Sandia National Laboratories SAND2016-4506C

Exploring Model Form Uncertainty Approaches with a Burgers' Equation Example

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ASME 2016 Verification & Validation Symposium
Las Vegas, NV
May 18, 2016

U.S. DEPARTMENT OF ENERGY

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ABSTRACT

Beyond considering uncertainty in model parameters and experimental data when quantifying predictive uncertainty, accounting for insufficiencies in the form of models has become an area of emphasis. Insufficiencies in the model form cause what is known as model form uncertainty, or the discrepancy between model predictions and the truth. Methods of accounting for model form uncertainty vary widely and no one method has been accepted across the VVUQ community. Model form uncertainty is known to cause identifiability issues when calibrating model parameters. Such issues have led many researchers to incorporate model validation activities prior to making predictions. Is it best to use the same approach towards accounting for model form uncertainty when making interpolations and extrapolations and should extrapolations in the parameter space be treaded in the same manner as extrapolations to new data types? The type of prediction that the model form uncertainty is influencing may impact how characterizing the uncertainty is approached and what methods should be applied. By differentiating and defining types of prediction problems, a analysis structure for considering methods of approaching model form uncertainty for each prediction type can be better understood.

Using the 1D viscous Burgers' equation as an application example, a survey of a few methods of addressing model form uncertainty will be considered. Inadequacy in the model form for the example problem is introduced by using the linear convective diffusion equation as the model form, while the data is generated by the Burgers' equation. Implications on predictions for data types similar to that used for calibration as well as extrapolations to different data types will be considered. Methods considered in this analysis include those with Bayesian foundations as well as engineering bounds based. Through applying a diverse set of methods to a single test problem, analysis of the application and results can illuminate strengths and weaknesses of current approaches.

