (Tw, Tw)_{X^2}, \qquad w \text{ given},$$

so for $v = Tw$

$$\frac{a(w,v)}{||v||_{X^2}} = \frac{||Tw||^2_{X^2}}{||Tw||_{X^2}} = ||Tw||_{X^2}.$$

Noncoercive Problems: Inf-Sup Elements - Supremizer

But by Cauchy-Schwarz inequality, for any $v \in X^2$

$$\frac{a(w,v)}{||v||_{X^2}} = \frac{(Tw,v)_{X^2}}{||v||_{X^2}} \leq \frac{||Tw||_{X^2}||v||_{X^2}}{||v||_{X^2}} \leq ||Tw||_{X^2},$$

which proves the result.

Note Tw is simply our $v^*(w)$ of earlier. Hence, for any $w \in X^1$,

$$a(w,Tw) \geq \beta ||w||_{X^1}||Tw||_{X^2}.$$

Noncoercive Problems: Inf-Sup Elements - Supremizer

We can also develop an alternative expansion for β:

$$\beta = \inf_{w \in X^1} \frac{\left(\sup_{v \in X^2} \frac{a(w,v)}{||v||_{X^2}} \right)}{||w||_{X^1}} \overset{(v=Tw)}{=} \inf_{w \in X^1} \frac{||Tw||_{X^2}}{||w||_{X^1}},$$

or

$$\beta^2 = \inf_{w \in X^1} \frac{(Tw, Tw)_{X^2}}{||w||^2_{X^1}}$$

which is in fact a Rayleigh quotient.

Noncoercive Problems: Abstract Problem - Approximation

Find $u(\mu) \in X$ such that

$$a(u(\mu), v; \mu) = f(v) \qquad \forall\, v \in X$$

and

$$s(\mu) = \ell(u(\mu)),$$

where $\beta(\mu) > 0,\ \forall \mu \in \mathcal{D}$, with

$$\beta(\mu) = \inf_{w \in X} \sup_{v \in X} \frac{a(w, v; \mu)}{||w||_X ||v||_X}.$$

Noncoercive Problems: Abstract Problem - Approximation

We further assume that $a(\cdot,\cdot;\mu)$ is affine,

$$a(w,v;\mu) = \sum_{q=1}^{Q} \Theta^q(\mu) a^q(w,v).$$

We now denote our supremizer as $T^\mu : X \to X$, where

$$(T^\mu w, v)_X = a(w,v;\mu), \qquad \forall\, v \in X$$

Note from our affine assumption it follows that

$$T^\mu w = \sum_{q=1}^{Q} \Theta^q(\mu) T^q w,$$

where $(T^q w, v)_X = a^q(w,v), \qquad \forall\, v \in X.$

Noncoercive Problems: Approximation - Petrov-Galerkin

We assume we are given two subspaces $\tilde{X}^1 \subset X, \tilde{X}^2 \subset X$. Then $\tilde{u}(\mu) \in \tilde{X}^1$ satisfies

$$a(\tilde{u}(\mu), v, \mu) = f(v), \quad \forall v \in \tilde{X}^2,$$

and

$$\tilde{s}(\mu) = \ell(\tilde{u}(\mu)).$$

We define

$$\tilde{\beta}(\mu) = \inf_{w \in \tilde{X}^1} \sup_{v \in \tilde{X}^2} \frac{a(w, v; \mu)}{||w||_X ||v||_X}$$

Noncoercive Problems: Approximation - Petrov-Galerkin

Our supremizer operator is then given by $\tilde{T}^{\mu} : \tilde{X}^1 \to \tilde{X}^2$

$$(\tilde{T}^{\mu} w, v)_X = a(w, v; \mu), \quad \forall v \in \tilde{X}^2.$$

It follows that, for any $w \in \tilde{X}^1$,

$$a(w, \tilde{T}^{\mu} w; \mu) \geq \tilde{\beta}(\mu) ||w||_X || T^{\mu} w||_X$$

We pursue here just a Primal approximation, however we can readily extend the approach to a Primal-Dual formulation as described for coercive problems.

Noncoercive Problems: Approximation - A Priori Theory

We know that

$$a(u(\mu), v; \mu) = f(v), \quad \forall v \in X$$

$$a(\tilde{u}(\mu), v; \mu) = f(v), \quad \forall v \in \tilde{X}^2$$

and hence

$$a(u - \tilde{u}, v; \mu) = 0, \quad \forall v \in \tilde{X}^2 (\subset X)$$

which is the usual (Petrov-)Galerkin orthogonality relationship.

