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1 Coercivity Lower Bounds

Contents

1.1 Introduction

"Truth" Problem Statement

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

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

$$s(\mu) = f(u(\mu); \mu)$$

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

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

Assumptions:

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

Reduced Basis Sample and Space

Parameter samples:

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

with

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

Lagrangian reduced basis spaces:

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

with

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

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: $X_N = \text{“Gram-Schmidt”}(W_N)$
- $u_N(\mu)$ unique (from coercivity, continuity, linear independence)

Hypotheses

We assume that $a : X \times X \times \mathcal{D} \rightarrow \mathbb{R}$ 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**)

$$((w, v))_\mu = a(w, v; \mu), \quad \forall w, v \in X$$

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

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

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

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

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 1 (Energy Error Bound). *For any $N = 1, \dots, N_{\text{max}}$, the effectivity, $\eta_N^{\text{en}}(\mu)$ satisfies*

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

Coercivity Lower Bound – Goal

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

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

II. $\partial t_{\text{comp}}(\mu \rightarrow \alpha_{\text{LB}}(\mu))$ 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 Θ " Approach
- Multiple Inner Products
- Successive Constraint Method

1.2 The “min Θ ” Approach

The “min Θ ” Approach

Lemma 2. *For a parametrically coercive, we have*

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

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

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

Recall X -inner product and 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 Θ ” Approach

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

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 Θ ” Approach

If \mathbf{a} is **parametrically coercive**, we may choose as a lower bound for the coercivity constant

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

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 \mathbf{a} .

The “min Θ ” Approach – non-symmetric forms

For \mathbf{a} parametrically coercive **but non-symmetric** we obtain

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

where the symmetric part is given by

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

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

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

and

$$a_s^q(v, v) \geq 0, \quad \forall v \in X, \quad 1 \leq q \leq Q_{a_s}.$$

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

1.3 Multiple Inner Products

Multiple Inner Products – Motivation

Upper bound for effectivity (\mathbf{a} parametrically coercive & symmetric)

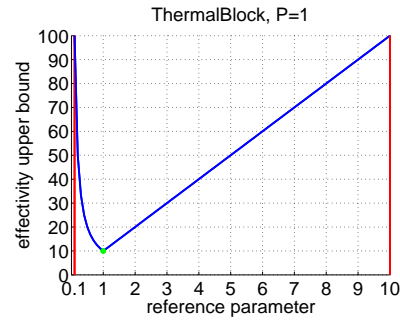
$$1 \leq \eta_N^s(\mu) \leq \frac{\gamma_{\text{UB}}(\mu)}{\alpha_{\text{LB}}(\mu)} = \frac{\Theta_a^{\text{max}, \bar{\mu}}(\mu)}{\Theta_a^{\text{min}, \bar{\mu}}(\mu)} = \theta^{\bar{\mu}}(\mu)$$

ThermalBlock: $P = 1$

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

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

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

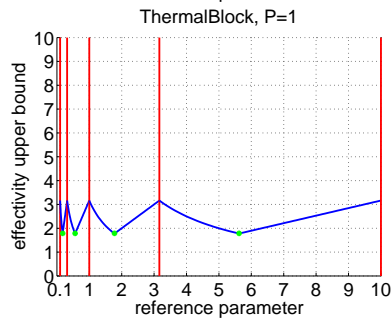
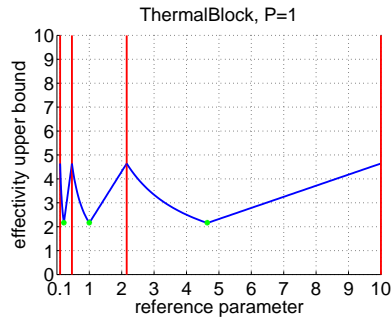
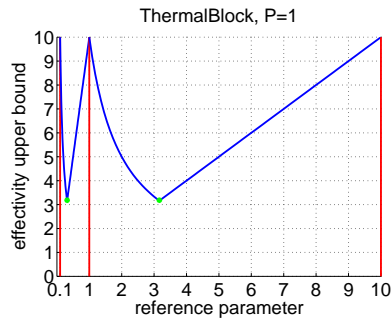