Outline

model form uncertainty issues / problem types

conceptual approaches to model form uncertainty problems

problem types of interest

overview of approaches considered / main approach concepts

Burgers' equation as analysis canvas

current thoughts on problem

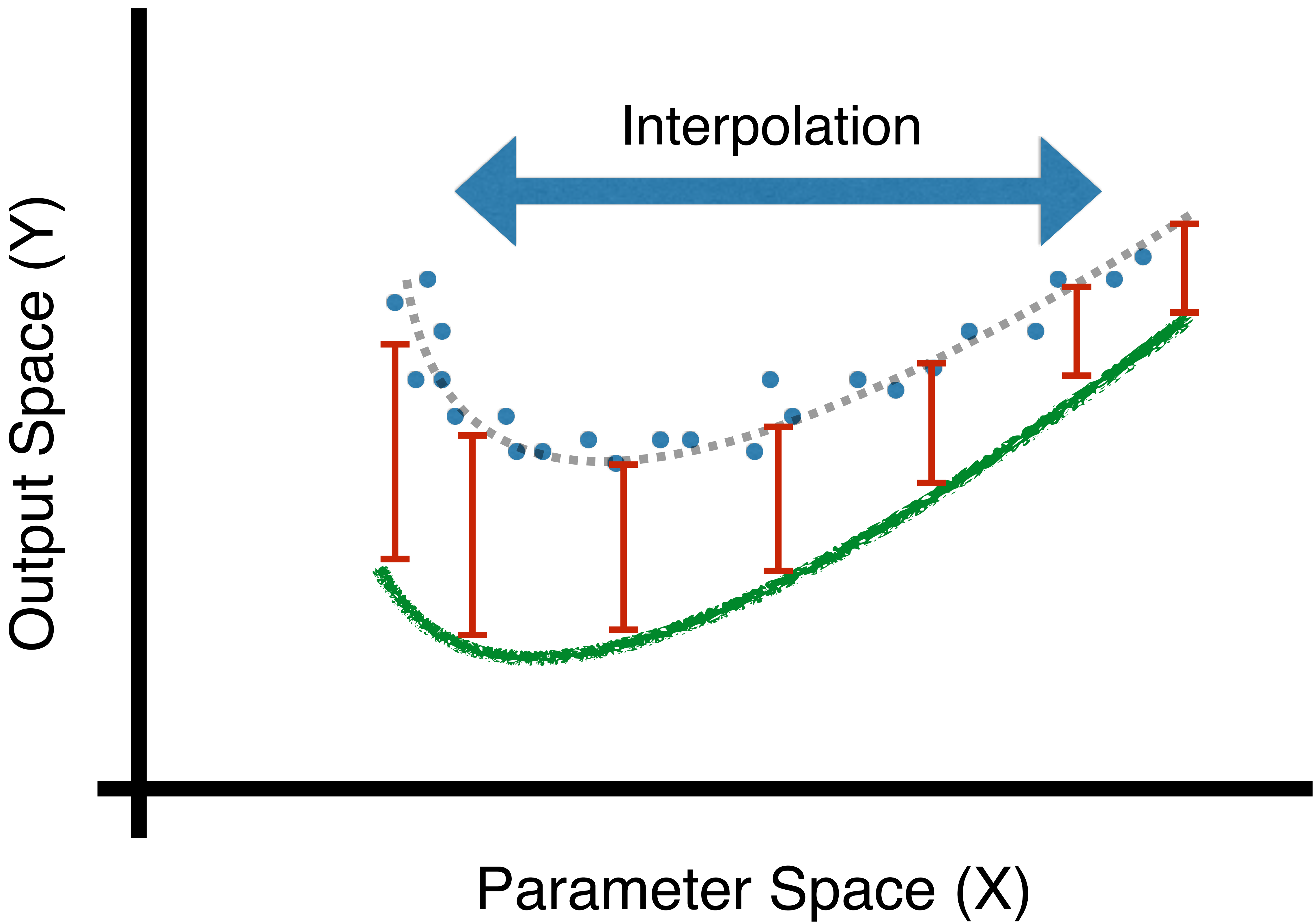
Model Form Uncertainty Issues

- the uncertainty attributed to the model form representing the truth in a less than perfect fashion
- all models are imperfect, the extent to which this impacts the desired predictions determines if the model form uncertainty is considered when making predictions
- methods of addressing this issue must also address parameter uncertainty and its propagation leading to identifiability issues

