Model Order Reduction Techniques I & II

RB: Coercivity Lower Bounds

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"Truth" Problem Statement

Given $\boldsymbol{\mu} \in \boldsymbol{\mathcal{D}} \subset \mathbb{R}^{P}$, evaluate

$(\cdot) = (\cdot)^{\mathcal{N}}$

$$s(\boldsymbol{\mu}) = f(u(\boldsymbol{\mu}); \boldsymbol{\mu})$$

where $u(x; \boldsymbol{\mu}) \in X$ satisfies

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

Assumptions:

- linearity, coercivity, continuity;
- affine parameter dependence; and
- compliance: $\ell = f$, a symmetric.

Reduced Basis Sample and Space

Parameter samples:

$$S_N = \{\mu^1 \in \mathcal{D}, \ldots, \mu^N \in \mathcal{D}\}, \quad 1 \le N \le N_{\max},$$

with

$$S_1 \subset S_2 \subset \ldots \subset S_{N_{\max}-1} \subset S_{N_{\max}} \subset \mathcal{D}.$$

Lagrangian reduced basis spaces:

$$W_N = \mathrm{span}\{ \underbrace{u(\mu^n)}_{\text{"snapshots"}}, 1 \le n \le N\}, \quad 1 \le N \le N_{\max},$$

with

$$W_1 \subset W_2 \subset \ldots \subset W_{N_{\max}-1} \subset W_{N_{\max}} (\subset X).$$

Reduced Basis Approximation

Given $\mu \in \mathcal{D} \subset \mathbb{R}^P$, evaluate

$$s_N(\mu) = f(u_N(\mu); \mu)$$

where $u_N(x; \mu) \in X_N \subset X$ satisfies

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

Recall:

- RB space: $X_N =$ "Gram-Schmidt"(W_N)
- $u_N(\mu)$ unique (from coercivity, continuity, linear independence)

Hypotheses

We assume that $a : X \times X \times \mathcal{D} \to \mathbb{R}$ is

- coercive

$$(0 <)\ \alpha(\mu) \equiv \inf_{w \in X} \frac{a(w, w; \mu)}{\|w\|_X^2};$$

- continuous

$$\gamma(\mu) \equiv \sup_{w \in X} \sup_{v \in X} \frac{a(w, v; \mu)}{\|w\|_X \|v\|_X}\ (< \infty).$$

- and affine parameter dependent

$$a(w, v; \mu) = \sum_{q=1}^{Q_a} \Theta_a^q(\mu)\, a^q(w, v), \quad \forall w, v \in X$$

Inner Products and Norms

We defined the

- energy inner product and induced norm (parameter-dependent)

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

$$|||w|||_{\mu} = \sqrt{a(w, w; \mu)}, \qquad \forall w \in X$$

- X^{e}-inner product and induced norm (parameter-independent)

$$(w, v)_X \equiv (((w, v)))_{\bar{\mu}} \,(= a(w, v; \bar{\mu})), \qquad \forall w, v \in X$$

$$\|w\|_X \equiv |||w|||_{\bar{\mu}} \,(= \sqrt{a(w, w; \bar{\mu})}), \qquad \forall w \in X$$

Energy Error Bound

Recall the definition of the

- error bound: $$\Delta_N^{\text{en}}(\mu) \equiv \frac{\|\hat{e}(\mu)\|_X}{\sqrt{\alpha_{\text{LB}}(\mu)}}$$
- and effectivity: $$\eta_N^{\text{en}}(\mu) \equiv \frac{\Delta_N^{\text{en}}(\mu)}{|||e(\mu)|||_\mu}$$

Proposition (Energy Error Bound)

For any $N = 1, \ldots, N_{\max}$, the effecitivity, $\eta_N^{\text{en}}(\mu)$ satisfies

$$1 \leq \eta_N^{\text{en}}(\mu) \leq \sqrt{\frac{\gamma_{\text{UB}}(\mu)}{\alpha_{\text{LB}}(\mu)}}, \qquad \forall \mu \in \mathcal{D}.$$

Coercivity Lower Bound – Goal

For our *a posteriori* error bounds we require a positive lower bound for the coercivity constant, $\alpha_{\mathrm{LB}} : \mathcal{D} \to \mathbb{R}$, such that

I. $0 < \alpha_{\mathrm{LB}}(\mu) \leq \alpha(\mu), \quad \forall \mu \in \mathcal{D}$

II. $\partial t_{\mathrm{comp}}(\mu \to \alpha_{\mathrm{LB}}(\mu))$ is $O(1)$,

where

$$\alpha(\mu) \equiv \inf_{w \in X} \frac{a(w, w; \mu)}{\|w\|_X^2}, \quad \forall \mu \in \mathcal{D}.$$

We consider

- "$\min \Theta$" Approach
- Multiple Inner Products
- Successive Constraint Method

The "$\min \Theta$" Approach

Lemma

For a parametrically coercive, we have

$$0 < \Theta_a^{\min,\bar{\mu}}(\mu) \le \alpha(\mu), \quad \forall \mu \in \mathcal{D},$$

where $\Theta_a^{\min,\bar{\mu}} : \mathcal{D} \to \mathbb{R}_+$ *is given by*

$$\Theta_a^{\min,\bar{\mu}}(\mu) = \min_{q \in \{1,\dots,Q_a\}} \frac{\Theta_a^q(\mu)}{\Theta_a^q(\bar{\mu})}.$$