Multiple Inner Products – Motivation

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

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

- $\bar{K} = 2$ $\theta^{\bar{\mu}_{\text{opt}}}(\mu_1) \lesssim 3.2$
- $\bar{K} = 3$ $\theta^{\bar{\mu}_{\text{opt}}}(\mu_1) \lesssim 2.2$
- $\bar{K} = 4$ $\theta^{\bar{\mu}_{\text{opt}}}(\mu_1) \lesssim 1.8$



Multiple Inner Products

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

- associated inner product

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

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

$$\Delta_{N,k}^s(\boldsymbol{\mu}) \equiv \frac{\|\hat{e}_k(\boldsymbol{\mu})\|_{X,k}^2}{\alpha_{\text{LB},k}(\boldsymbol{\mu})}, \quad 1 \leq k \leq \bar{K}$$

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

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

and

$$\alpha_{\text{LB},k}(\boldsymbol{\mu}) \equiv \Theta_a^{\min, \bar{\mu}^k}(\boldsymbol{\mu}).$$

Multiple Inner Products

We can then introduce the effectivities

$$\eta_{N,k}^s(\boldsymbol{\mu}) \equiv \frac{\Delta_{N,k}^s(\boldsymbol{\mu})}{s(\boldsymbol{\mu}) - s_N(\boldsymbol{\mu})}, \quad 1 \leq k \leq \bar{K},$$

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

$$1 \leq \eta_{N,k}^s(\boldsymbol{\mu}) \leq \theta^{\bar{\mu}^k}(\boldsymbol{\mu}), \quad \forall \boldsymbol{\mu} \in \mathcal{D}.$$

We finally define the error bound

$$\Delta_N^s(\boldsymbol{\mu}) = \Delta_{N,k^*}^s(\boldsymbol{\mu})$$

where $k^* : \mathcal{D} \rightarrow \{1, \dots, \bar{K}\}$ is an appropriate indicator function.

Multiple Inner Products

Indicator strategy k^* :

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

$$k^*(\boldsymbol{\mu}) = \arg \min_{k \in \{1, \dots, \bar{K}\}} |\boldsymbol{\mu} - \bar{\boldsymbol{\mu}}^k|,$$

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

- (O2) Minimum effectivity upper bound

$$k^*(\boldsymbol{\mu}) = \arg \min_{k \in \{1, \dots, \bar{K}\}} \theta^{\bar{\mu}^k}(\boldsymbol{\mu}).$$

- (O1) Smallest (hence sharpest) error bound

$$k^*(\boldsymbol{\mu}) = \arg \min_{k \in \{1, \dots, \bar{K}\}} \Delta_{N,k}^s(\boldsymbol{\mu}).$$

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

ThermalBlock: $P = 1$

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

Single inner product: $\bar{\mu}_1 = 1 \Rightarrow \eta_{N,\max}^s = \sqrt{\mu_r}$.

We introduce a grid $G_{[\mu_1^{\min}, \mu_1^{\max}; \bar{K}+1]}^{\text{In}} = [z_1, \dots, z_{\bar{K}+1}]$ and set

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

We then obtain

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

and

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

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

It follows that, for (O2), we obtain

$$\eta_{N, \max}^s \leq (\sqrt{\mu_r})^{\frac{1}{\bar{K}}} \left(= e^{\frac{1}{2\bar{K}} \ln \mu_r} \right).$$

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

$$\eta_{N, \max}^s \leq \sqrt{\mu_r} \quad \text{for } G_{[\mu_1^{\min}, \mu_1^{\max}; 2]}^{\ln} = [\mu_1^{\min}, \mu_1^{\max}],$$

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

Furthermore:

