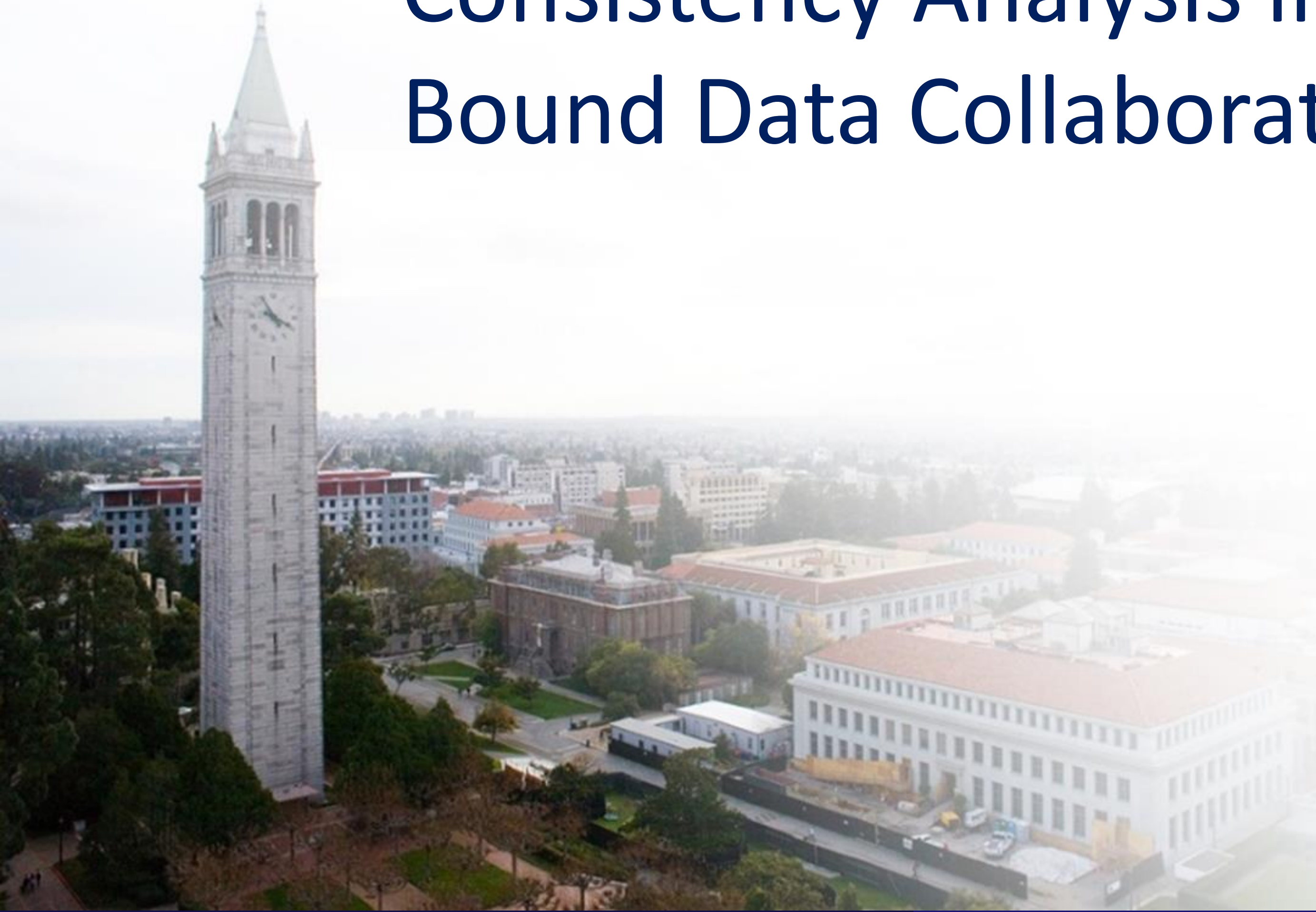
Consistency Analysis in Bound-to-Bound Data Collaboration



Arun Hegde
(PhD candidate,
UC Berkeley)

About Me

- Academic Background
  - 2014 – Present:
    - PhD **Mechanical Engineering** – UC Berkeley
    - Major: **Controls**
    - Minors: **Optimization**, **Mathematics**
    - Advisors: Andy Packard (Controls), Michael Frenklach (Combustion)
  - 2009-2013:
    - B.S. Mechanical Engineering / Applied Math – UConn
- Research Background
  - *uncertainty quantification*, *optimization* (“keywords”)

Overview:

- Bound-to-Bound Data Collaboration
  - notation: parameters, models, data ➔ dataset, feasible set
  - toy example: 2-parameter reaction system
- Dataset Consistency – agreement between models and data
  - scalar consistency measure – **is there agreement?**
  - **vector consistency measure – resolve conflict between models and data**
- Dataset examples
  - GRI-Mech 3.0
  - DLR-SynG
- “The Big Picture”
- Summary

What is Bound-to-Bound Data Collaboration?

- Deterministic, optimization-based approach to UQ.

Uncertainties modeled as **sets**, **bounded regions**, **intervals**, etc.

Inference and prediction addressed through **constrained optimization** (min/max s.t. uncertainty).

- General problem setup:
  - A physical model is being compared to **experimental data**
  - Uncertainty in experimental data
  - Model uncertainty primarily rests in the **model parameters**
  - Prior knowledge on parameters is available

Components of B2BDC:

Model parameters

$$x \in \mathbb{R}^n$$

Prior knowledge

$$x \in \mathcal{H} \subseteq \mathbb{R}^n$$

Prediction model P

$$f_P(x)$$

Observables / QOIs

$$e = 1, \ldots, N$$

Models

$$f_e : \mathbb{R}^n \to \mathbb{R}$$

Measurements

$$L_e \leq y_e \leq U_e$$

Constraints on x

$$L_e \leq f_e(x) \leq U_e \quad \forall e$$

$$\min_x \; f_P(x) \quad \text{s.t.} \; x \in \mathcal{H}, \quad L_e \leq f_e(x) \leq U_e \quad \forall e$$

$$\max_x \; f_P(x) \quad \text{s.t.} \; x \in \mathcal{H}, \quad L_e \leq f_e(x) \leq U_e \quad \forall e$$

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What are the "models"?

Input: x

Output: response $r(t)$

QOIs

$$f_1(x) = \max_t \ r(t)$$

$$f_2(x) = r(t)|_{t=0.5}$$

$$\vdots$$

Components of B2BDC: surrogate models

Model parameters

$$x \in \mathbb{R}^n$$

Prior knowledge

$$x \in \mathcal{H} \subseteq \mathbb{R}^n$$

Prediction model P

$$M_P(x) \approx f_P(x)$$

Observables / QOIs

$$e = 1, \ldots, N$$

Models

$$f_e : \mathbb{R}^n \to \mathbb{R}$$

Measurements

$$L_e \le y_e \le U_e$$

Constraints on x

$$L_e \le f_e(x) \le U_e \quad \forall e$$

Surrogate models

$$M_e(x) \approx f_e(x)$$

Error estimate

$$|M_e(x) - f_e(x)| \le \epsilon_e$$

Dataset

$$\boxed{\begin{gathered} x \in \mathcal{H} \subseteq \mathbb{R}^n \\ L_e - \epsilon_e \le M_e(x) \le U_e + \epsilon_e \\ \text{for } e = 1, \ldots, N \end{gathered}}$$

Feasible Set

$$\boxed{\mathcal{F} \subseteq \mathcal{H}}$$

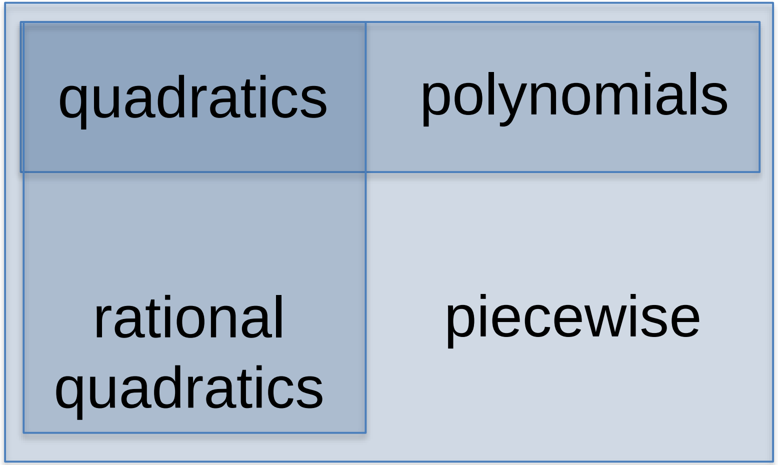
$$\min_x \; M_P(x) \quad \text{s.t.} \quad x \in \mathcal{F}$$

$$\max_x \; M_P(x) \quad \text{s.t.} \quad x \in \mathcal{F}$$

Surrogate models in B2BDC

Desirable properties for the surrogate models:

- Built using samples from $\mathcal{H}$ and evaluations of f
- Leads to **tractable B2BDC inference and prediction** (prefer global results)



Convex relaxations of inference and prediction can be cast as semidefinite programs ➔ global results

Notable features of semidefinite programming

- Generalizes linear programming
- Very active research (sparsity, structure, first order methods, etc.)
- Open source, free/commercial software, parsers
  - SeDuMi, CVX, MOSEK, CDCS, etc.…

Surrogate models in B2BDC

Desirable properties for the surrogate models:
- Built using samples from $\mathcal{H}$ and evaluations of f
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quadratics

polynomials

rational quadratics

piecewise

Convex relaxations of inference and prediction can be cast as semidefinite programs ➔ global results

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- Generalizes linear programming
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Example: 2-parameter reaction

Setup:

$$\frac{da}{dt} = -k_1 a(t)$$
$$\frac{db}{dt} = k_1 a(t) - k_2 b(t)$$
$$\frac{dc}{dt} = k_2 b(t)$$