Recall X-inner product an norm

$$(w,v)_X \equiv a(w,v;\bar{\mu}), \quad \forall w,v \in X$$

$$||w||_X \equiv (w,w)_X^{1/2}, \quad \forall w \in X$$

The "$\min \Theta$" Approach

Proof.

$$\begin{aligned} a(w,w;\mu) &= \sum_{q=1}^{Q_a} \Theta_a^q(\mu)\, a^q(w,w) \\ &= \sum_{q=1}^{Q_a} \frac{\Theta_a^q(\mu)}{\Theta_a^q(\bar{\mu})} \Theta_a^q(\bar{\mu})\, a^q(w,w) \\ &\geq \left(\min_{q \in \{1,\ldots,Q_a\}} \frac{\Theta_a^q(\mu)}{\Theta_a^q(\bar{\mu})} \right) \; a^q(w,w;\bar{\mu}) \\ &= \Theta_a^{\min,\bar{\mu}}(\mu)\, \|w\|_X^2, \quad \forall w \in X,\ \forall \mu \in \mathcal{D} \end{aligned}$$

It thus follows that

$$\alpha(\mu) = \inf_{w \in X} \frac{a(w,w;\mu)}{\|w\|_X^2} \geq \Theta_a^{\min,\bar{\mu}}(\mu) > 0, \quad \forall \mu \in \mathcal{D}.$$

□

The "$\min \Theta$" Approach

If a is parametrically coercive, we may choose as a lower bound for the coercivity constant

$$\alpha_{\mathrm{LB}}(\mu) \equiv \Theta_a^{\min,\bar{\mu}}(\mu) = \min_{q \in \{1,\ldots,Q_a\}} \frac{\Theta_a^q(\mu)}{\Theta_a^q(\bar{\mu})}.$$

Note:

- Online cost to evaluate $\Theta_a^{\min,\bar{\mu}}(\mu)$: $O(Q_a)$.
- Choice of inner product important: $(w,v)_X \equiv a(w,v;\bar{\mu})$.
- Lower bound directly extends to non-symmetric forms a.

The "$\min \Theta$" Approach – non-symmetric forms

For a parametrically coercive but non-symmetric we obtain

$$a_s(w, v; \mu) = \sum_{q=1}^{Q_{a_s}} \Theta_{a_s}^q(\mu)\, a_s^q(w, v), \quad \forall w, v \in X,$$

where the symmetric part is given by

$$a_s(w, v; \mu) = \frac{1}{2}(a(w, v; \mu) + a(v, w; \mu)),$$

and the $\Theta_{a_s}^q(\mu)$ and $a_s^q(w, v)$ satisfy

$$\Theta_{a_s}^q(\mu) > 0, \qquad \forall \mu \in \mathcal{D},\ 1 \leq q \leq Q_a,$$

and

$$a_s^q(v, v) \geq 0, \qquad \forall v \in X,\ 1 \leq q \leq Q_a.$$

$$\Rightarrow \alpha_{\mathrm{LB}}(\mu) \equiv \Theta_{a_s}^{\min,\bar{\mu}}(\mu) = \min_{q \in \{1,\ldots,Q_{a_s}\}} \frac{\Theta_{a_s}^q(\mu)}{\Theta_{a_s}^q(\bar{\mu})}.$$

Multiple Inner Products – Motivation

Upper bound for effectivity (a parametrically coercive & symmetric)

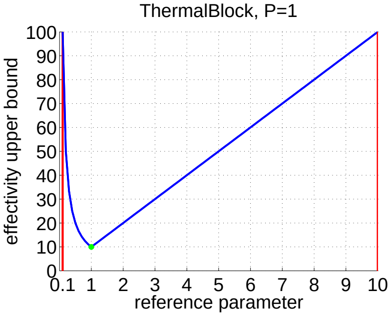
$$1 \le \eta_N^s(\mu) \le \frac{\gamma_{\mathrm{UB}}(\mu)}{\alpha_{\mathrm{LB}}(\mu)} = \frac{\Theta_a^{\max,\bar{\mu}}(\mu)}{\Theta_a^{\min,\bar{\mu}}(\mu)} = \theta^{\bar{\mu}}(\mu)$$

ThermalBlock: $P = 1$

$$\theta^{\bar{\mu}}(\mu_1) = \mathrm{Max}\left(\frac{\bar{\mu}_1}{\mu_1}, \frac{\mu_1}{\bar{\mu}_1}\right)$$

and for $\mu_1 \in [0.1, 10]$ we thus obtain

- $\bar{\mu}_1 = 0.1 : \theta^{\bar{\mu}}(\mu_1) \le 100$
- $\bar{\mu}_1 = 1 : \theta^{\bar{\mu}}(\mu_1) \le 10$
- $\bar{\mu}_1 = 10 : \theta^{\bar{\mu}}(\mu_1) \le 100$



Multiple Inner Products – Motivation

Idea: Introduce $\overline{K}$ reference parameter values $\overline{\mu}^k$, $1 \leq k \leq \overline{K}$, with associated inner product and error bound.