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

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

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

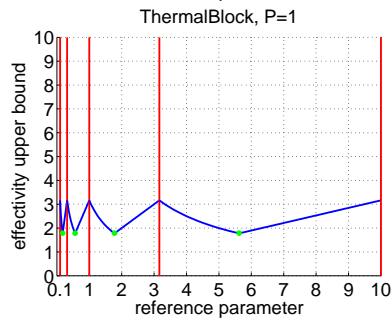
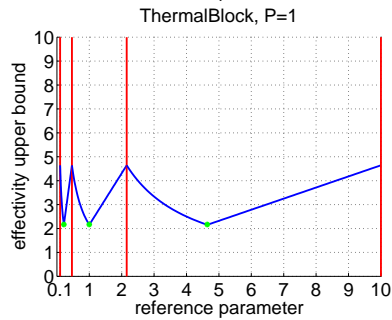
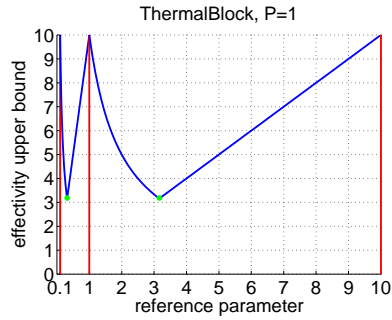
Grid: $G_{[\mu_1^{\min}, \mu_1^{\max}; \bar{K}+1]}^{\ln} = [z_1, \dots, z_{\bar{K}+1}]$

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

$$1 \leq k \leq \bar{K}.$$

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

- $\bar{K} = 2$ $\theta^{\bar{\mu}^{\text{opt}}}(\mu_1) \lesssim 3.2$
- $\bar{K} = 3$ $\theta^{\bar{\mu}^{\text{opt}}}(\mu_1) \lesssim 2.2$
- $\bar{K} = 4$ $\theta^{\bar{\mu}^{\text{opt}}}(\mu_1) \lesssim 1.8$



Multiple Inner Products – Summary

Remarks

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

- to achieve $\eta_{\mathcal{N}, \max}^s \leq 10$ for $P > 1$ (ThermalBlock) we require roughly $\bar{K} = \lceil \ln \mu_r / \ln 10 \rceil_+^P$ inner products.

1.4 Successive Constraint Method

Successive Constraint Method

The “**min Θ** ” 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 $\mathcal{J}^{\text{obj}} : \mathcal{D} \times \mathbb{R}^{Q_a} \rightarrow \mathbb{R}$ given by

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

We can then write

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

where

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

Note:

- $\mathbf{y} = (\mathbf{y}^1, \dots, \mathbf{y}^{Q_a}) \in \mathbb{R}^{Q_a}$ 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}_{LB} to \mathcal{Y} such that

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

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

very efficiently.

We can then define

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

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

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

We first define

$$b_q^- \equiv \inf_{v \in X} \frac{a^q(v, v)}{\|v\|_X^2}, \quad 1 \leq q \leq Q_a,$$

$$b_q^+ \equiv \sup_{v \in X} \frac{a^q(v, v)}{\|v\|_X^2}, \quad 1 \leq q \leq Q_a,$$

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

$\forall \mathbf{w}_y \in X$

$$\inf_{v \in X} \frac{a^q(v, v)}{\|v\|_X^2} \leq \underbrace{\frac{a^q(\mathbf{w}_y, \mathbf{w}_y)}{\|\mathbf{w}_y\|_X^2}}_{y_q} \leq \sup_{v \in X} \frac{a^q(v, v)}{\|v\|_X^2}.$$

Lower Bound: \mathcal{Y}_{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

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

Proposition 3. For given $\mathcal{P}_M \subset \mathcal{D}$, $M \in \mathbb{N}_+$,

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

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

We may now define the coercivity lower bound

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

Proposition 4. For given $\mathcal{P}_M \subset \mathcal{D}$, $M \in \mathbb{N}_+$,

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

Proof: ...

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

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

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

Upper Bound

Two questions remain:

- I. How do we choose \mathcal{P}_M ?
- II. How do we know that $\alpha_{\text{LB}}(\mu)$ is accurate?

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

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

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

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

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

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

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

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

very efficiently.