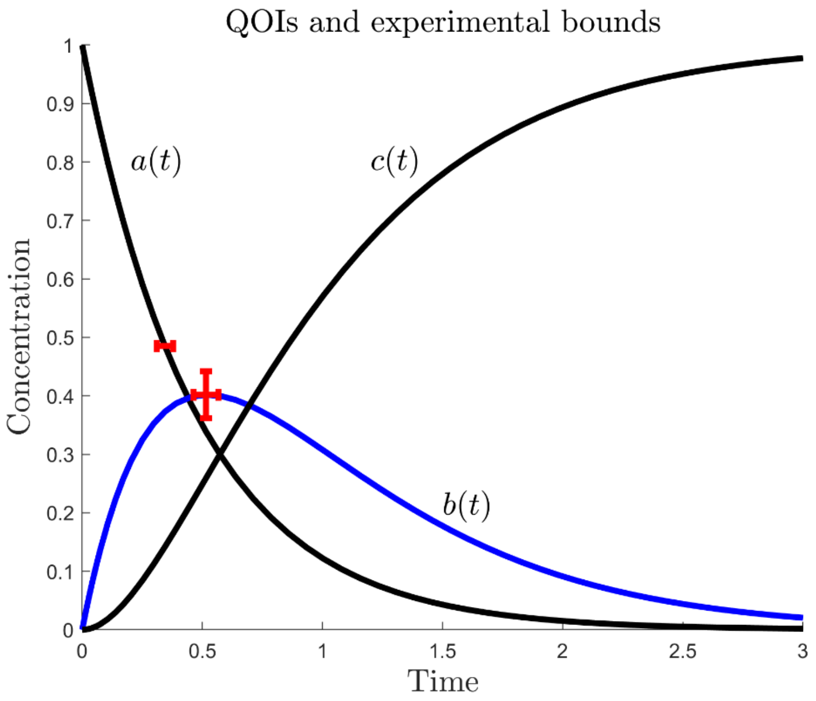
$a(0) = 1$
$b(0) = 0$
$c(0) = 0$

Prior uncertainty

$k_1 \in [1, 4]$
$k_2 \in [0.5, 2]$

3 QOIs

Peak response and time of $b(t)$
Half time of $a(t)$



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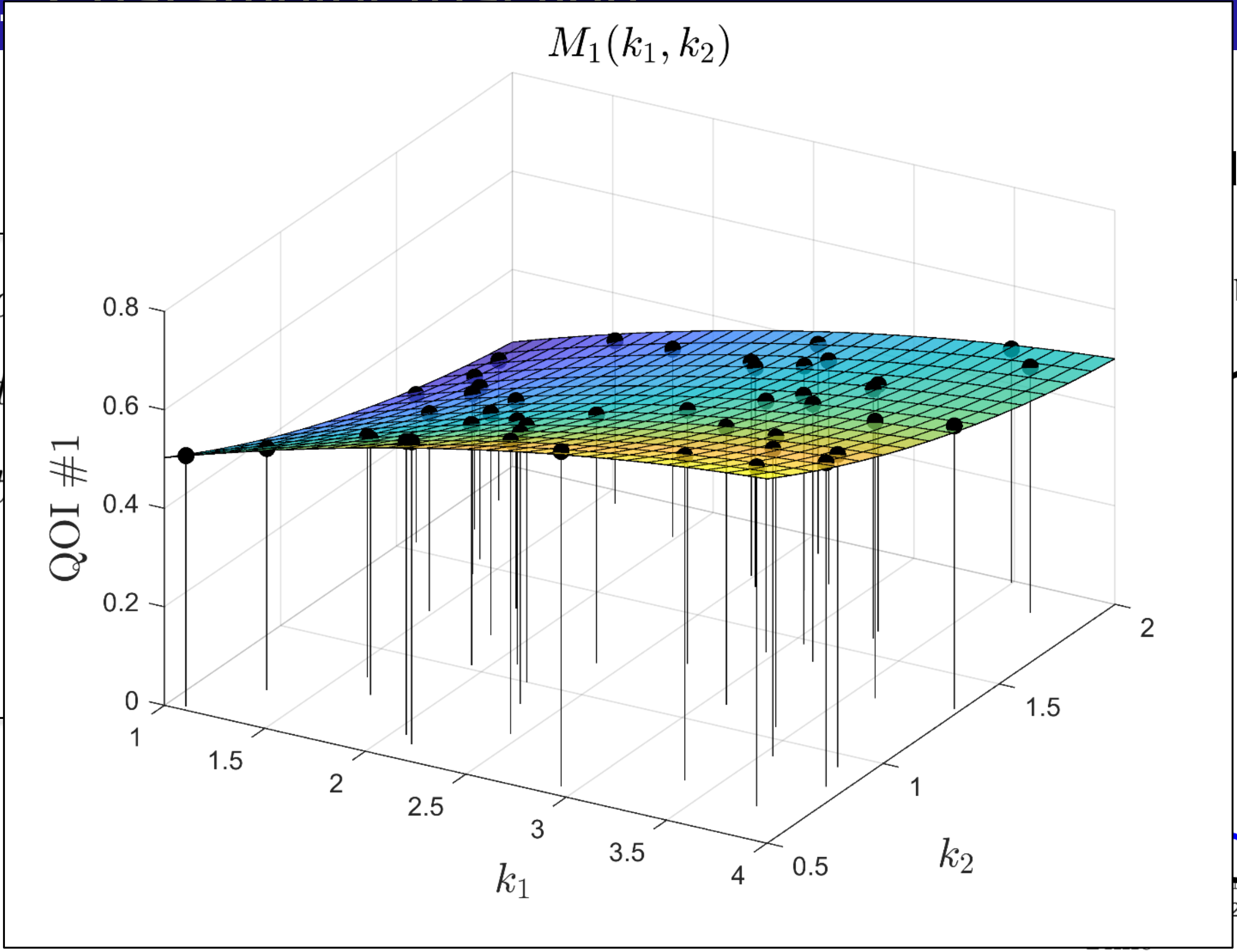

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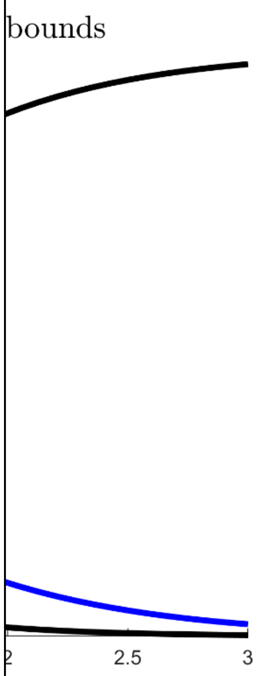

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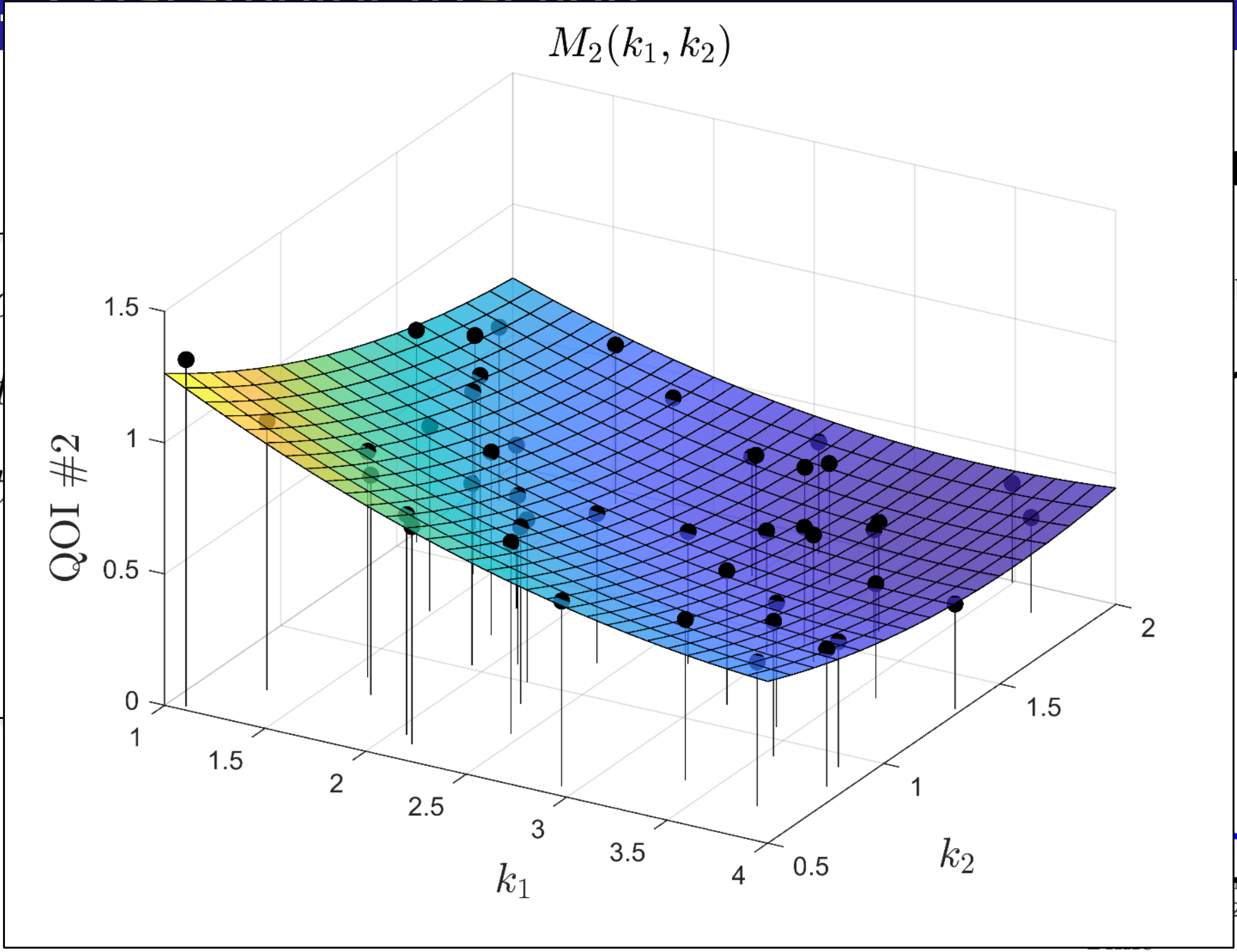
bounds



Example: 2 parameter reaction

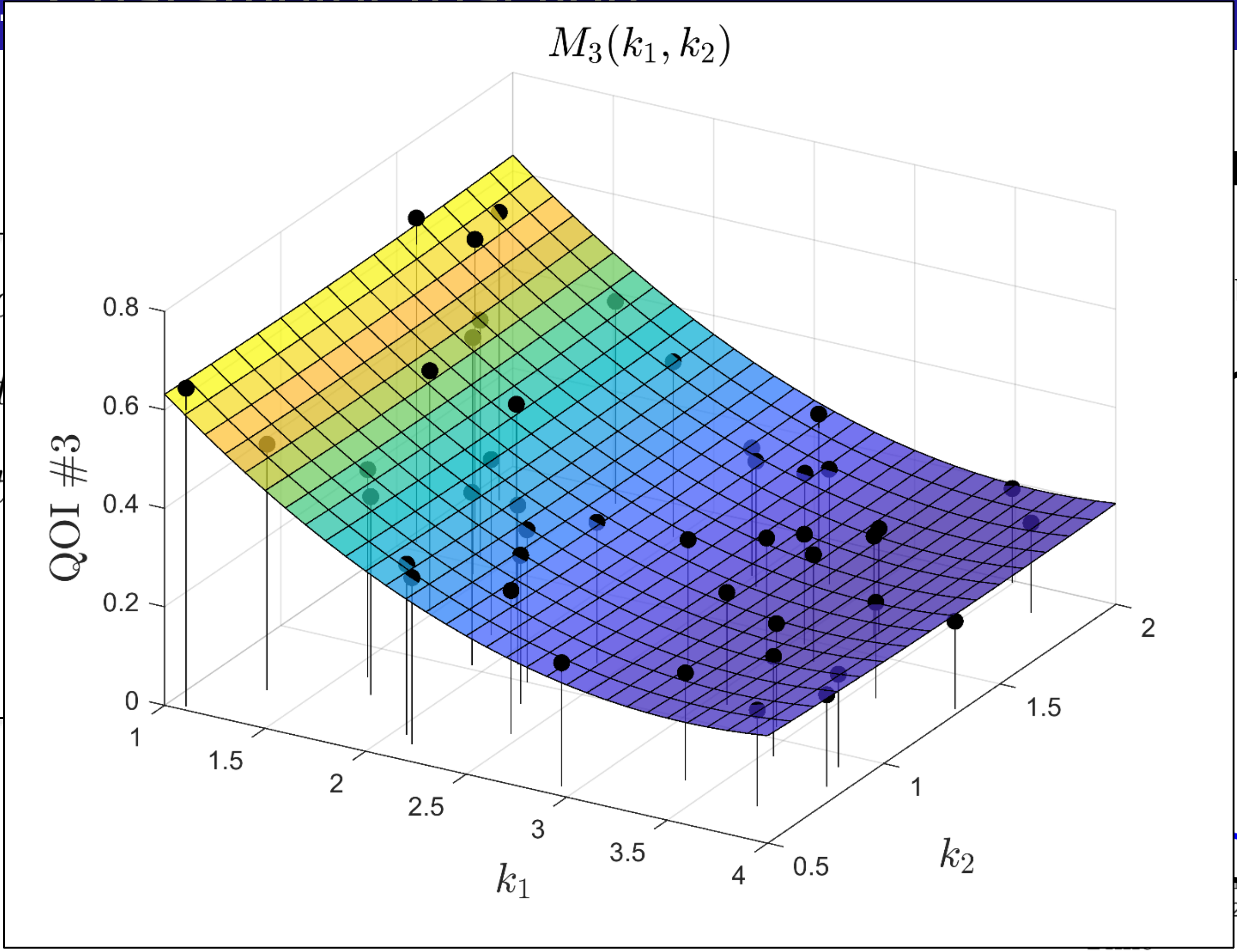
Setup:

$$\frac{da}{dt} = -k_1 \ldots$$
$$\frac{db}{dt} = k_1 a(\ldots$$
$$\frac{dc}{dt} = k_2 b(\ldots$$