Noncoercive Problems: Approximation - A Priori Theory

We can write, for any $\tilde{w} \in \tilde{X}^1$,

$$\tilde{\beta}||\tilde{u} - \tilde{w}||_X||\tilde{T}^\mu(\tilde{u} - \tilde{w})||_X \leq a(\tilde{u} - \tilde{w}, \tilde{T}^\mu(\tilde{u} - \tilde{w}); \mu)$$
$$= a((\tilde{u} - \tilde{w}) + (u - \tilde{u}), \underbrace{\tilde{T}^\mu(\tilde{u} - \tilde{w})}; \mu)$$

(T^μ must be member of $\tilde{X}^2$, hence can not use stabler T^μ)

$$= a(u - \tilde{w}, \tilde{T}^\mu(\tilde{u} - \tilde{w}); \mu)$$
$$\leq \gamma||u - \tilde{w}||_X||\tilde{T}^\mu(\tilde{u} - \tilde{w})||_X$$

so

$$||\tilde{u} - \tilde{w}||_X \leq \frac{\gamma}{\tilde{\beta}}||u - \tilde{w}||_X,$$

and hence

$$||u - \tilde{u}||_X \leq \inf_{\tilde{w} \in \tilde{X}^1}(||u - \tilde{w}||_X + ||\tilde{u} - \tilde{w}||_X)$$

Noncoercive Problems: Approximation - A Priori Theory

Note it is not necessarily the case that $\tilde{\beta} \geq \beta$ or even $\tilde{\beta} > \mathbf{0}$ ($\tilde{\beta}$ may tend to zero as $\tilde{X}^1, \tilde{X}^2$ are refined);

in this sense, noncoercive problems are much more difficult than coercive problems.

We observe that approximation is provided by $\tilde{X}^1$ and stability (through $\tilde{\beta}$) by $\tilde{X}^2$.

Noncoercive Problems: RB Approximation - Galerkin

$$\tilde{X}^1 = \tilde{X}^2 = W_N$$

Introduce

$$W_N = span\left\{u(\mu_{pr}^n), 1 \leq n \leq N\right\}, \quad 1 \leq N \leq N_{max}.$$

Then $u_N(\mu) \in W_N$ satisfies

$$a(u_N(\mu), v; \mu) = f(v), \quad \forall v \in W_N,$$

and

$$s_N(\mu) = \ell(u_N(\mu)).$$

Noncoercive Problems: RB Approximation - Galerkin

If we define

$$\beta_N(\mu) \equiv \inf_{w \in W_N} \sup_{v \in W_N} \frac{a(w, v; \mu)}{||w||_X ||v||_X},$$

then

$$||u - u_N||_X \leq (1 + \frac{\gamma}{\beta_N}) \inf_{w_N \in W_N} ||u - w_N||_X$$

(and $|s - s_N| \leq ||\ell||_{(X^{\mathcal{N}})'} ||u - u_N||_X$).
In practice this often works very well. In theory, however, it is not in general possible to ensure $\beta_N \geq \beta(\mu)$ and thus in principle we could (though typically do not) observe $\beta_N \to 0$ as $N \to \infty$.

Noncoercive Problems: RB Approximation - Petrov-Galerkin

$$\tilde{X}^1 = W_N, \tilde{X}^2 = V_N^\mu$$

Introduce

$$W_N = span\left\{u(\mu_{pr}^n), 1 \leq n \leq N\right\}, 1 \leq N \leq N_{max}$$

and

$$V_N^\mu = span\left\{T^\mu u(\mu_{pr}^n), 1 \leq n \leq N\right\}, 1 \leq N \leq N_{max}$$

Note V_N^μ is parameter dependent.

Noncoercive Problems: RB Approximation - Petrov-Galerkin

Then $u_N(\mu) \in W_N$ satisfies

$$a(u_N(\mu), v; \mu) = f(v), \quad \forall v \in V_N^\mu,$$

and

$$s_N(\mu) = \ell(u_N(\mu)).$$

If we define

$$\beta_N(\mu) \equiv \inf_{w \in W_N} \sup_{v \in V_N^\mu} \frac{a(w, v; \mu)}{||w||_X ||v||_X},$$

then

$$||u - u_N||_X \leq \left(1 + \frac{\gamma}{\beta_N}\right) \inf_{w_N \in W_N} ||u - w_N||_X,$$

(and $|s - s_N| \leq ||\ell||_{(X^{\mathcal{N}})'} ||u - u_N||_X$.)

Noncoercive Problems: RB Approximation - Petrov-Galerkin

But in this case we can show that $\beta_N(\mu) \geq \beta(\mu), \forall \mu \in \mathcal{D}$.
To wit

$$\beta_N(\mu) \geq \inf_{w \in W_N} \frac{a(w, T^\mu w; \mu)}{||w||_X ||T^\mu w||_X} \qquad T^\mu : X^\mathcal{N} \to X^\mathcal{N}$$

since for any $w \in W_N, T^\mu w \in V_N^\mu$. But $a(w, T^\mu w; \mu) = (T^\mu w, T^\mu w)_X$ and hence

$$\beta_N(\mu) = \inf_{w \in W_N} \frac{||T^\mu w||_X}{||w||_X} \geq \inf_{w \in X} \frac{||T^\mu w||_X}{||w||_X} = \beta(\mu),$$

given that $W_N \subset X$.