We can then define

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

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

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

We introduce a set of K parameter values

$$\mathcal{C}_K \equiv \{\boldsymbol{\mu}_{\text{SCM}}^1 \in \mathcal{D}, \dots, \boldsymbol{\mu}_{\text{SCM}}^K \in \mathcal{D}\}$$

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

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

We may now define

$$\mathcal{Y}_{\text{UB}}(\boldsymbol{\mu}; \mathcal{C}_K, K) \equiv \{\mathbf{y}^*(\boldsymbol{\mu}) \mid \boldsymbol{\mu} \in \mathcal{C}_K\}.$$

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

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

We may now define the coercivity upper bound

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

Proposition 5. For given $\mathcal{C}_K \subset \mathcal{D}$, $K \in \mathbb{N}_+$,

$$\alpha_{\text{UB}}(\boldsymbol{\mu}) \leq \alpha(\boldsymbol{\mu}), \quad \forall \boldsymbol{\mu} \in \mathcal{D}.$$

Proof: ...

Note:

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

Computation of $\mathbf{y}^*(\boldsymbol{\mu})$

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

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

such that

$$\alpha(\boldsymbol{\mu}) = \frac{\mathbf{a}(\mathbf{v}^*(\boldsymbol{\mu}), \mathbf{v}^*(\boldsymbol{\mu}); \boldsymbol{\mu})}{\|\mathbf{v}^*(\boldsymbol{\mu})\|_{\mathcal{X}}^2}$$

then the components of $\mathbf{y}^*(\boldsymbol{\mu})$ are given by

$$\mathbf{y}^{*q}(\boldsymbol{\mu}) = \frac{\mathbf{a}^q(\mathbf{v}^*(\boldsymbol{\mu}), \mathbf{v}^*(\boldsymbol{\mu}); \boldsymbol{\mu})}{\|\mathbf{v}^*(\boldsymbol{\mu})\|_{\mathcal{X}}^2},$$

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

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 $\alpha(\boldsymbol{\mu}')$ for all $\boldsymbol{\mu}' \in \mathcal{P}_M$ to obtain \mathcal{Y}_{LB} , where

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

- But from computation of $\mathbf{y}^*(\boldsymbol{\mu})$ for all $\boldsymbol{\mu} \in \mathcal{C}_K$ we essentially already know the $\alpha(\boldsymbol{\mu})$ for all $\boldsymbol{\mu} \in \mathcal{C}_K$, where

$$\mathcal{C}_K \equiv \{\boldsymbol{\mu}_{\text{SCM}}^1 \in \mathcal{D}, \dots, \boldsymbol{\mu}_{\text{SCM}}^K \in \mathcal{D}\}.$$

- We thus choose

$$\begin{aligned} \mathcal{P}_M &= \{M \text{ points in } \mathcal{C}_K \text{ closest to } \boldsymbol{\mu}\}, \\ \text{or } \mathcal{P}_M &= \mathcal{C}_K \text{ if } M \geq K, \end{aligned}$$

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;
- $\Xi_{\text{train}}^{\text{SCM}}$: training sample.

II. Compute b_q^\pm , $1 \leq q \leq Q_a$:

- Solve $2Q$ generalized eigenvalue problems

$$\underline{\mathbb{A}}^{\mathcal{N}^q} \underline{\mathbf{v}} = \lambda \underline{\mathbb{X}}^{\mathcal{N}} \underline{\mathbf{v}}, \quad q = 1, \dots, Q_a.$$

- Set $b_q^- = \lambda_{\min}$, $b_q^+ = \lambda_{\max}$.

III. Set $K = 1$, and choose $C_1 = \{\mu_{\text{SCM}}^1\}$ arbitrarily.

Offline-Online Procedure

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

1. Compute $\alpha(\mu_{\text{SCM}}^K)$ and $y^*(\mu_{\text{SCM}}^K)$:

- Solve generalized eigenvalue problem

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

for $\underline{\mathbf{v}}_{\min}$ and λ_{\min} .

- Set: $\alpha(\mu_{\text{SCM}}^K) = \lambda_{\min}$,

$$y^{*q}(\mu_{\text{SCM}}^K) = \underline{\mathbf{v}}_{\min}^T \underline{\mathbf{A}}^{\mathcal{N}q} \underline{\mathbf{v}}_{\min} / (\underline{\mathbf{v}}_{\min}^T \underline{\mathbf{X}}^{\mathcal{N}q} \underline{\mathbf{v}}_{\min}),$$

$q = 1, \dots, Q_a$.