Then "switch" to the best error bound, e.g., for

- $\overline{K} = 2$
  $\theta^{\bar{\mu}_{\text{opt}}}(\mu_1) \lessapprox 3.2$
- $\overline{K} = 3$
  $\theta^{\bar{\mu}_{\text{opt}}}(\mu_1) \lessapprox 2.2$
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  $\theta^{\bar{\mu}_{\text{opt}}}(\mu_1) \lessapprox 1.8$

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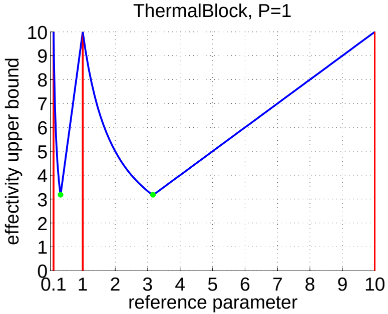

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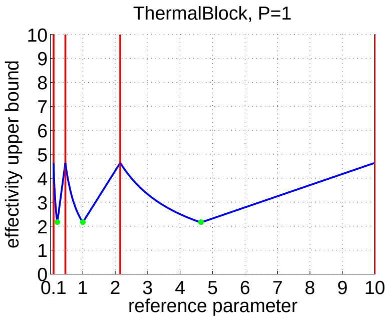

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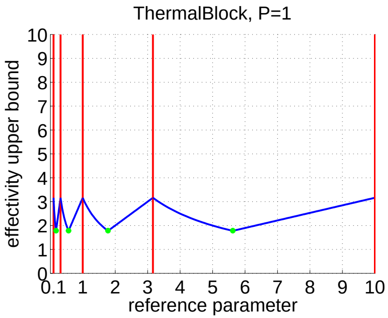

Multiple Inner Products

Introduce sample $\mathcal{V}^{\overline{K}} = \{\overline{\mu}^1 \in \mathcal{D}, \ldots, \overline{\mu}^{\overline{K}} \in \mathcal{D}\}$ with $\overline{K}$ points in $\mathcal{D}$ and

- associated inner product

$$(w, v)_{X,k} = a(w, v; \overline{\mu}^k), \ \forall w, v \in X, \ 1 \leq k \leq \overline{K}$$

- and error bounds (for $s(\mu) - s_N(\mu)$)

$$\Delta^s_{N,k}(\mu) \equiv \frac{\|\hat{e}_k(\mu)\|^2_{X,k}}{\alpha_{\mathrm{LB},k}(\mu)}, \quad 1 \leq k \leq \overline{K}$$

where $\hat{e}_k(\mu) \in X, \ 1 \leq k \leq \overline{K}$, satisfies

$$(\hat{e}_k(\mu), v)_{X,k} = r(v; \mu), \quad \forall v \in X,$$

and

$$\alpha_{\mathrm{LB},k}(\mu) \equiv \Theta_a^{\min, \overline{\mu}^k}(\mu).$$

Multiple Inner Products

We can then introduce the effectivities

$$\eta^s_{N,k}(\mu) \equiv \frac{\Delta^s_{N,k}(\mu)}{s(\mu) - s_N(\mu)}, \quad 1 \leq k \leq \overline{K},$$

and it follows that, for $1 \leq N \leq N_{\max}$,

$$1 \leq \eta^s_{N,k}(\mu) \leq \theta^{\overline{\mu}^k}(\mu), \quad \forall \mu \in \mathcal{D}.$$

We finally define the error bound

$$\Delta^s_N(\mu) = \Delta^s_{N,k^*}(\mu)$$

where $k^* : \mathcal{D} \to \{1, \ldots, \overline{K}\}$ is an appropriate indicator function.

Multiple Inner Products

Indicator strategy k^*:

(O1) Partition $\mathcal{D}$ into $\overline{K}$ subdomains $\mathcal{D}_k$ such that $k^*(\mu \in \mathcal{D}_k) = k$, e.g.,

$$k^*(\mu) = \arg \min_{k \in \{1,\ldots,\overline{K}\}} |\mu - \overline{\mu}^k|,$$

where $|\cdot|$ denotes the Euclidean norm in $\mathbb{R}^P$.

(O2) Minimum effectivity upper bound

$$k^*(\mu) = \arg \min_{k \in \{1,\ldots,\overline{K}\}} \theta^{\overline{\mu}^k}(\mu).$$

(O1) Smallest (hence sharpest) error bound

$$k^*(\mu) = \arg \min_{k \in \{1,\ldots,\overline{K}\}} \Delta^s_{N,k}(\mu).$$

Multiple Inner Products – Example: TB $P = 1$

ThermalBlock: $P = 1$

$$1/\mu_1^{\min} = \sqrt{\mu_r},\ \mu_1^{\max} = \sqrt{\mu_r} \Rightarrow \mu_1^{\max}/\mu_1^{\min} = \mu_r$$

Single inner product: $\overline{\mu}_1 = 1 \Rightarrow \eta^s_{N,\max} = \sqrt{\mu_r}.$

We introduce a grid $G^{\ln}_{[\mu_1^{\min},\mu_1^{\max};\overline{K}+1]} = [z_1, \ldots, z_{\overline{K}+1}]$ and set

$$\ln \overline{\mu}_1^k = \tfrac{1}{2}(\ln z_k + \ln z_{k+1}), \quad 1 \leq k \leq \overline{K}.$$

We then obtain

$$\theta^{\bar{\mu}^k}(\mu_1) = \mathrm{Max}\left(\frac{\overline{\mu}_1^k}{\mu_1}, \frac{\mu_1}{\overline{\mu}_1^k}\right)$$

and

$$\min_{k \in \{1,\ldots,\overline{K}\}} \max_{\mu_1 \in \mathcal{D}} \theta^{\overline{\mu}^k}(\mu_1) = (\sqrt{\mu_r})^{\frac{1}{\overline{K}}}.$$