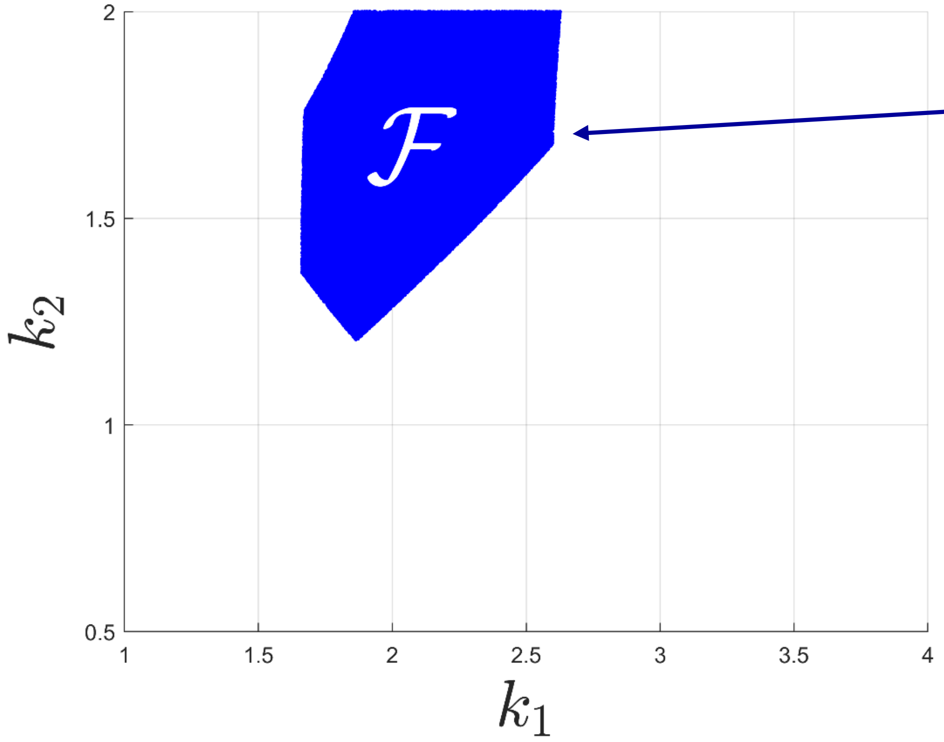
$a(0) = 1$
$b(0) = 0$
$c(0) = 0$

... time of $b(t)$

bounds



Example: feasible set

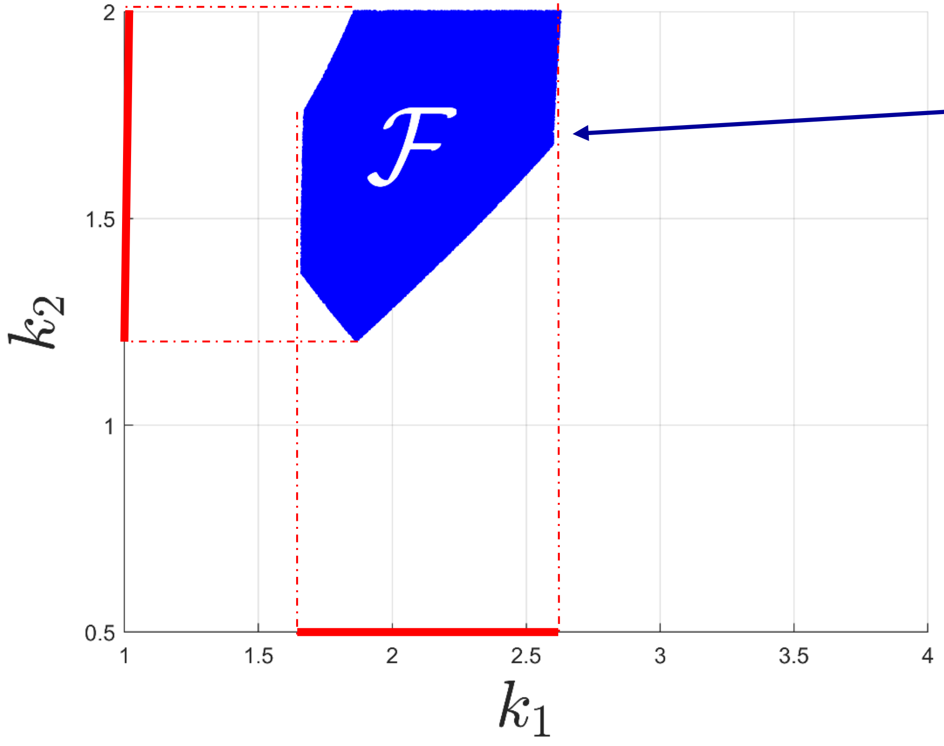


$$\begin{gathered} L_1 \leq M_1(k_1, k_2) \leq U_1 \\ L_2 \leq M_2(k_1, k_2) \leq U_2 \\ L_3 \leq M_3(k_1, k_2) \leq U_3 \\ (k_1, k_2) \in \mathcal{H} \end{gathered}$$

What inferences might we be interesting in?

Axes display prior range

Example: feasible set



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What inferences might we be interesting in?

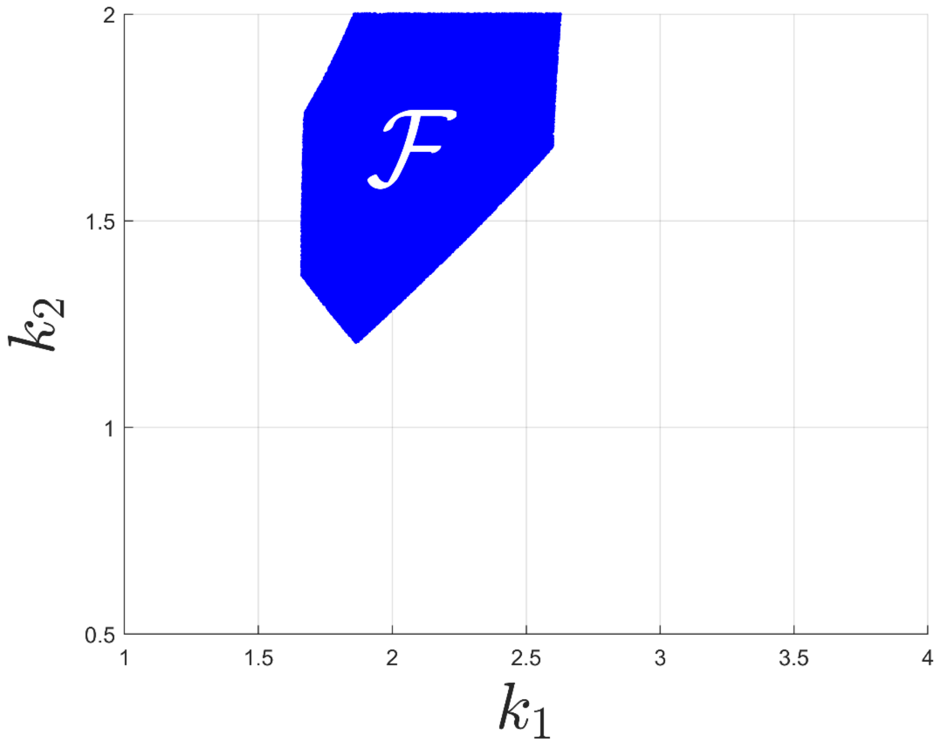
$$\left[\min_{(k_1,k_2)\in\mathcal{F}} k_1, \quad \max_{(k_1,k_2)\in\mathcal{F}} k_1 \right]$$

"posterior bounds"

Axes display prior range

Example: prediction

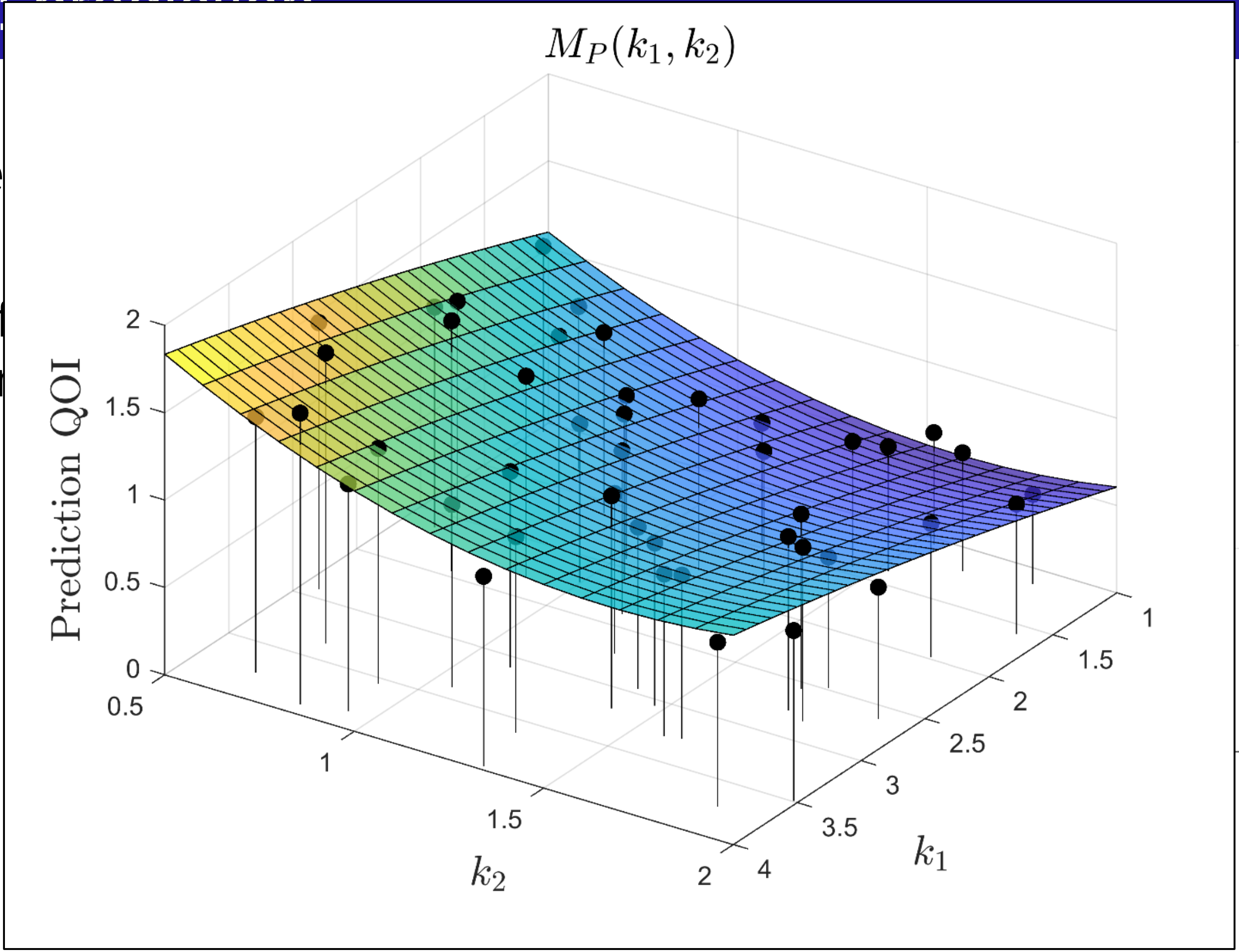
- Suppose we were interested in the prediction of an unmeasured property:
  - **ratio** of $c(t)$ to $a(t)$ @ the peak time of $b(t)$

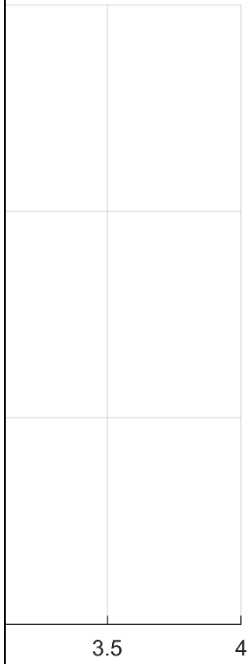


Axes display prior range

Example: prediction

- Suppose
  in the pre
  unmeasu
  - **ratio** of
    peak ti

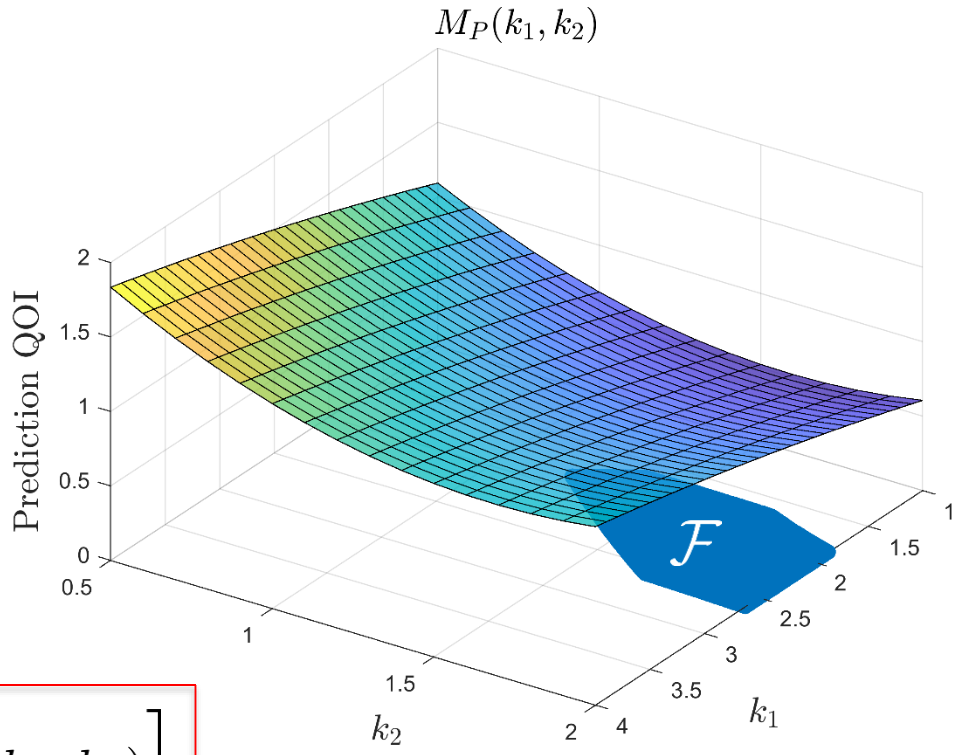




Example: prediction

- Suppose we were interested in the prediction of an unmeasured property:
  - **ratio** of $c(t)$ to $a(t)$ @ the peak time of $b(t)$

$$\left[\min_{(k_1,k_2)\in\mathcal{F}} M_P(k_1,k_2),\quad \max_{(k_1,k_2)\in\mathcal{F}} M_P(k_1,k_2)\right]$$