Noncoercive Problems: RB Approximation - Petrov-Galerkin

Hence this Petrov-Galerkin scheme is guaranteed to be stable.
Re Offline-Online, we note that if

$$W_N = span\left\{\zeta^n, 1 \le n \le N\right\}$$

then

$$V_N^\mu = span\left\{\sum_{q=1}^{Q} \Theta^q(\mu) T^q \zeta^n, 1 \le n \le N\right\}$$

and hence

$$a(u_N(\mu), v; \mu) = \cdots$$

$$a\left(\sum_{j=1}^{N} u_{Nj}(\mu)\zeta^j, \sum_{q'=1}^{Q} \Theta^{q'}(\mu) T^{q'} \zeta^i; \mu\right) 1 \le i \le N$$

Noncoercive Problems: RB Approximation - Petrov-Galerkin

stored

$$\sum_{j=1}^{N} \underbrace{\left(\sum_{q=1}^{Q} \sum_{q'=1}^{Q} \Theta^q(\mu)\Theta^{q'}(\mu) \overbrace{a^q(\zeta^j, T^{q'}\zeta^i)} \right)} u_{Nj}(\mu)$$

$1 \leq i \leq N \quad O(Q^2N^2)$ Online operations.

(not particular onerous since there is already a $O(Q^2N^2)$ operation associated with a posteriori error bound.)

Noncoercive Problems: RB Approximation -A Posteriori Error Estimation

We know that

$$a(u - u_N, v; \mu) = r(v; \mu), \forall v \in X$$
$$= (\hat{e}(\mu), v)_X, \forall v \in X$$

where

$$r(v; \mu) = f(v) - a(u_N, v; \mu)$$

Here u_N can be either our Galerkin or Petrov-Galerkin approximation.

Noncoercive Problems: RB Approximation -A Posteriori Error Estimation

It thus follows that

$$\beta(\mu)||u - u_N||_X||T^\mu(u - u_N)||_X \leq$$

$$a(u - u_N, T^\mu(u - u_N); \mu) =$$

$$= (\hat{e}(\mu), T^\mu(u - u_N))_X$$

$$\leq ||\hat{e}(\mu)||_X||T^\mu(u - u_N)||_X$$

or

$$||u - u_N||_X \leq \frac{||\hat{e}(\mu)||_X}{\beta(\mu)}$$

Noncoercive Problems: RB Approximation -A Posteriori Error Estimation

Thus, for $\beta_{LB}(\mu)$ a positive lower bound for $\beta(\mu)$, and

$$\Delta_N(\mu) \equiv \frac{||\hat{e}(\mu)||_X}{\beta_{LB}(\mu)},$$

we obtain

$$||u - u_N||_X \leq \Delta_N(\mu)$$

(and also $|s - s_N| \leq ||l||_{(X^{\mathcal{N}})'} \Delta_N(\mu)$: a Primal-Dual approach / result is also possible).
Re Offline-Online, the calculation of $||\hat{e}(\mu)||_X$ is identical to the coercive case. It only remains to construct $\beta_{LB}(\mu)$ by the SCM.

Noncoercive Problems: RB Approximation -SCM for $\beta_{LB}(\mu)$

We recall that

$$\beta^2(\mu) = \inf_{w \in X^{\mathcal{N}}} \frac{(T^\mu w, T^\mu w)_X}{||w||_X^2}$$

but since a is affine,

$$\beta^2(\mu) = \inf_{w \in X^{\mathcal{N}}} \sum_{q=1}^{Q} \sum_{q'=1}^{Q} \Theta^q(\mu) \Theta^{q'}(\mu) \frac{(T^q w, T^{q'} w)_X}{||w||_X^2}$$

$$= \inf_{w \in X^{\mathcal{N}}} \sum_{q=1}^{Q} \sum_{q'=q}^{Q} (2 - \delta_{qq'}) \Theta^q(\mu) \Theta^{q'}(\mu) \frac{(T^q w, T^{q'} w)_X}{||w||_X^2}$$

Noncoercive Problems: RB Approximation -SCM for $\beta_{LB}(\mu)$

Hence

$$\beta^2(\mu) = \underbrace{\inf_{w \in X^{\mathcal{N}}} \sum_{q=1}^{\hat{Q}} \hat{\Theta}^q(\mu) \frac{\hat{a}^q(w,w)}{||w||_X^2}}_{\text{apply standard SCM}}$$

where

$$\begin{matrix} (2-\delta_{q'q''})\Theta^{q'}(\mu)\Theta^{q''}(\mu) \\ 1 \le q' < q'' \le Q \end{matrix} \longmapsto \begin{matrix} \hat{\Theta}^q(\mu) \\ 1 \le q \le \hat{Q} \equiv \frac{Q(Q+1)}{2} \end{matrix}$$

$$\begin{matrix} \frac{1}{2}\left((T^{q'}w, T^{q''}v)_X + (T^{q'}v, T^{q''}w)_X\right) \\ 1 \le q' < q'' \le Q \end{matrix}$$

$$\longmapsto \begin{matrix} \hat{a}^q(w,v) \\ 1 \le q \le \hat{Q} \equiv \frac{Q(Q+1)}{2} \end{matrix}$$