Multiple Inner Products – Example: TB $P = 1$

It follows that, for (O2), we obtain

$$\eta^s_{N,\max} \leq (\sqrt{\mu_r})^{\frac{1}{\overline{K}}} \left(= e^{\frac{1}{2\overline{K}} \ln \mu_r} \right).$$

Recall: Effectivity bound for single inner product ($\overline{K} = 1$)

$$\eta^s_{N,\max} \leq \sqrt{\mu_r} \quad \text{for} \quad G^{\ln}_{[\mu_1^{\min}, \mu_1^{\max}; 2]} = [\mu_1^{\min}, \mu_1^{\max}],$$

and hence $\overline{\mu}^1_1 = 1$ for $\mu_1^{\min} = 1/\sqrt{\mu_r}$, $\mu_1^{\max} = \sqrt{\mu_r}$.

Furthermore:
Set of points $\mathcal{V}^{\overline{K}} \equiv \{\overline{\mu}^1, \dots, \overline{\mu}^{\overline{K}}\}$ is optimal in the (O2) sense

$$\overline{K} = 1 \Rightarrow \overline{\mu}^1 = 1.$$

Multiple Inner Products – Example: TB $P = 1$

Grid: $G^{\ln}_{[\mu_1^{\min},\mu_1^{\max};\overline{K}+1]} = [z_1, \ldots, z_{\overline{K}+1}]$

Reference Parameters: $\ln \overline{\mu}_1^k = \frac{1}{2}(\ln z_k + \ln z_{k+1}),$
$1 \leq k \leq \overline{K}.$

We obtain with (O2), for all $\mu_1 \in [0.1, 10]$:

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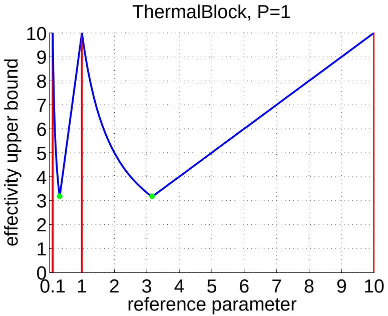

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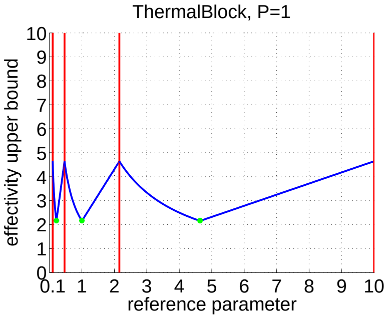

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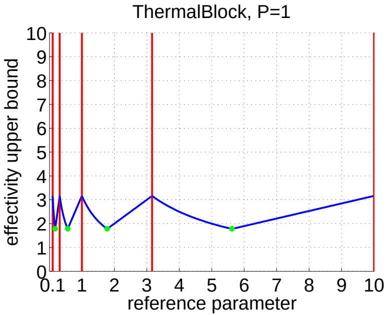

Multiple Inner Products – Summary

Remarks

- We can "control" the effectivity upper bound, e.g.,
  - to achieve $\eta^s_{N,\max} \leq 10$ we need $\overline{K} = [\ln \mu_r / 2 \ln 10]_+$.
  - For $\mu_r = 10^6 \Rightarrow \mathcal{D} = [10^{-3}, 10^3]$ we obtain $\overline{K} = 6$.
- Offline operation count & Online storage scale linearly with $\overline{K}$.
- Online operation count for (O1) and (O2) is insensitive to $\overline{K}$ and scales linearly for (O3).
- Approach limited to modest $\overline{K}$ and rather modest P, e.g.,
  - to achieve $\eta^s_{N,\max} \leq 10$ for $P > 1$ (ThermalBlock) we require roughly $\overline{K} = [\ln \mu_r / \ln 10]^P_+$ inner products.

Successive Constraint Method

The "$\mathbf{min}\,\boldsymbol{\Theta}$" Approach with one or multiple inner products is

- straightforward and efficient to implement, and
- returns sharp lower bounds for the coercivity constant

but is restricted to parametrically coercive problems.

How do we deal with general (non-)coercive problems?

Successive Constraint Method

- Construction of lower bounds for
  - coercivity constants, and
  - inf-sup stability constants (for non-coercive problems).
- Offline-Online Computational Procedure
  - Offline: eigenproblems, inner products, LPs.
  - Online: one LP of small size (independent of $\mathcal{N}$).