Axes display prior range

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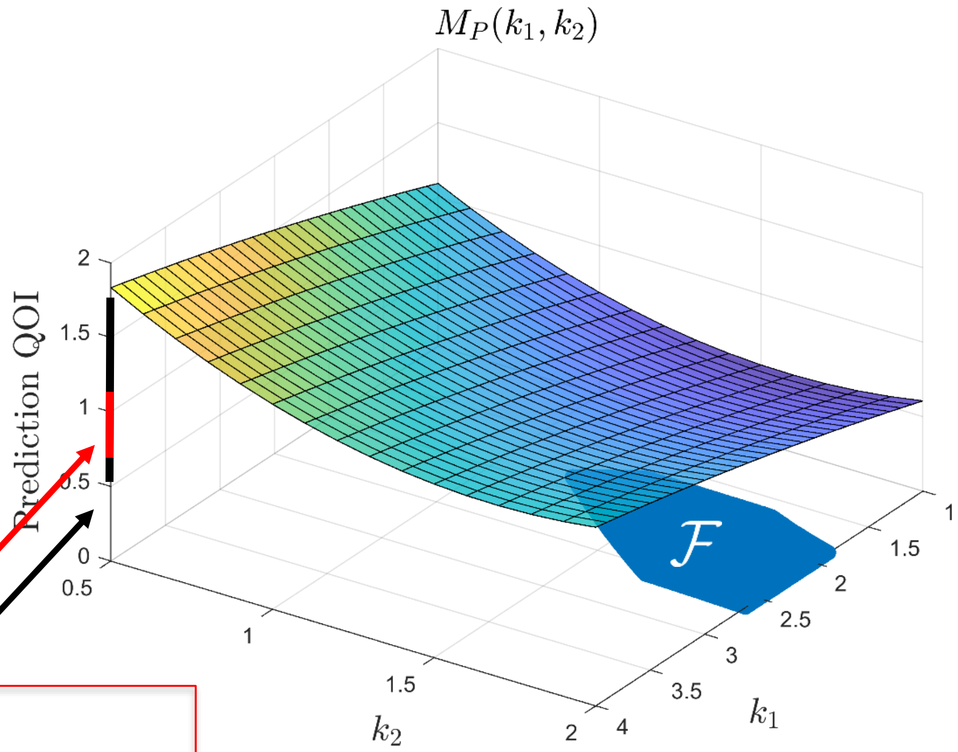

Prediction over $\mathcal{F}$: $[0.68,\ 1.1]$

Prediction over $\mathcal{H}$: $[0.52,\ 1.8]$

Axes display prior range

Computational strategy (e.g. for prediction)

$$p := \min_{x \in \mathcal{F}} \; M_P(x)$$

challenging,
nonconvex
optimization

$$r := \max_{x \in \mathcal{F}} \; M_P(x)$$

challenging,
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Computational strategy (e.g. for prediction)

Computable bounds, easily verified as valid

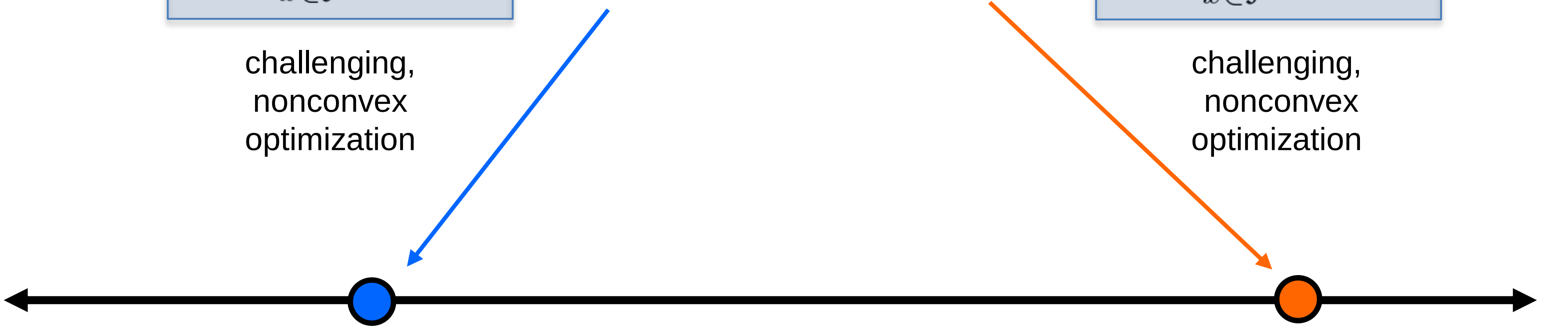
$$p := \min_{x \in \mathcal{F}} M_P(x) \leq p^U$$

challenging, nonconvex optimization

Computable bounds, easily verified as valid

$$r^L \leq r := \max_{x \in \mathcal{F}} M_P(x)$$

challenging, nonconvex optimization



Computational strategy (e.g. for prediction)

Computable bounds, **easily verified as valid**

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challenging, nonconvex optimization

Computable bounds, **easily verified as valid**

$$r^L \leq r := \max_{x \in \mathcal{F}} M_P(x)$$

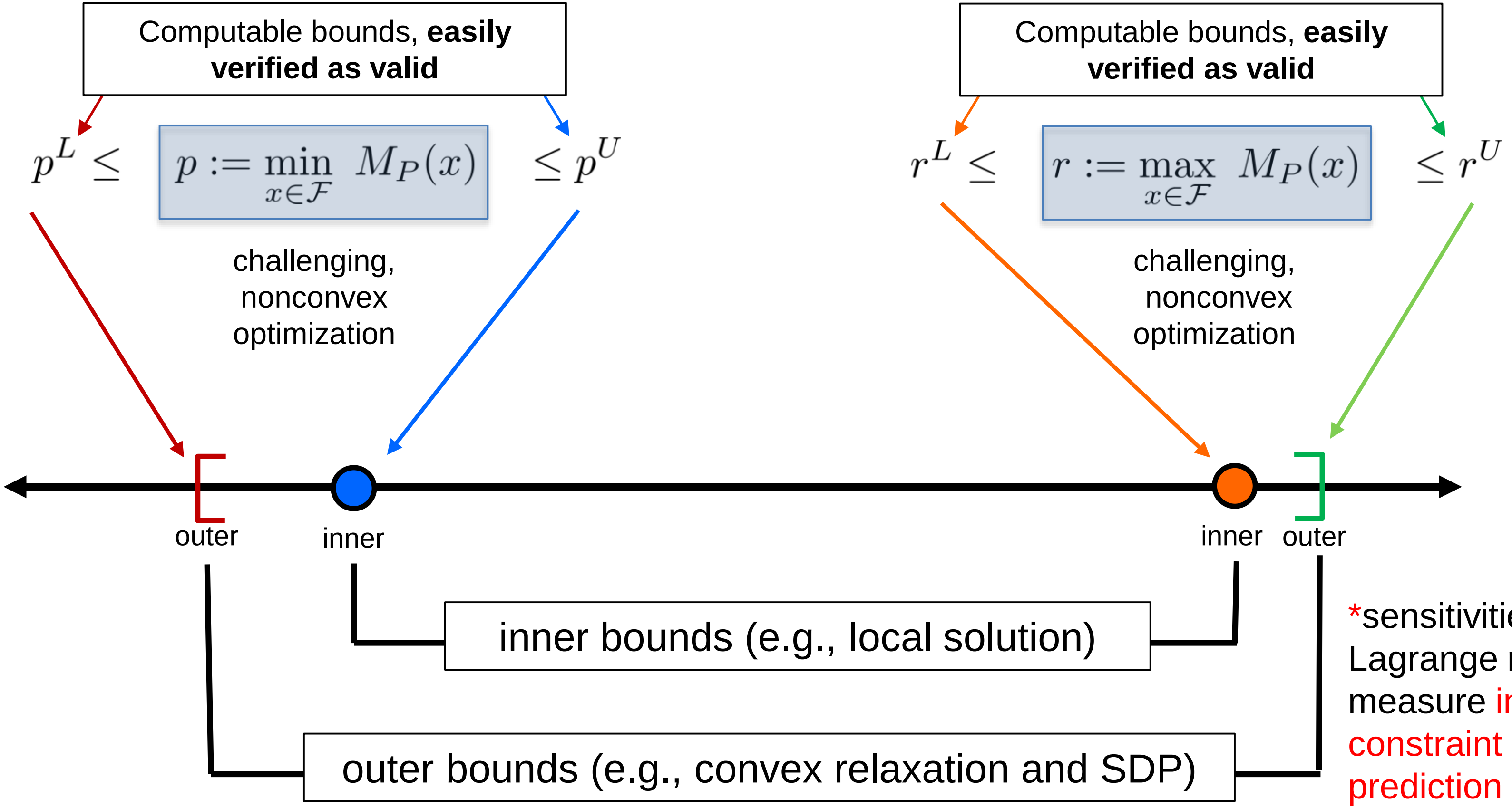
challenging, nonconvex optimization

inner

inner

inner bounds (e.g., local solution)

Computational strategy (e.g. for prediction)



*sensitivities / Lagrange multipliers measure influence of constraint bounds on prediction bounds

Computational strategy – convex relaxation

$p^L \Rightarrow$ <u>NQCQP:</u>

$$\boxed{\begin{aligned} \min_{x\in\mathbb{R}^n} \quad & \begin{bmatrix}1\\x\end{bmatrix}^{\mathsf{T}} Q_0 \begin{bmatrix}1\\x\end{bmatrix} \\ \text{s.t.} \quad & \begin{bmatrix}1\\x\end{bmatrix}^{\mathsf{T}} Q_i \begin{bmatrix}1\\x\end{bmatrix} \leq 0 \\ & \text{for } i = 1, \ldots, m \end{aligned}}$$

General form of the optimization <u>(**inference** and **prediction**)</u> for **quadratic** surrogate models

NQCQP:

$$\min_{x\in\mathbb{R}^n} \operatorname{Tr}\left(Q_0 \begin{bmatrix}1\\x\end{bmatrix}\begin{bmatrix}1\\x\end{bmatrix}^\intercal\right)$$

$$\text{s.t. } \operatorname{Tr}\left(Q_i \begin{bmatrix}1\\x\end{bmatrix}\begin{bmatrix}1\\x\end{bmatrix}^\intercal\right) \le 0$$

$$\text{for } i = 1, \ldots, m$$

… equivalent!

NQCQP:

$$
\begin{aligned}
\min_{X \in \mathcal{S}^n} \ & \operatorname{Tr}(Q_0 X) \\
\text{s.t.} \ & \operatorname{Tr}(Q_i X) \leq 0 \\
& X_{11} = 1 \\
& X \succeq 0 \\
& \operatorname{rank}(X) = 1 \\
& \text{for } i = 1, \ldots, m
\end{aligned}
$$

… still equivalent!

NQCQP:

$$
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\end{aligned}
$$

… still equivalent!

Source of nonconvexity.

Computational strategy – convex relaxation

~~NQCQP:~~ Semidefinite program

$$
\begin{aligned}
\min_{X \in \mathcal{S}^n} \ & \mathrm{Tr}\left(Q_0 X\right) \\
\text{s.t. } & \mathrm{Tr}\left(Q_i X\right) \leq 0 \\
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& X \succeq 0 \\
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& \text{for } i = 1, \ldots, m
\end{aligned}
$$

… No longer equivalent, lower bound on the NQCQP!

NQCQP

$$\begin{aligned}\min_{x \in \mathbb{R}^n} \quad & \begin{bmatrix} 1 \\ x \end{bmatrix}^\intercal Q_0 \begin{bmatrix} 1 \\ x \end{bmatrix} \\ \text{s.t.} \quad & \begin{bmatrix} 1 \\ x \end{bmatrix}^\intercal Q_i \begin{bmatrix} 1 \\ x \end{bmatrix} \leq 0 \\ & \text{for } i = 1, \ldots, m\end{aligned}$$

SDP relaxation

$\leq$

SDP #1

$$\begin{aligned}\min_{X \in \mathcal{S}^n} \quad & \mathrm{Tr}\left(Q_0 X\right) \\ \text{s.t.} \quad & \mathrm{Tr}\left(Q_i X\right) \leq 0 \\ & X_{11} = 1 \\ & X \succeq 0 \\ & \text{for } i = 1, \ldots, m\end{aligned}$$

Computational strategy – convex relaxation

NQCQP

$$\min_{x\in\mathbb{R}^n} \begin{bmatrix}1\\x\end{bmatrix}^\top Q_0 \begin{bmatrix}1\\x\end{bmatrix}$$
$$\text{s.t.} \begin{bmatrix}1\\x\end{bmatrix}^\top Q_i \begin{bmatrix}1\\x\end{bmatrix} \leq 0$$
$$\text{for } i = 1, \ldots, m$$