Offline-Online Procedure

2. Calculate $\alpha_{\text{LB}}(\mu)$ and $\alpha_{\text{UB}}(\mu)$ for all $\mu \in \Xi_{\text{train}}^{\text{SCM}}$:

- Lower Bound: find \mathcal{P}_M and solve LP

$$\begin{aligned} \alpha_{\text{LB}}(\mu) &= \min_{y \in \mathcal{B}} \sum_{q=1}^{Q_a} \Theta_a^q(\mu) y^q \\ \text{s.t. } \sum_{q=1}^{Q_a} \Theta_a^q(\mu') y^q &\geq \alpha(\mu'), \quad \forall \mu' \in P_M, \end{aligned}$$

- Upper Bound

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

Offline-Online Procedure

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

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

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

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

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

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^+ , $q = 1, \dots, Q_a$;
 - $\alpha(\mu)$, for all $\mu \in \mathcal{C}_K$.
 - KQ_a inner products over $X^{\mathcal{N}}$ to form
 - y^{*q} , $q = 1, \dots, Q_a$, for all $\mu \in \mathcal{C}_K$.
 - $n_{\text{train}}^{\text{SCM}}K$ LPs of size Q_a with $2Q_a + M$ inequality constraints to choose the “next” $\mu_{\text{SCM}} \in \mathcal{C}_K$.
- \Rightarrow Cost depends on \mathcal{N} , but no “cross-term” $O(n_{\text{train}}^{\text{SCM}}\mathcal{N})$.

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 $\mu' \rightarrow \Theta_a^q(\mu')$ $O((K + 1)Q_a)$
- perform M look-ups $\mu' \rightarrow \alpha(\mu')$
- solve LP

$$\begin{aligned}
\alpha_{\text{LB}}(\mu) &= \min_{y \in \mathcal{B}} \sum_{q=1}^{Q_a} \Theta_a^q(\mu) y^q \\
\text{s.t. } \sum_{q=1}^{Q_a} \Theta_a^q(\mu') y^q &\geq \alpha(\mu'), \quad \forall \mu' \in \mathcal{P}_M,
\end{aligned}$$

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

SCM – Parametric Coercivity

If \mathbf{a} is also parametrically coercive, i.e.,

$$\Theta_a^q(\boldsymbol{\mu}) > \mathbf{0}, \quad \forall \boldsymbol{\mu} \in \mathcal{D}, \quad 1 \leq q \leq Q_a,$$

$$\mathbf{a}^q(\mathbf{v}, \mathbf{v}) \geq \mathbf{0}, \quad \forall \mathbf{v} \in \mathbf{X}, \quad 1 \leq q \leq Q_a,$$

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

$$\mathcal{J}^{\text{obj}}(\boldsymbol{\mu}; \mathbf{y}) = \sum_{q=1}^{Q_a} \Theta_a^q(\boldsymbol{\mu}) \mathbf{y}^q \geq \min_{q=1, \dots, Q_a} \frac{\Theta_a^q(\boldsymbol{\mu})}{\Theta_a^q(\boldsymbol{\mu}')} \alpha(\boldsymbol{\mu}'),$$

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

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

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

SCM – Sharpness of bound

Recall that output effectivity satisfies

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

Furthermore, it follows from

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

that

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

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

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

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 \mathbf{P} to ensure that $\alpha_{\text{LB}}(\boldsymbol{\mu})$ is viable (positive) for all $\boldsymbol{\mu} \in \mathcal{D}$.
- High accuracy for $\alpha_{\text{LB}}(\boldsymbol{\mu})$ not required – increase of ε_{SCM} from $\approx \mathbf{0}$ to **0.75** increases output bound effectivities only by a factor of roughly **4**.
- Choice of \mathbf{M} balances offline vs. online effort
 - \mathbf{M} very large economizes offline performance (reduces \mathbf{K}) but degrades online performance.
 - \mathbf{M} very small increases offline cost (increases \mathbf{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** Θ ” Approach), i.e., replace $\mathbf{a}(\mathbf{w}, \mathbf{v}; \boldsymbol{\mu})$ by

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

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