Reformulation – Coercivity

It follows from affine parameter dependence

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

and coercivity

$$0 < \alpha(\mu) \equiv \inf_{w \in X} \frac{a(w,w;\mu)}{\|w\|_X^2},$$

that we can write

$$\alpha(\mu) \equiv \inf_{w \in X} J_w^{\text{obj}}(\mu; w),$$

where

$$J_w^{\text{obj}}(\mu; w) \equiv \sum_{q=1}^{Q_a} \Theta_a^q(\mu) \frac{a^q(w,w)}{\|w\|_X^2}.$$

Reformulation – Coercivity

We first introduce an objective function $\mathcal{J}^{\text{obj}} : \mathcal{D} \times \mathbb{R}^{Q_a} \to \mathbb{R}$ given by

$$\mathcal{J}^{\text{obj}}(\mu; y) \equiv \sum_{q=1}^{Q_a} \Theta_a^q(\mu)\, y^q.$$

We can then write

$$\alpha(\mu) \equiv \inf_{y \in \mathcal{Y}} \mathcal{J}^{\text{obj}}(\mu; y),$$

where

$$\mathcal{Y} \equiv \left\{ y \in \mathbb{R}^{Q_a} \,\middle|\, \exists\, w_y \in X \text{ s.t. } y^q = \frac{a^q(w_y, w_y)}{\|w_y\|_X^2},\ 1 \le q \le Q_a \right\}.$$

Note:

- $y = (y^1, \ldots, y^{Q_a}) \in \mathbb{R}^{Q_a}$ is a vector of Rayleigh quotients.
- so far this is just a change of notation.

Lower Bound

Assume we are given an approximation $\mathcal{Y}_{\mathbf{LB}}$ to $\mathcal{Y}$ such that

- $\mathcal{Y}$ is a subset of $\mathcal{Y}_{\mathbf{LB}}$, i.e., $\mathcal{Y} \subset \mathcal{Y}_{\mathbf{LB}}$, and
- we can solve

$$\inf_{y \in \mathcal{Y}_{\mathbf{LB}}} \mathcal{J}^{\mathbf{obj}}(\mu; y)$$

very efficiently.

We can then define

$$\begin{aligned} \alpha_{\mathbf{LB}}(\mu) &\equiv \inf_{y \in \mathcal{Y}_{\mathbf{LB}}} \mathcal{J}^{\mathbf{obj}}(\mu; y) \\ &\leq \inf_{y \in \mathcal{Y}} \mathcal{J}^{\mathbf{obj}}(\mu; y) \\ &= \alpha(\mu), \quad \forall \mu \in \mathcal{D}, \end{aligned}$$

that is, $\alpha_{\mathbf{LB}}(\mu)$ is a lower bound to $\alpha(\mu)$.

Lower Bound: $\mathcal{Y}_{\mathrm{LB}}$

We first define

$$\begin{aligned} b_q^- &\equiv \inf_{v \in X} \frac{a^q(v,v)}{\|v\|_X^2}, \quad 1 \le q \le Q_a, \\ b_q^+ &\equiv \sup_{v \in X} \frac{a^q(v,v)}{\|v\|_X^2}, \quad 1 \le q \le Q_a, \end{aligned}$$

and the "continuity constraint" box

$$\mathcal{B} \equiv \prod_{q=1}^{Q_a} [b_q^-, b_q^+].$$

It follows that $\mathcal{Y} \subset \mathcal{B}$, since $\forall w_y \in X$

$$\inf_{v \in X} \frac{a^q(v,v)}{\|v\|_X^2} \le \underbrace{\frac{a^q(w_y,w_y)}{\|w_y\|_X^2}}_{y_q} \le \sup_{v \in X} \frac{a^q(v,v)}{\|v\|_X^2}.$$

Lower Bound: $\mathcal{Y}_{\mathrm{LB}}$

We then introduce a set of M parameter values

$$\mathcal{P}_M = \{\mu'_i \in \mathcal{D}, i = 1, \dots, M\}$$

at which we pre-compute $\alpha(\mu')$ for all $\mu' \in \mathcal{P}_M$.

We may now define

$$\mathcal{Y}_{\mathrm{LB}}(\mu; \mathcal{P}_M, M) \equiv \left\{ y \in \mathbb{R}^{Q_a} \;\middle|\; \begin{array}{l} y \in \mathcal{B}, \\ \sum_{q=1}^{Q_a} \Theta_a^q(\mu') y^q \geq \alpha(\mu'), \ \forall \mu' \in \mathcal{P}_M \end{array} \right\}.$$

Proposition

For given $\mathcal{P}_M \subset \mathcal{D}$, $M \in \mathbb{N}_+$,

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

Coercivity Lower Bound $\alpha_{\mathrm{LB}}(\mu)$

We may now define the coercivity lower bound

$$\alpha_{\mathrm{LB}}(\mu) \equiv \min_{y \in \mathcal{Y}_{\mathrm{LB}}(\mu; \mathcal{P}_M, M)} \mathcal{J}^{\mathrm{obj}}(\mu; y).$$

Proposition

For given $\mathcal{P}_M \subset \mathcal{D}$, $M \in \mathbb{N}_+$,

$$\alpha_{\mathrm{LB}}(\mu) \leq \alpha(\mu), \quad \forall \mu \in \mathcal{D}.$$

Proof: ...

Note: $\alpha_{\mathrm{LB}}(\mu)$ is a linear optimization problem (LP) with

- Q_a design variables,
- $2Q_a + M$ inequality constraints.

$\Rightarrow$ cost to evaluate $\mu \to \alpha_{\mathrm{LB}}(\mu)$ is independent of $\mathcal{N}$.