SDP relaxation $\leq$

Lagrangian / weak duality $\geq$

SDP #1

$$\min_{X\in\mathcal{S}^n} \mathrm{Tr}(Q_0 X)$$
$$\text{s.t. } \mathrm{Tr}(Q_i X) \leq 0$$
$$X_{11} = 1$$
$$X \succeq 0$$
$$\text{for } i = 1, \ldots, m$$

strong duality

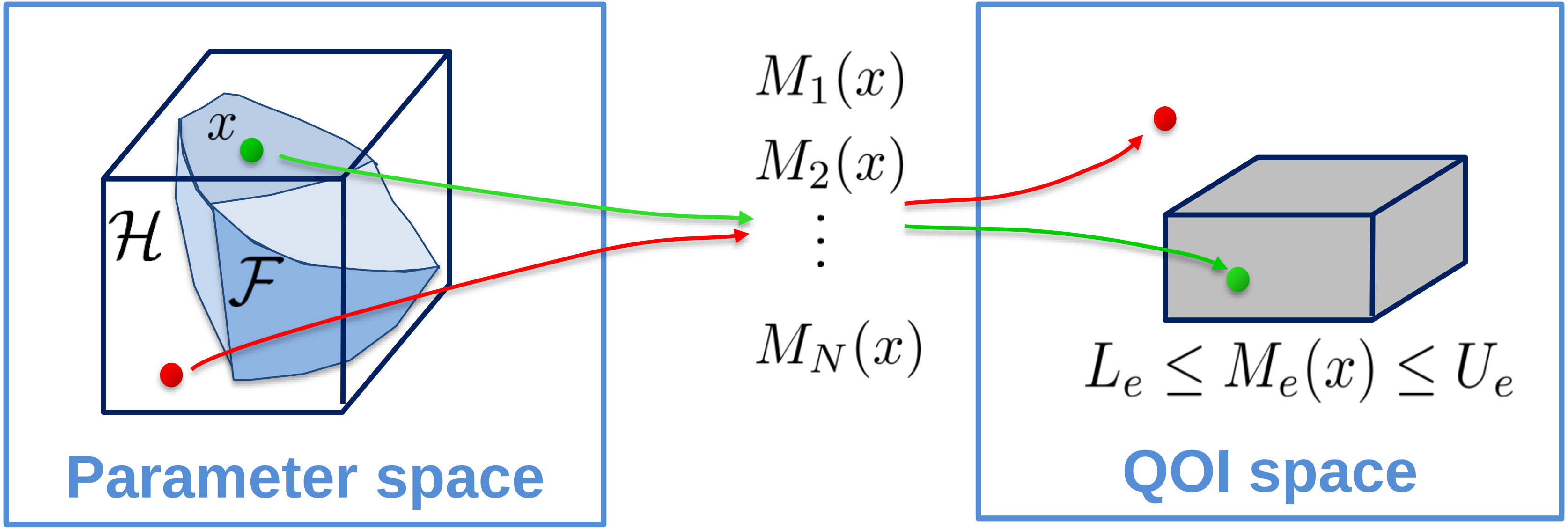
SDP #2

$$\max_{\lambda\geq 0,\rho} \rho$$
$$\text{s.t. } Q_0 - \begin{bmatrix}\rho & 0\\0 & 0\end{bmatrix} + \textstyle\sum_{i=1}^m \lambda_i Q_i \succeq 0$$

λ_i provide **sensitivity** estimates of the **optimal value** with respect to **perturbations of the constraints**.

Consistency and Feasible Sets

- A dataset is **consistent** if it is feasible
  - Parameters exist for which model predictions match the experiments



- Consistency analysis provides measures of validation

Quantifying Consistency

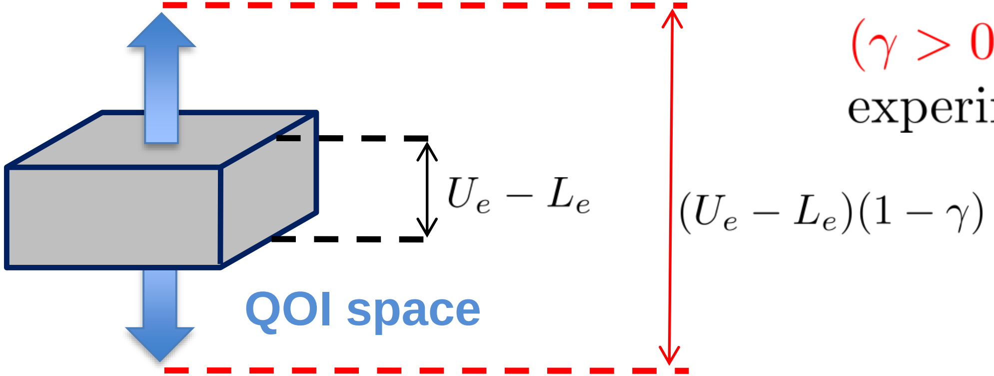
Q: Does there exist a parameter vector $x \in \mathcal{H}$ for which the models and data agree, within uncertainty?

A: Compute the *scalar consistency measure* (**SCM**)

Scalar Consistency Measure (SCM)*

$$
\begin{aligned}
\max_{x,\gamma} \quad & \gamma \\
\text{s.t.} \quad & L_e + \frac{(U_e - L_e)}{2}\gamma \le M_e(x) \le U_e - \frac{(U_e - L_e)}{2}\gamma \\
& x \in \mathcal{H}, \gamma \in \mathbb{R} \\
& \text{for } e = 1, \ldots, N
\end{aligned}
$$

The SCM produces a symmetric tightening $(\gamma > 0)$ or stretching $(\gamma < 0)$ of all experimental bounds.



*Feeley, R.; Seiler, P.; Packard, A.; Frenklach., M.; *J. Phys. Chem. A.* 2004, *108*, 9573.

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$$

If consistent, go to prediction

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If inconsistent, … ???

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- Inconsistency → models and data disagree
- Follow-up questions:
  - **What** are the sources of inconsistency?
  - **Where** do we begin to look?

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Quantifying Consistency

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Lagrange multipliers from dual form

Sensitivities

Local: $\lambda_j \approx \dfrac{\partial(\text{SCM})}{\partial(\text{bound } j)}$

Global: $\Delta(\text{SCM}) \le \lambda^T \Delta(\text{bounds})$

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Quantifying Consistency

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Scalar Consistency Measure (SCM)

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& x \in \mathcal{H}, \gamma \in \mathbb{R} \\
& \text{for } e = 1, \ldots, N
\end{aligned}
$$

New question: What is the **fewest** number of constraint relaxations required to render the dataset consistent?

Vector Consistency

Q: Does there exist a parameter vector $x \in \mathcal{H}$ for which the models and data agree, within uncertainty?

A: Compute the *scalar consistency measure* (**SCM**)

Scalar Consistency Measure (SCM)

$$\begin{aligned} \max_{x,\gamma} \quad & \gamma \\ \text{s.t.} \quad & L_e + \frac{(U_e - L_e)}{2}\gamma \leq M_e(x) \leq U_e - \frac{(U_e - L_e)}{2}\gamma \\ & x \in \mathcal{H}, \gamma \in \mathbb{R} \\ & \text{for } e = 1, \ldots, N \end{aligned}$$

If inconsistent, compute the *vector consistency measure* (**VCM**)

- Offers detailed analysis of inconsistency by allowing independent relaxations.
- Can be used to flag constraints contributing to inconsistency

Vector Consistency Measure (VCM)

$$\begin{aligned} \min_{x,\Delta} \quad & \|\Delta^L\|_1 + \|\Delta^U\|_1 \\ \text{s.t.} \quad & L_e - \Delta_e^L \leq M_e(x) \leq U_e + \Delta_e^U \\ & \Delta_e^L, \Delta_e^U \in \mathbb{R}, x \in \mathcal{H} \\ & \text{for } e = 1, \ldots, N \end{aligned}$$

Q: Does there exist a parameter vector $x \in \mathcal{H}$ for which the models and data agree, within uncertainty?

A: Compute the *scalar consistency measure* (**SCM**)

Scalar Consistency Measure (SCM)

$$\begin{aligned} \max_{x,\gamma} \quad & \gamma \\ \text{s.t.} \quad & L_e + \frac{(U_e - L_e)}{2}\gamma \leq M_e(x) \leq U_e - \frac{(U_e - L_e)}{2}\gamma \\ & x \in \mathcal{H}, \gamma \in \mathbb{R} \\ & \text{for } e = 1, \ldots, N \end{aligned}$$

If inconsistent, compute the *vector consistency measure* (**VCM**)

- Offers detailed analysis of inconsistency by allowing independent relaxations.
- Can be used to flag constraints contributing to inconsistency

Vector Consistency Measure (VCM)

$$\begin{aligned} \min_{x,\Delta} \quad & \boxed{\|\Delta^L\|_1 + \|\Delta^U\|_1} \\ \text{s.t.} \quad & L_e - \Delta_e^L \leq M_e(x) \leq U_e + \Delta_e^U \\ & \Delta_e^L, \Delta_e^U \in \mathbb{R}, x \in \mathcal{H} \\ & \text{for } e = 1, \ldots, N \end{aligned}$$

heuristic for fewest # of nonzeros (sparsity)

Examples*

* Hegde, A.; Li, W.; Oreluk, J.; Packard, A.; Frenklach, M., *SIAM/ASA J. Uncert. Quantif.,* 2018, 6(2), 429-456.

Example datasets

GRI-Mech 3.0

- Chemical kinetic model for natural gas combustion.
  - Nonlinear ODE system
- GRI-Mech 3.0 dataset
  - **77 experimental QOIs** with expert-assessed uncertainty
    - 54 shock-tube ignition delay
    - 23 laminar flame speeds
    - QOI models represented by quadratic surrogates
  - **102 uncertain parameters** with prior bounds
    - parameters ~ rate coefficients

DLR-SynG

- Syngas combustion model developed at DLR
- DLR-SynG dataset
  - **159 experimental QOIs** with expert-assessed uncertainty
    - 114 shock-tube ignition delay
    - 45 laminar flame speeds
    - QOI models represented by quadratic surrogates
  - **55 uncertain parameters** with prior bounds
    - parameters ~ rate coefficients

Example 1: GRI-Mech 3.0

GRI-Mech 3.0 dataset (**77 QOIs, 102 uncertain parameters**) for natural gas combustion.

Scalar Consistency

- **Procedure:** apply SCM, use sensitivities to flag problems.

Vector Consistency

Example 1: GRI-Mech 3.0

GRI-Mech 3.0 dataset (**77 QOIs, 102 uncertain parameters**) for natural gas combustion.

Scalar Consistency

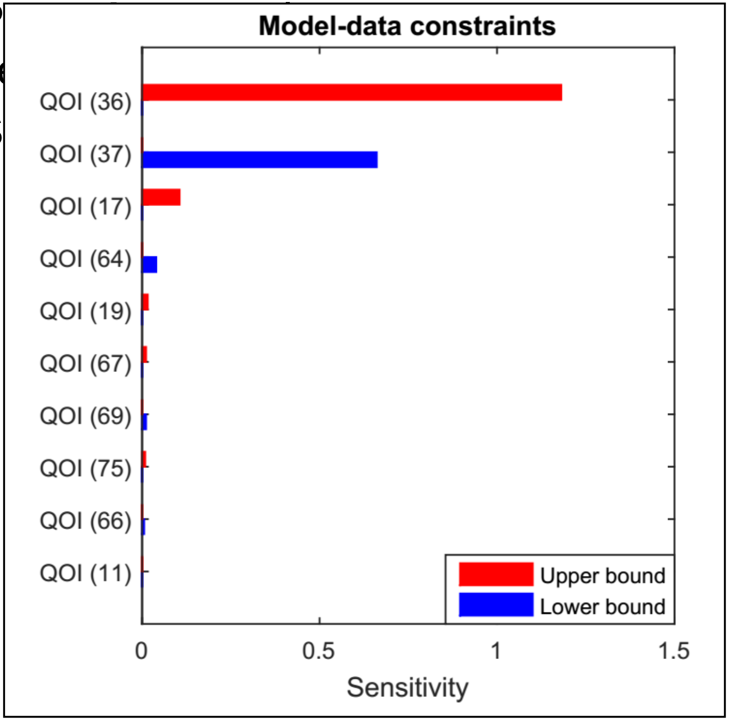
- **Procedure:** apply SCM, use sensitivities to flag problems.
- SCM < 0. Analyze ranked sensitivities

Vector Consistency

GRI-Mech 3.0 dataset (**77 QOIs, 102 uncertain parameters**) for natural gas combustion.

Scalar Consistency

- **P**
  se
- S



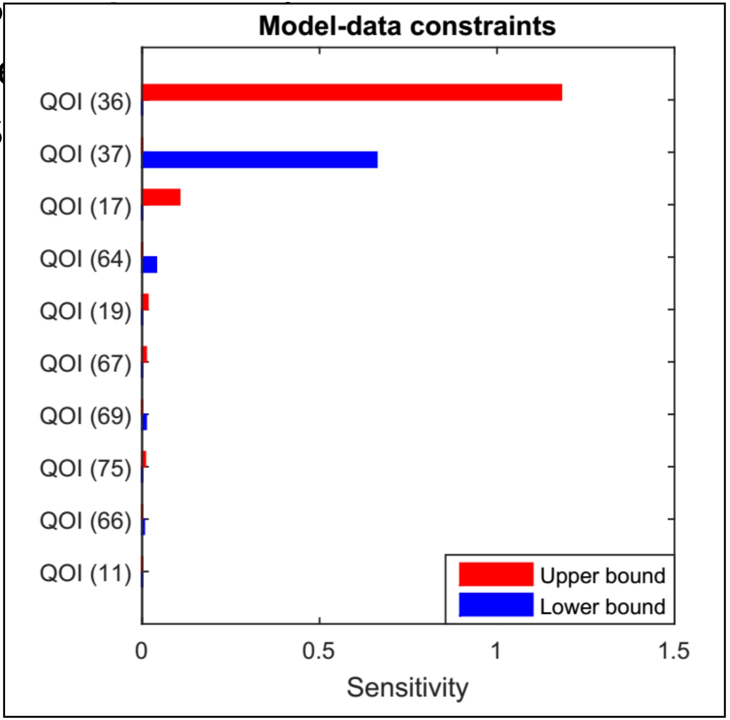
Vector Consistency

Example 1: GRI-Mech 3.0

GRI-Mech 3.0 dataset (**77 QOIs, 102 uncertain parameters**) for natural gas combustion.