Upper Bound

Two questions remain:

I. How do we choose $\mathcal{P}_M$?

II. How do we know that $\alpha_{\mathrm{LB}}(\mu)$ is accurate?

Recall that we require that $\alpha_{\mathrm{LB}}(\mu)$ be

- positive: $\alpha_{\mathrm{LB}}(\mu) > 0, \quad \forall \mu \in \mathcal{D}$, but also
- accurate: $\dfrac{\alpha(\mu) - \alpha_{\mathrm{LB}}(\mu)}{\alpha(\mu)} < \varepsilon_{\mathrm{SCM}}, \quad \forall \mu \in \mathcal{D}.$

Since we do not know $\alpha(\mu)$, we introduce an (easily computable) upper bound, $\alpha_{\mathrm{UB}}(\mu)$, and instead require

$$\frac{\alpha_{\mathrm{UB}}(\mu) - \alpha_{\mathrm{LB}}(\mu)}{\alpha_{\mathrm{LB}}(\mu)} < \varepsilon_{\mathrm{SCM}}, \quad \forall \mu \in \mathcal{D}.$$

Upper Bound: $\mathcal{Y}_{\mathrm{UB}}$

Assume we are given an approximation $\mathcal{Y}_{\mathrm{UB}}$ to $\mathcal{Y}$ such that

- $\mathcal{Y}_{\mathrm{UB}}$ is a subset of $\mathcal{Y}$, i.e., $\mathcal{Y}_{\mathrm{UB}} \subset \mathcal{Y}$, and
- we can solve

$$\inf_{y \in \mathcal{Y}_{\mathrm{UB}}} \mathcal{J}^{\mathrm{obj}}(\mu; y) \left(\equiv \sum_{q=1}^{Q_a} \Theta_a^q(\mu)\, y^q \right)$$

very efficiently.

We can then define

$$\begin{aligned} \alpha_{\mathrm{UB}}(\mu) &\equiv \inf_{y \in \mathcal{Y}_{\mathrm{UB}}} \mathcal{J}^{\mathrm{obj}}(\mu; y) \\ &\geq \inf_{y \in \mathcal{Y}} \mathcal{J}^{\mathrm{obj}}(\mu; y) \\ &= \alpha(\mu), \quad \forall \mu \in \mathcal{D}, \end{aligned}$$

that is, $\alpha_{\mathrm{UB}}(\mu)$ is an upper bound to $\alpha(\mu)$.

Upper Bound: $\mathcal{Y}_{\mathrm{UB}}$

We introduce a set of K parameter values

$$\mathcal{C}_K \equiv \{\mu^1_{\mathrm{SCM}} \in \mathcal{D}, \ldots, \mu^K_{\mathrm{SCM}} \in \mathcal{D}\}$$

and define, for any $\mu \in \mathcal{D}$,

$$y^*(\mu) \equiv \arg \inf_{y \in \mathcal{Y}} \sum_{q=1}^{Q_a} \Theta^q_a(\mu) y^q.$$

We may now define

$$\mathcal{Y}_{\mathrm{UB}}(\mu; \mathcal{C}_K, K) \equiv \left\{ y^*(\mu) \,|\, \mu \in \mathcal{C}_K \right\}.$$

Since any $y \in \mathcal{Y}_{\mathrm{UB}}$ is also a member of $\mathcal{Y}$, it follows that $\mathcal{Y}_{\mathrm{UB}} \subset \mathcal{Y}$ as desired.

Coercivity Upper Bound $\alpha_{\mathrm{UB}}(\mu)$

We may now define the coercivity upper bound

$$\alpha_{\mathrm{UB}}(\mu) \equiv \min_{y \in \mathcal{Y}_{\mathrm{UB}}(\mu; \mathcal{C}_K, K)} \mathcal{J}^{\mathrm{obj}}(\mu; y).$$

Proposition

For given $\mathcal{C}_K \subset \mathcal{D}$, $K \in \mathbb{N}_+$,

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

Proof: ...

Note:

- Accuracy of $\alpha_{\mathrm{UB}}(\mu)$ depends on K (the size of $\mathcal{C}_K$);
- Evaluation of $\alpha_{\mathrm{UB}}(\mu)$ is a simple enumeration exercise
  $\Rightarrow$ cost to evaluate $\mu \rightarrow \alpha_{\mathrm{UB}}(\mu)$ is independent of $\mathcal{N}$.

Computation of $y^*(\mu)$

Note that if $v^*(\mu)$ is the eigenvector associated with $\alpha(\mu)$, i.e.,

$$v^*(\mu) \equiv \arg \inf_{v \in X} \frac{a(v, v; \mu)}{\|v\|_X^2}$$

such that

$$\alpha(\mu) = \frac{a(v^*(\mu), v^*(\mu); \mu)}{\|v^*(\mu)\|_X^2}$$

then the components of $y^*(\mu)$ are given by

$$y^{*q}(\mu) = \frac{a^q\left(v^*(\mu), v^*(\mu)\right)}{\|v^*(\mu)\|_X^2},$$

and $y^*(\mu) = (y^{*1}(\mu), y^{*2}(\mu), \ldots, y^{*Q_a}(\mu)) \in \mathbb{R}^{Q_a}$.

Set $\mathcal{P}_M$ and $\mathcal{C}_K$

I. How do we choose $\mathcal{P}_M$?

- Recall that we need to pre-compute the minimum eigenvalues $\alpha(\mu')$ for all $\mu' \in \mathcal{P}_M$ to obtain $\mathcal{Y}_{\text{LB}}$, where
$$\mathcal{P}_M = \{\mu'_i \in \mathcal{D}, i = 1, \ldots, M\}.$$
- But from computation of $y^*(\mu)$ for all $\mu \in \mathcal{C}_K$ we essentially already know the $\alpha(\mu)$ for all $\mu \in \mathcal{C}_K$, where
$$\mathcal{C}_K \equiv \{\mu^1_{\text{SCM}} \in \mathcal{D}, \ldots, \mu^K_{\text{SCM}} \in \mathcal{D}\}.$$
- We thus choose
$$\begin{aligned} \mathcal{P}_M &= \{M \text{ points in } \mathcal{C}_K \text{ closest to } \mu\}, \\ \text{or } \mathcal{P}_M &= \mathcal{C}_K \text{ if } M \geq K, \end{aligned}$$
and we select $\mathcal{C}_K$ using a greedy procedure.

Offline-Online Procedure

Offline Stage: Greedy Procedure

Initialize (once):

I. Given

- M: number of points in $\mathcal{P}_M$;
- $\epsilon \in (0,1]$: relative error tolerance;
- $\Xi^{\mathrm{SCM}}_{\mathrm{train}}$: training sample.

II. Compute $b_q^{\pm}, \; 1 \le q \le Q_a$:

- Solve $2Q$ generalized eigenvalue problems
$$\underline{\mathbb{A}}^{\mathcal{N}q}\,\underline{v} = \lambda\,\underline{\mathbb{X}}^{\mathcal{N}}\,\underline{v}, \quad q = 1, \ldots, Q_a.$$
- Set $b_q^- = \lambda_{\min}, \; b_q^+ = \lambda_{\max}$.

III. Set $K = 1$, and choose $C_1 = \{\mu^1_{\mathrm{SCM}}\}$ arbitrarily.

Offline-Online Procedure

$$\texttt{While} \quad \max_{\mu \in \Xi_{\text{train}}^{\text{SCM}}} \frac{\alpha_{\text{UB}}(\mu) - \alpha_{\text{LB}}(\mu)}{\alpha_{\text{LB}}(\mu)} > \varepsilon_{\text{SCM}}$$

1. Compute $\alpha(\mu_{\text{SCM}}^{K})$ and $y^*(\mu_{\text{SCM}}^{K})$:
   - Solve generalized eigenvalue problem

     $$\underline{A}^{\mathcal{N}} \underline{v} = \lambda \underline{\mathbb{X}}^{\mathcal{N}} \underline{v}$$

     for $\underline{v}_{\min}$ and $\lambda_{\min}$.
   - Set: $\alpha(\mu_{\text{SCM}}^{K}) = \lambda_{\min}$,

     $$y^{*q}(\mu_{\text{SCM}}^{K}) = \underline{v}_{\min}^{T} \underline{\mathbb{A}}^{\mathcal{N}q} \underline{v}_{\min} / (\underline{v}_{\min}^{T} \underline{\mathbb{X}}^{\mathcal{N}} \underline{v}_{\min}), \quad q = 1, \dots, Q_a.$$

Offline-Online Procedure

2. Calculate $\alpha_{\mathrm{LB}}(\mu)$ and $\alpha_{\mathrm{UB}}(\mu)$ for all $\mu \in \Xi_{\mathrm{train}}^{\mathrm{SCM}}$:
   - Lower Bound: find $\mathcal{P}_M$ and solve LP

$$\alpha_{\mathrm{LB}}(\mu) = \min_{y \in \mathcal{B}} \sum_{q=1}^{Q_a} \Theta_a^q(\mu)\, y^q$$

$$\text{s.t.} \quad \sum_{q=1}^{Q_a} \Theta_a^q(\mu')\, y^q \geq \alpha(\mu'), \quad \forall \mu' \in P_M,$$

   - Upper Bound

$$\alpha_{\mathrm{UB}}(\mu) = \min_{k=1,\ldots,K} \sum_{q=1}^{Q_a} \Theta_a^q(\mu)\, y^{*q}(\mu_{\mathrm{SCM}}^k).$$

Offline-Online Procedure

3. `if` $\min_{\mu \in \Xi_{\mathrm{train}}^{\mathrm{SCM}}} \alpha_{\mathrm{LB}}(\mu) \leq 0$

$$\begin{aligned} \mu^*_{K+1} &= \arg \min_{\mu \in \Xi_{\mathrm{train}}^{\mathrm{SCM}}} \alpha_{\mathrm{LB}}(\mu) \\ C_{K+1} &= C_K \cup \mu^*_{K+1} \\ K &\leftarrow K+1 \end{aligned}$$

`elseif` $\max_{\mu \in \Xi_{\mathrm{train}}^{\mathrm{SCM}}} \frac{\alpha_{\mathrm{UB}}(\mu) - \alpha_{\mathrm{LB}}(\mu)}{\alpha_{\mathrm{LB}}(\mu)} > \varepsilon_{\mathrm{SCM}}$

$$\begin{aligned} \mu^*_{K+1} &= \arg \max_{\mu \in \Xi_{\mathrm{train}}^{\mathrm{SCM}}} \frac{\alpha_{\mathrm{UB}}(\mu) - \alpha_{\mathrm{LB}}(\mu)}{\alpha_{\mathrm{LB}}(\mu)} \\ C_{K+1} &= C_K \cup \mu^*_{K+1} \\ K &\leftarrow K+1 \end{aligned}$$

`else` $K_{\max} = K$.