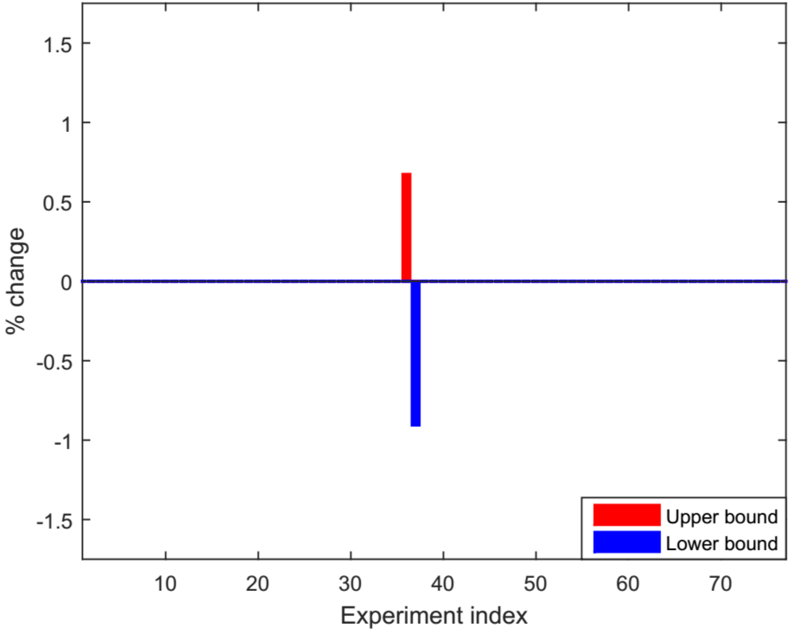
Scalar Consistency

- **P**
  se
- S



Vector Consistency

- Compute VCM.



Example 1: GRI-Mech 3.0

GRI-Mech 3.0 dataset (**77 QOIs, 102 uncertain parameters**) for natural gas combustion.

Scalar Consistency

- **Procedure:** apply SCM, use sensitivities to flag problems.
- SCM < 0. Analyze ranked sensitivities
- SCM > 0. Two QOIs removed, dataset consistent.

Vector Consistency

- Compute VCM.
- Two QOIs relaxed (same as in SCM), dataset consistent.

Example 1: GRI-Mech 3.0

GRI-Mech 3.0 dataset (**77 QOIs, 102 uncertain parameters**) for natural gas combustion.

Scalar Consistency

- **Procedure:** apply SCM, use sensitivities to flag problems.

Rapid and interpretable resolution of inconsistency

Vector Consistency

- Compute VCM.
- Two QOIs relaxed (same as in SCM),

Rapid and interpretable resolution of inconsistency

Example 2: DLR-SynG

DLR-SynG dataset (**159 QOIs, 55 uncertain parameters**) for syngas combustion developed at DLR*.

Scalar Consistency

Vector Consistency

* Slavinskaya, N.; et al. *Energy & Fuels.* 2017, 31, pp 2274–2297

Example 2: DLR-SynG

DLR-SynG dataset (**159 QOIs, 55 uncertain parameters**) for syngas combustion developed at DLR.

Scalar Consistency

- SCM < 0. Analyze ranked sensitivities.

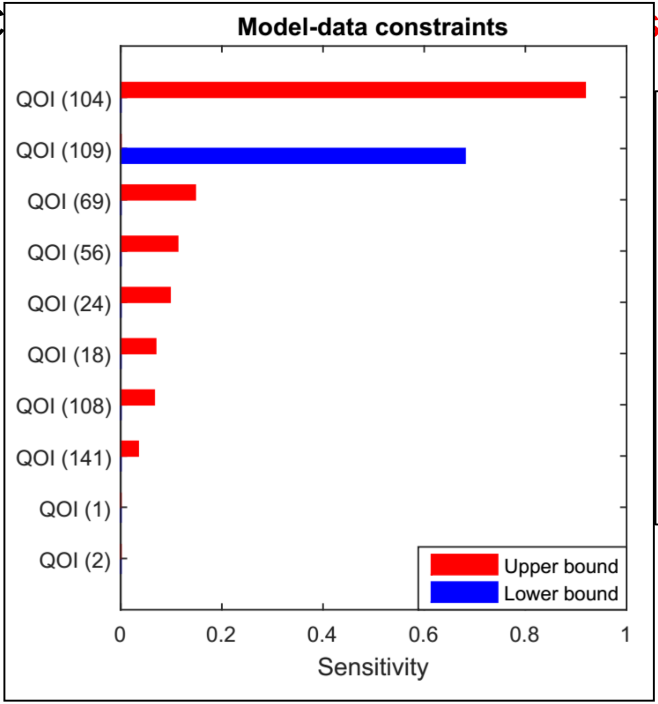
Vector Consistency

Example 2: DLR-SynG

DLR-SynG dataset (**159 QOIs, 55 uncertain parameters**) for syngas combustion developed at DLR.

Scalar Consistency

- SC



Vector Consistency

Set aside the top most sensitive QOI
Set aside the top two most sensitive QOIs
Set aside the top *n* most sensitive QOIs
Set aside the second most sensitive QOI (counter intuitive)

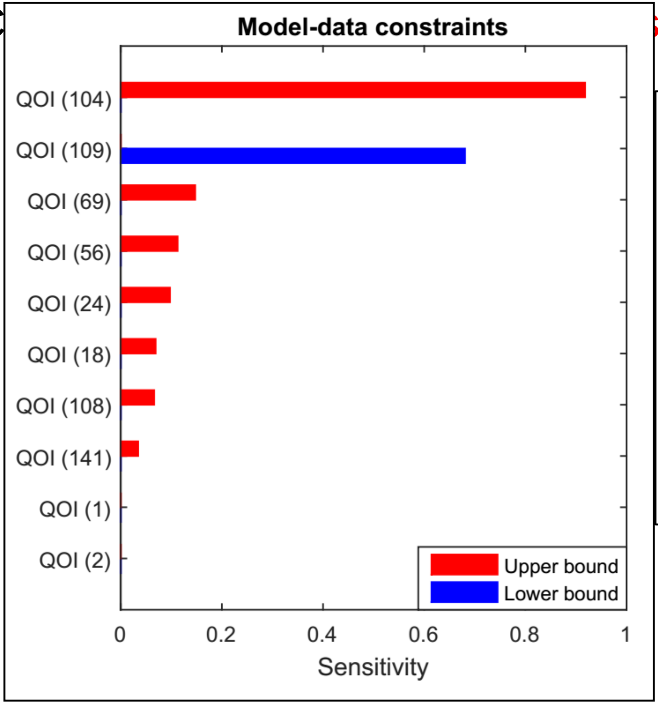
.
.
.

Example 2: DLR-SynG

DLR-SynG dataset (**159 QOIs, 55 uncertain parameters**) for syngas combustion developed at DLR.

Scalar Consistency

- SC



Vertical Consistency

Set aside the top most sensitive QOI

~~Set aside the top two most sensitive QOIs~~

~~Set aside the top *n* most sensitive QOIs~~

~~Set aside the second most sensitive QOI (counter intuitive)~~

.

.

.

Example 2: DLR-SynG

DLR-SynG dataset (**159 QOIs, 55 uncertain parameters**) for syngas combustion developed at DLR.

Scalar Consistency

- SCM < 0. Analyze ranked sensitivities.
  - Remove QOI #104 from dataset.

Vector Consistency

Example 2: DLR-SynG

DLR-SynG dataset (**159 QOIs, 55 uncertain parameters**) for syngas combustion developed at DLR.

Scalar Consistency

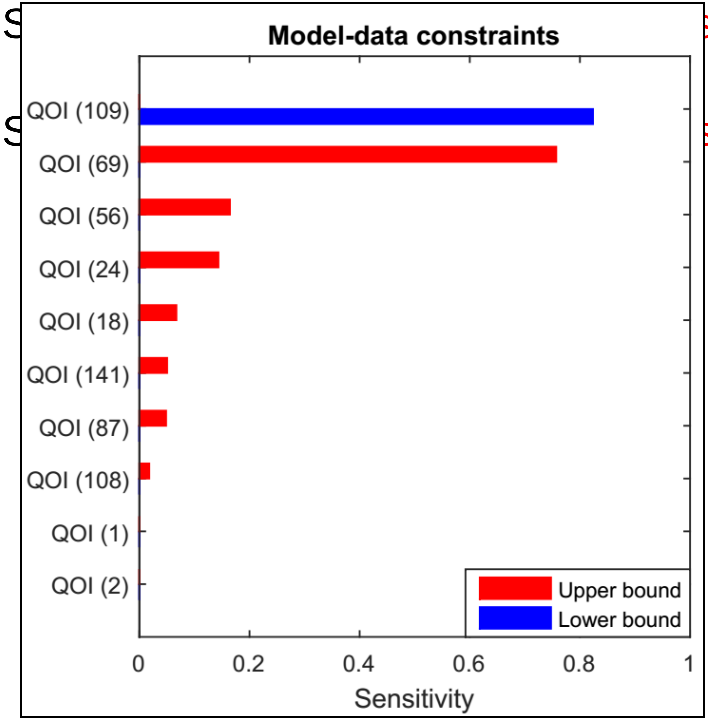
- SCM < 0. Analyze ranked sensitivities.
  - Remove QOI #104 from dataset.
- SCM < 0. Analyze ranked sensitivities.

Vector Consistency

DLR-SynG dataset (**159 QOIs, 55 uncertain parameters**) for syngas combustion developed at DLR.

Scalar Consistency

- S... s.
- S... s



Vector Consistency

Set aside the top most sensitive QOI

~~Set aside the top two most sensitive QOIs~~

~~Set aside the top *n* most sensitive QOIs~~

~~Set aside the second most sensitive QOI (counter intuitive)~~

.
.
.

Example 2: DLR-SynG

DLR-SynG dataset (**159 QOIs, 55 uncertain parameters**) for syngas combustion developed at DLR.

Scalar Consistency

- SCM < 0. Analyze ranked sensitivities.
  - Remove QOI #104 from dataset.
- SCM < 0. Analyze ranked sensitivities.
  - Remove QOI # 109.

Vector Consistency

Example 2: DLR-SynG

DLR-SynG dataset (**159 QOIs, 55 uncertain parameters**) for syngas combustion developed at DLR.

Scalar Consistency

- SCM < 0. Analyze ranked sensitivities.
  - Remove QOI #104 from dataset.
- SCM < 0. Analyze ranked sensitivities.
  - Remove QOI # 109.

Repeat until consistent

Vector Consistency

Example 2: DLR-SynG

DLR-SynG dataset (**159 QOIs, 55 uncertain parameters**) for syngas combustion developed at DLR.

Scalar Consistency

- SCM < 0. Analyze ranked sensitivities.
  - Remove QOI #104 from dataset.
- SCM < 0. Analyze ranked sensitivities.
  - Remove QOI # 109.

Repeat until consistent

- This strategy results in the removal of 73 QOIs.

Vector Consistency

Example 2: DLR-SynG

DLR-SynG dataset (**159 QOIs, 55 uncertain parameters**) for syngas combustion developed at DLR.

Scalar Consistency

- SCM < 0. Analyze ranked sensitivities.
  - Remove QOI #104 from dataset.
- SCM < 0. Analyze ranked sensitivities.
  - Remove QOI # 109.

Repeat until consistent

- This strategy results in the removal of 73 QOIs.
- Another strategy results in 56 QOIs removed.

Vector Consistency

Example 2: DLR-SynG

DLR-SynG dataset (**159 QOIs, 55 uncertain parameters**) for syngas combustion developed at DLR.

Scalar Consistency

- SCM < 0. Analyze ranked sensitivities.
  - Remove QOI #104 from dataset.
- SCM < 0. Analyze ranked sensitivities.
  - Remove QOI # 109.

Repeat until consistent

- This strategy results in the removal of 73 QOIs.
- Another strategy results in 56 QOIs removed.

Vector Consistency

- Compute VCM.

Example 2: DLR-SynG

DLR-SynG dataset (**159 QOIs, 55 uncertain parameters**) for syngas combustion developed at DLR.