`end.`

Offline-Online Procedure – Summary

Offline Stage: *once, parameter-independent*

- $2Q + K$ eigenproblems over $X^{\mathcal{N}}$ to form
  - $\mathcal{B}$, i.e., $b_q^-,\ b_q^+,\ q = 1, \ldots, Q_a$;
  - $\alpha(\mu)$, for all $\mu \in \mathcal{C}_K$.
- KQ_a inner products over $X^{\mathcal{N}}$ to form
  - $y^{*q},\ q = 1, \ldots, Q_a$, for all $\mu \in \mathcal{C}_K$.
- $n_{\mathrm{train}}^{\mathrm{SCM}} K$ LPs of size Q_a with $2Q_a + M$ inequality constraints to choose the "next" $\mu_{\mathrm{SCM}} \in \mathcal{C}_K$.

$\Rightarrow$ Cost depends on $\mathcal{N}$, but no "cross-term" $O(n_{\mathrm{train}}^{\mathrm{SCM}} \mathcal{N})$.

Offline-Online Procedure – Summary

Online Stage: given $\mu \in \mathcal{D}$ many times

- sort K points in $\mathcal{C}_K$ to determine $\mathcal{P}_M$ $O(MK)$
- $(M+1)K$ evaluations $\mu' \to \Theta_a^q(\mu')$ $O((K+1)Q_a)$
- perform M *look-ups* $\mu' \to \alpha(\mu')$
- solve LP

$$\alpha_{\mathrm{LB}}(\mu) \;=\; \min_{y \in \mathcal{B}} \sum_{q=1}^{Q_a} \Theta_a^q(\mu)\, y^q$$

$$\text{s.t.} \quad \sum_{q=1}^{Q_a} \Theta_a^q(\mu')\, y^q \;\geq\; \alpha(\mu'), \quad \forall \mu' \in P_M,$$

$\Rightarrow$ cost is independent of $\mathcal{N}$.

SCM – Parametric Coercivity

If a is also parametrically coercive, i.e.,

$$\Theta_a^q(\mu) > 0, \quad \forall \mu \in \mathcal{D}, \ 1 \le q \le Q_a,$$
$$a^q(v,v) \ge 0, \quad \forall v \in X, \ 1 \le q \le Q_a,$$

we obtain, for any $y \in \mathcal{Y}_{\mathrm{LB}}(\mu; \mathcal{P}_M, M)$,

$$\mathcal{J}^{\mathrm{obj}}(\mu; y) = \sum_{q=1}^{Q_a} \Theta_a^q(\mu)\, y^q \ge \min_{q=1,\ldots,Q_a} \frac{\Theta_a^q(\mu)}{\Theta_a^q(\mu')} \alpha(\mu'),$$

for any $\mu \in \mathcal{D}$, any $\mu' \in \mathcal{P}$. We obtain, for $K \ge 1$,

$$\alpha_{\mathrm{LB}}(\mu) \ge \max_{\mu' \in \mathcal{P}_M} \left(\min_{q=1,\ldots,Q_a} \frac{\Theta_a^q(\mu)}{\Theta_a^q(\mu')} \alpha(\mu') \right).$$

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

SCM – Sharpness of bound

Recall that output effectivity satisfies

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

Furthermore, it follows from

$$\frac{\alpha_{\mathrm{UB}}(\mu) - \alpha_{\mathrm{LB}}(\mu)}{\alpha_{\mathrm{LB}}(\mu)} < \varepsilon_{\mathrm{SCM}}, \quad \forall \mu \in \mathcal{D}.$$

that

$$\frac{\alpha^{\mathcal{N}}(\mu)}{\alpha_{\mathrm{LB}}(\mu)} \leq \frac{1}{1 - \varepsilon_{\mathrm{SCM}}}.$$

Since $\alpha^{\mathrm{e}}(\mu) \leq \alpha^{\mathcal{N}}(\mu)$, we thus have

$$\eta_N^s(\mu) \leq \frac{\alpha^{\mathcal{N}}(\mu)}{\alpha_{\mathrm{LB}}(\mu)} \frac{\gamma^{\mathrm{e}}(\alpha)}{\alpha^{\mathrm{e}}(\mu)} \leq \frac{1}{1 - \varepsilon_{\mathrm{SCM}}} \frac{\gamma^{\mathrm{e}}(\mu)}{\alpha^{\mathrm{e}}(\mu)}.$$

SCM Summary

Remarks:

- SCM does not require parametric coercivity, and can improve upon simple "$\min \Theta$" approach.
- $\Xi_{\text{train}}^{\text{SCM}}$ must be chosen quite large for high P to ensure that $\alpha_{\text{LB}}(\mu)$ is viable (positive) for all $\mu \in \mathcal{D}$.
- High accuracy for $\alpha_{\text{LB}}(\mu)$ not required – increase of ε_{SCM} from ≈ 0 to 0.75 increases output bound effectivities only by a factor of roughly 4.
- Choice of M balances offline vs. online effort
  - M very large economizes offline performance (reduces K) but degrades online performance.
  - M very small increases offline cost (increases K) but improves online response.

SCM Summary

Remarks:

- K may increase exponentially with P (for problems that are not parametrically coercive).
- Extension to non-symmetric forms by considering only symmetric part (analogous to "$\min \Theta$" Approach), i.e., replace $a(w, v; \mu)$ by

$$a_s(w, v; \mu) = \sum_{q=1}^{Q_{a_s}} \Theta_{a_s}^q(\mu)\, a_s^q(w, v), \quad \forall w, v \in X.$$

- We can also treat non-coercive operators, i.e., construct lower bounds for the inf-sup constant $\beta(\mu)$.