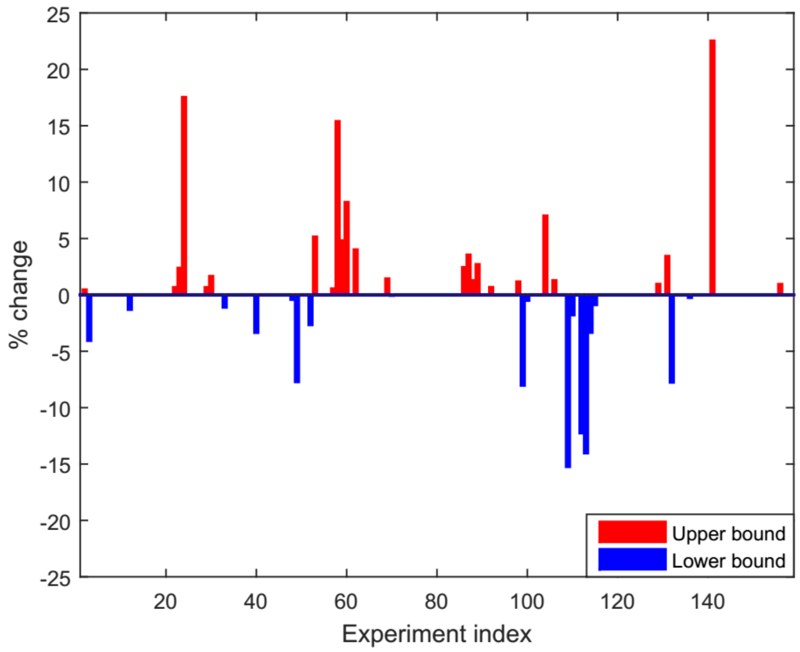
Scalar Consistency

- SCM < 0. Analyze ranked sensitivities.
  - Remove QOI #104 from dataset.
- SCM < 0. Analyze ranked sensitivities.
  - Remove QOI # 109.

Repeat until consistent

- This strategy results in the removal of 73 QOIs.
- Another strategy results in 56 QOIs removed.

Implementing 43 relaxations results in a consistent dataset



Example 2: DLR-SynG

DLR-SynG dataset (**159 QOIs, 55 uncertain parameters**) for syngas combustion developed at DLR.

Scalar Consistency

- SCM < 0. Analyze ranked sensitivities.
  - Remove QOI #104 from dataset.
- SCM < 0. Analyze ranked sensitivities.
  - Remove QOI # 109.

Repeat until consistent

- This strategy results in the removal of 73 QOIs.
- Another strategy results in 56 QOIs removed.

Vector Consistency

- Compute VCM.
  - Recommends 43 relaxations (18 to lower bounds, 25 to upper bounds)

Example 2: DLR-SynG

DLR-SynG dataset (**159 QOIs, 55 uncertain parameters**) for syngas combustion developed at DLR.

Scalar Consistency

- SCM < 0. Analyze ranked sensitivities.
  - Remove QOI #104 from dataset.
- SCM < 0. Analyze ranked sensitivities.
  - Remove QOI # 109.

Repeat until consistent

- This strategy results in the removal of 73 QOIs.
- Another strategy results in 56 QOIs removed.

Vector Consistency

- Compute VCM.
  - Recommends 43 relaxations (18 to lower bounds, 25 to upper bounds)

Example of what we termed **massive inconsistency**

Example 2: DLR-SynG

DLR-SynG dataset (**159 QOIs, 55 uncertain parameters**) for syngas combustion developed at DLR.

Scalar Consistency

- SCM < 0. Analyze ranked sensitivities.
  - Remove QOI #104 from dataset.
- SCM < 0. Analyze ranked sensitivities

Indirect and inefficient resolution of inconsistency

73 QOIs.

- Another strategy results in 56 QOIs removed.

Vector Consistency

- Compute VCM.
  - Recommends 43 relaxations (18 to lower bounds, 25 to upper bounds)

Direct, one-shot resolution of inconsistency

Example 2: DLR-SynG

DL

- S
- S

“For the particular system that we analyzed, the suspicion is on the instrumental models used to simulate the ignition. The future will tell if our present speculation on the possible source of the inconsistency is correct or not.”

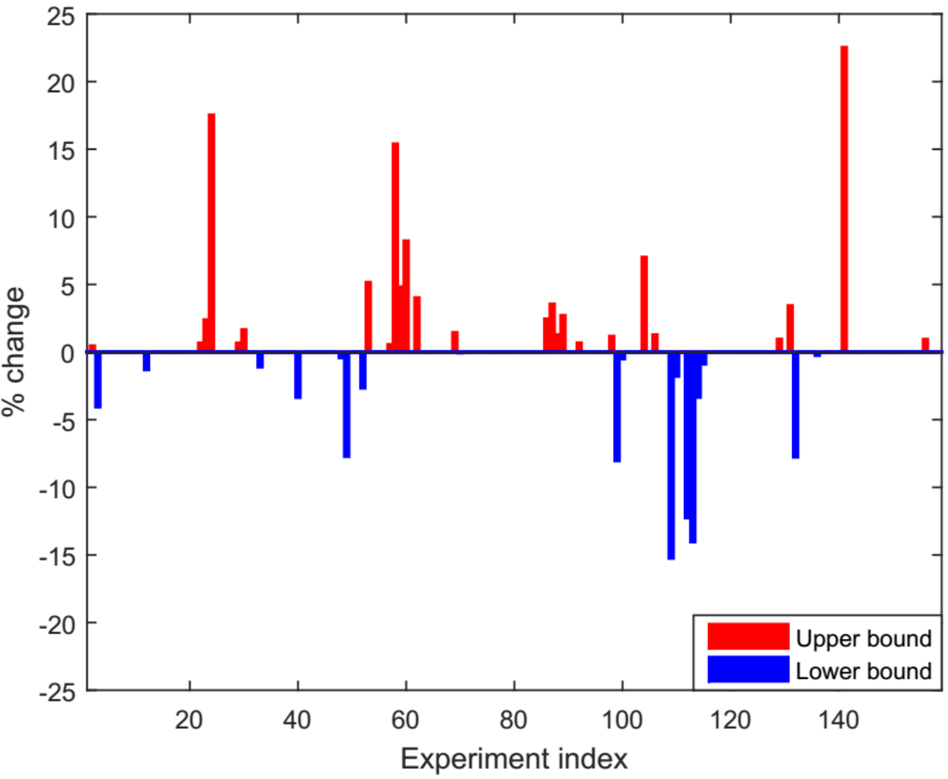
resolution of inconsistency

73 QOIs.

- Another strategy results in 56 QOIs removed.

inconsistency

Including weights in the VCM



What if we are unwilling to change certain experimental bounds?

Including weights in the VCM

- **Goal:** To allow domain expert knowledge and opinions enter VCM as weights.

- **Motivation:** If a dataset is inconsistent, one should be less willing to relax model-data constraints they trust and more willing to relax constraints that are less reliable. The same goes for parameter bounds.

Weighted VCM

$$
\begin{aligned}
\min_{x,\Delta^L,\Delta^U,\delta^l,\delta^u} \quad & \|\Delta^L\|_1 + \|\Delta^U\|_1 + \|\delta^l\|_1 + \|\delta^u\|_1 & \\
\text{s.t.} \quad & L_e - W_e^L \Delta_e^L \leq M_e(x) \leq U_e + W_e^U \Delta_e^U & \text{for } e = 1, \ldots, N \\
& l_i - w_i^l \delta_i^l \leq x_i \leq u_i + w_i^u \delta_i^u & \text{for } i = 1, \ldots, n
\end{aligned}
$$

- Small weight - less willing to change bound.
- Large weight - more willing to change bound.

Including weights in the VCM

- **Goal:** To allow domain expert knowledge and opinions enter VCM as weights.

- **Motivation:** If a dataset is inconsistent, one should be less willing to relax model-data constraints they trust and more willing to relax constraints that are less reliable. The same goes for parameter bounds.

Weighted VCM

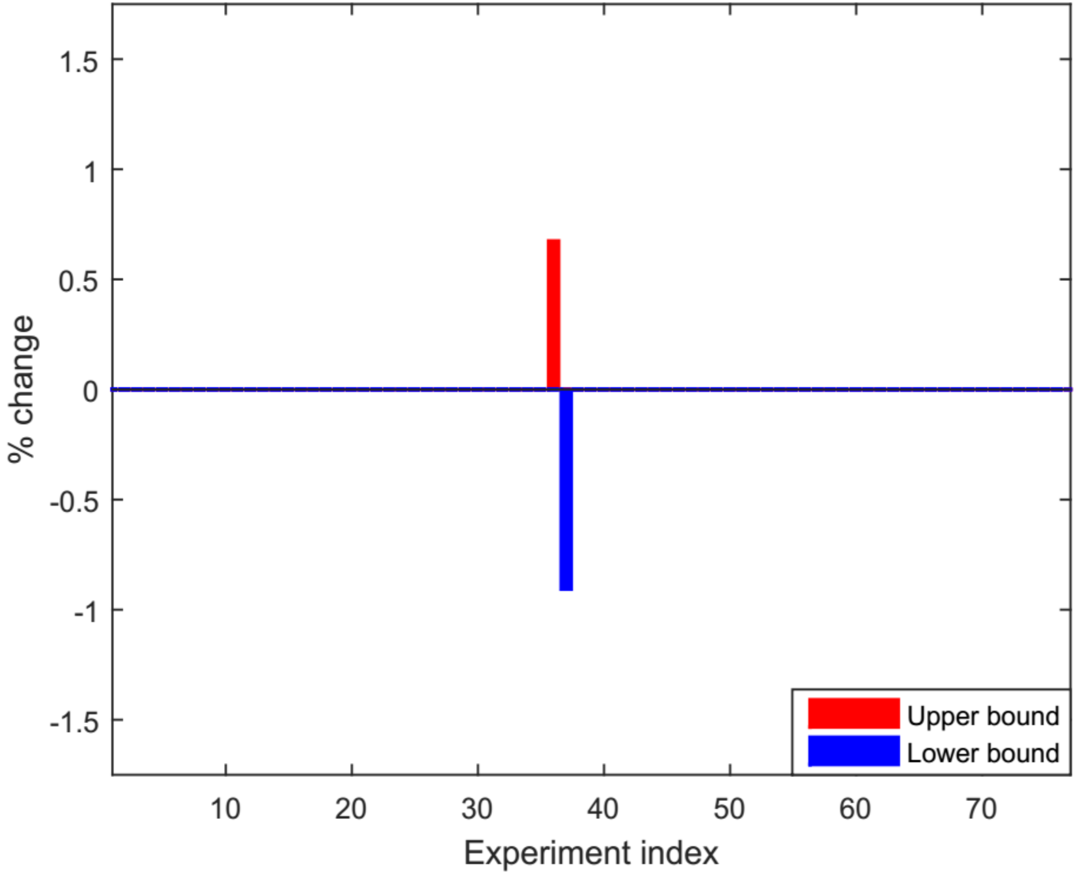
$$\begin{aligned} \min_{x,\Delta^L,\Delta^U,\delta^l,\delta^u} \quad & \|\Delta^L\|_1 + \|\Delta^U\|_1 + \|\delta^l\|_1 + \|\delta^u\|_1 \\ \text{s.t.} \quad & L_e - W_e^L \Delta_e^L \leq M_e(x) \leq U_e + W_e^U \Delta_e^U \qquad \text{for } e = 1, \ldots, N \\ & l_i - w_i^l \delta_i^l \leq x_i \leq u_i + w_i^u \delta_i^u \qquad \text{for } i = 1, \ldots, n \end{aligned}$$

$$W_e^{L/U} = U_e - L_e$$

With these weights, DLR-SynG can be made consistent by adjusting 37 QOIs.

Weights and GRI-Mech 3.0

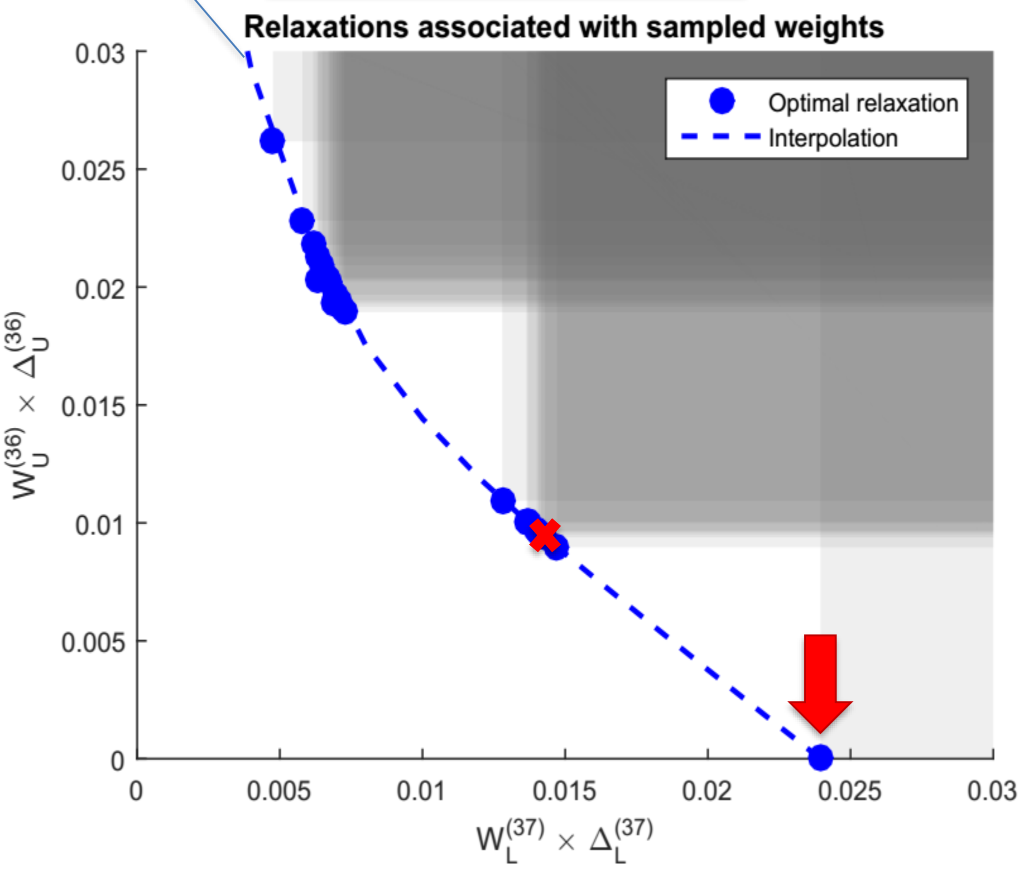
- Single application of VCM identifies two experimental bounds.



Weights and GRI-Mech 3.0

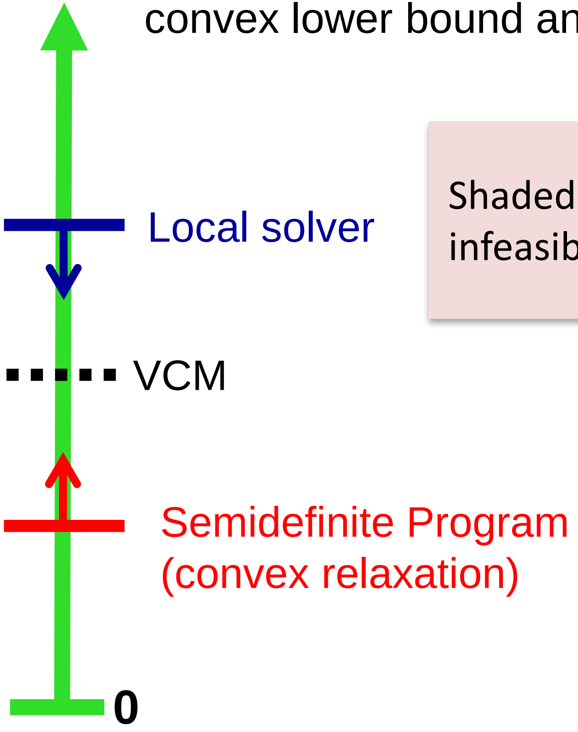
- Single application of VCM identifies two experimental bounds.
- Weights applied to only the previous two bounds.

Tradeoff effect from using different weights



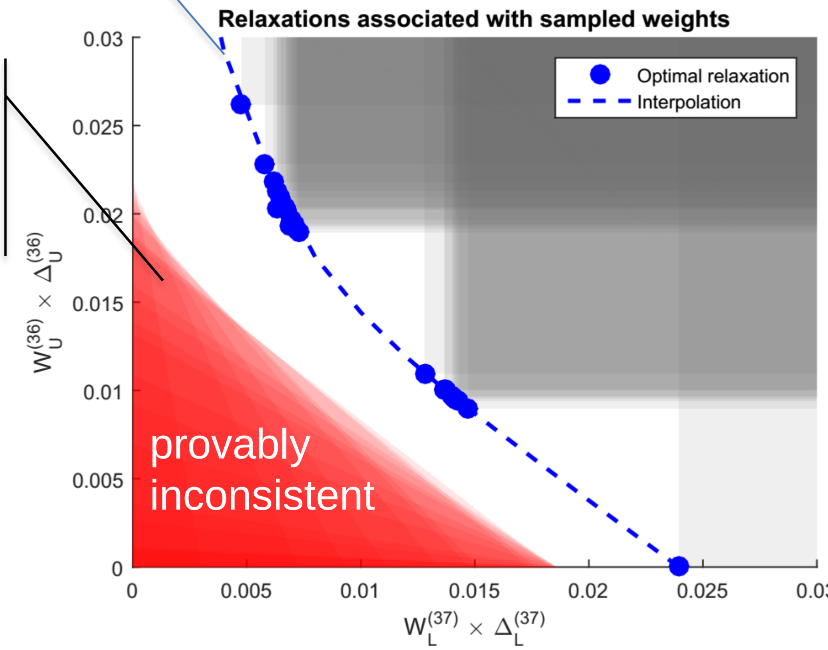
Computing the VCM

For **quadratic surrogate models**, we can approximate the true solution (NP-hard) using convex lower bound and local optima.



Shaded red region certified infeasible by SDP.

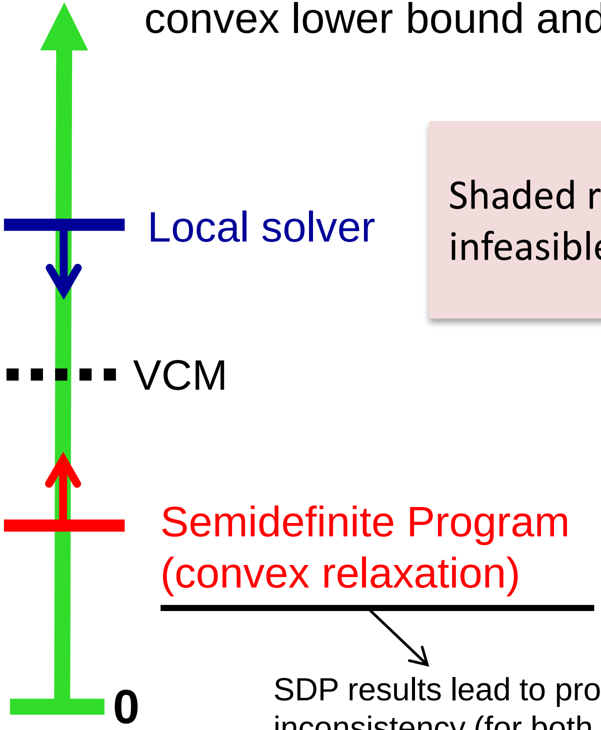
Tradeoff effect from using different weights



Example: GRI-Mech 3.0 dataset – VCM relaxations with varying weights, relaxations allowed to two constraints

Computing the VCM

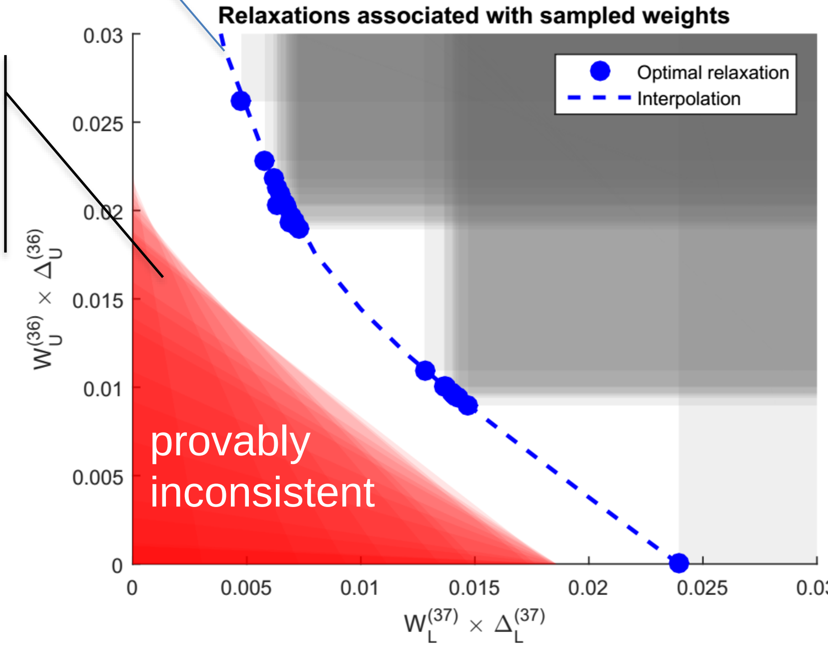
For **quadratic surrogate models**, we can approximate the true solution (NP-hard) using convex lower bound and local optima.



Shaded red region certified infeasible by SDP.

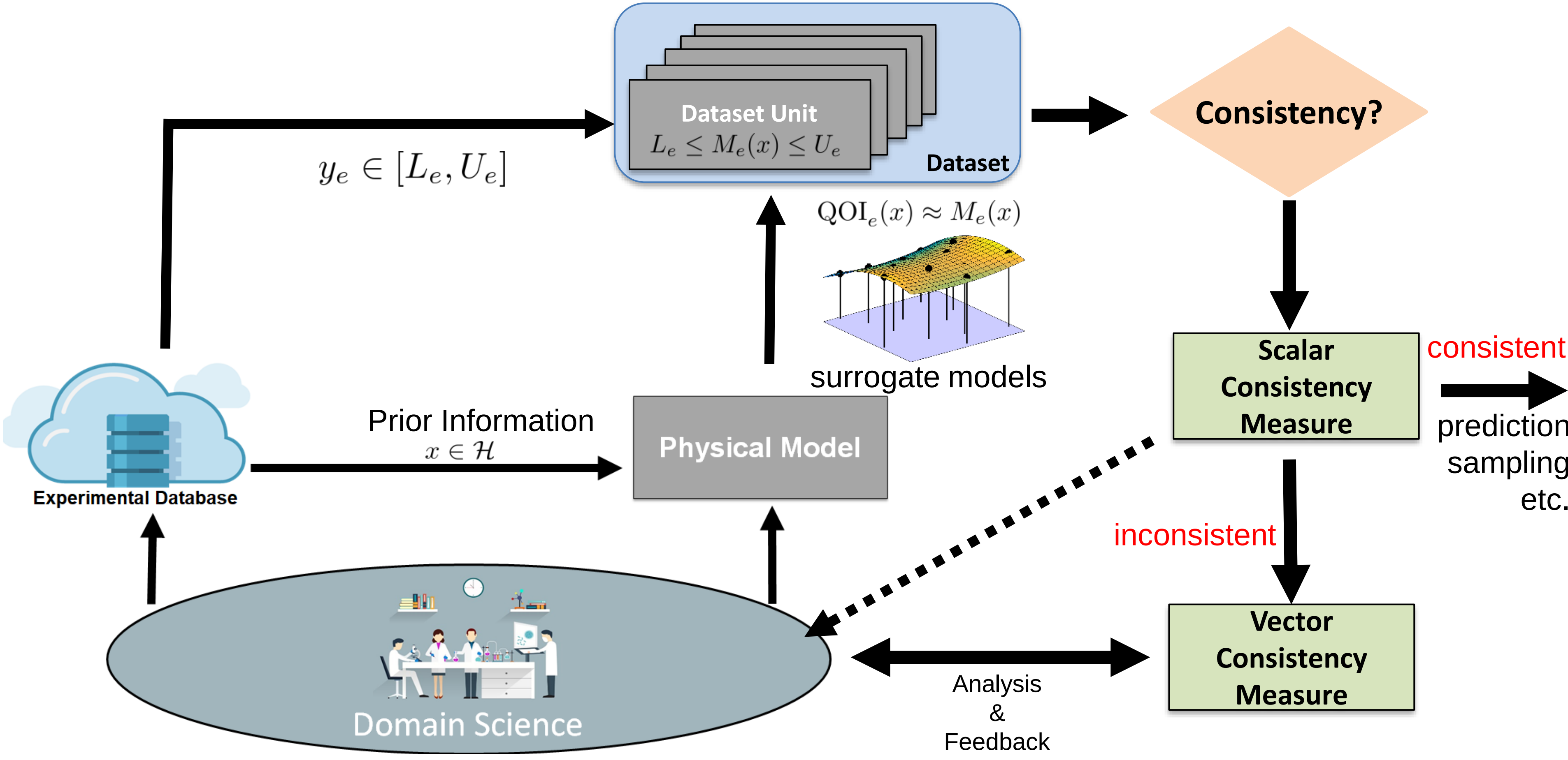
SDP results lead to proofs of inconsistency (for both VCM and SCM)

Tradeoff effect from using different weights



Example: GRI-Mech 3.0 dataset – VCM relaxations with varying weights, relaxations allowed to two constraints

"The Big Picture"



Summary

- **B2BDC** – constrained-optimization approach to UQ
  - Combines solution mapping (surrogate modeling) + semidefinite programming

- **Consistency measures** are tools to accomplish **validation**
  - **Scalar Consistency Measure (SCM)** – are we consistent?
  - **Vector Consistency Measure (VCM)** – diagnose inconsistency
    - **VCM** particularly efficient for resolving **massive inconsistency**
  - **Application:** GRI-Mech 3.0, DLR-SynG

- **Future directions**
  - Q: In what other applications do the mentioned surrogate model classes provide reasonable approximations?

Some references

- M. Frenklach, A. Packard, G. Garcia-Donato, R. Paulo, and J. Sacks, *Comparison of statistical and deterministic frameworks of uncertainty quantification*, SIAM/ASA JUQ, 2016.
  - comparison of B2BDC and Bayesian Calibration via example
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  - details numerical implementation of several B2BDC techniques, extension to polynomial surrogates
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  - highlights sensitivity aspect of prediction

Acknowledgements

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National Nuclear Security Administration

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Questions?