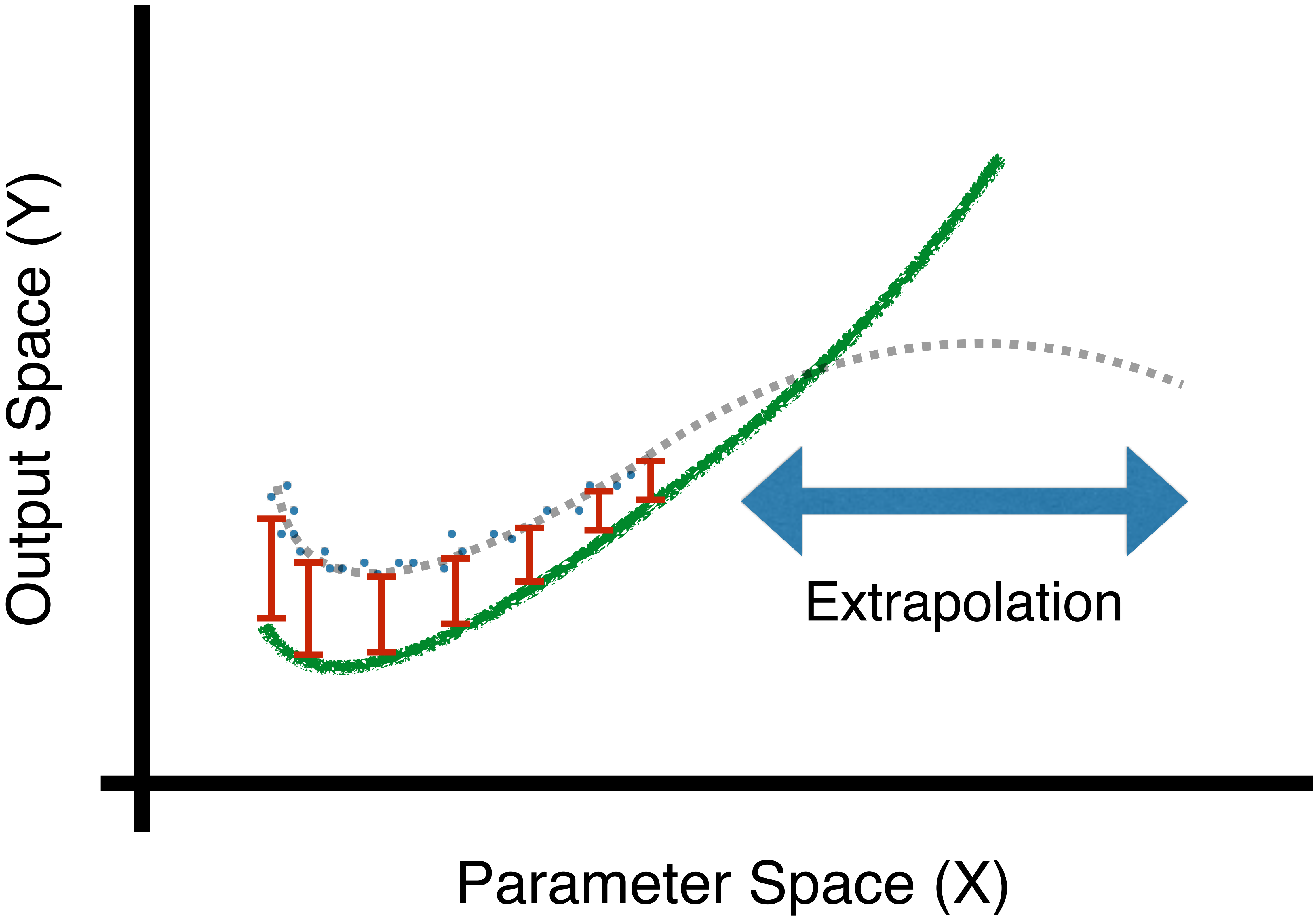
Hypotheses

- many different types of problems include an element of model form uncertainty
- different types of model form uncertainty problems will benefit from different solution strategies

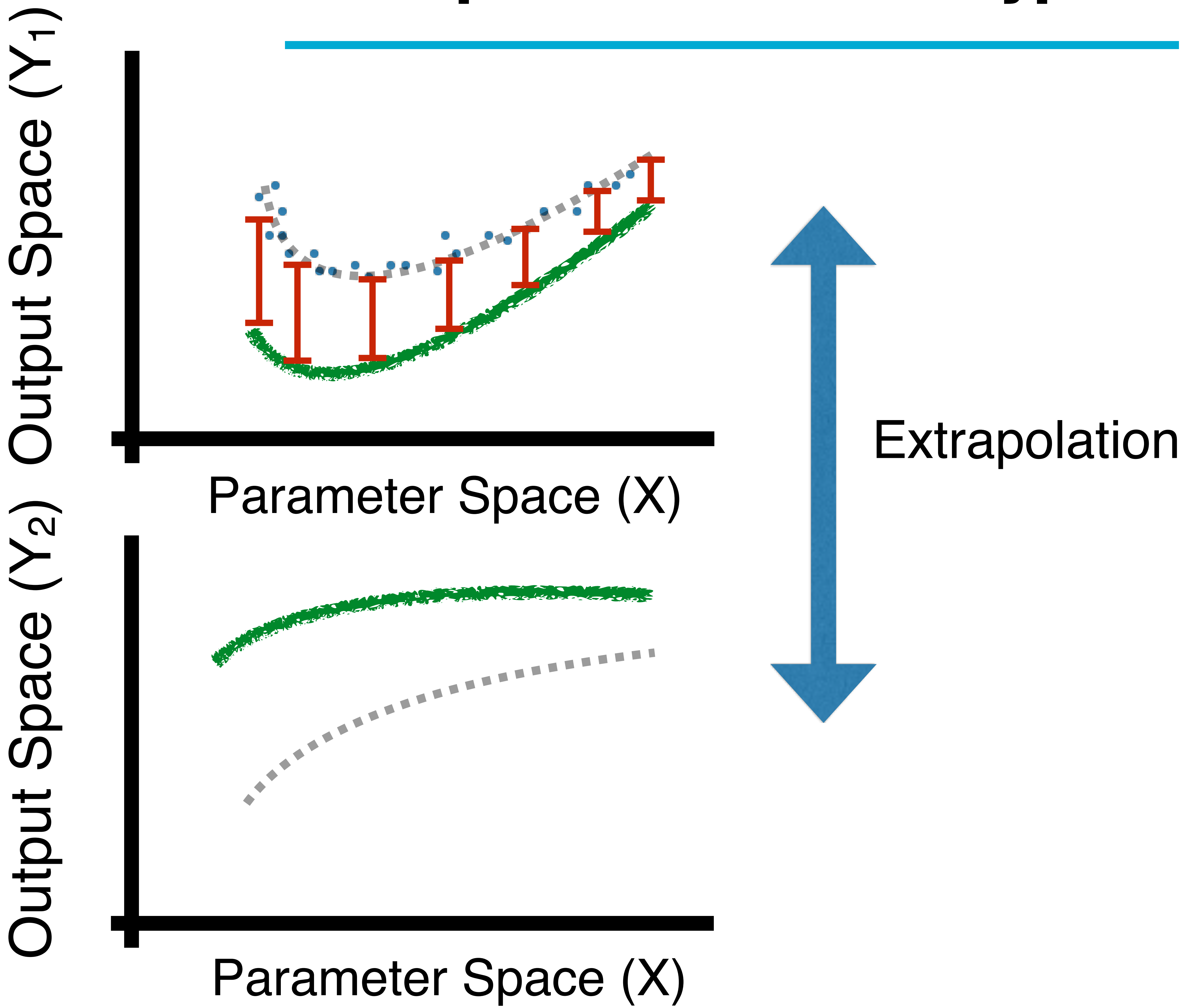
Interpolation Problem

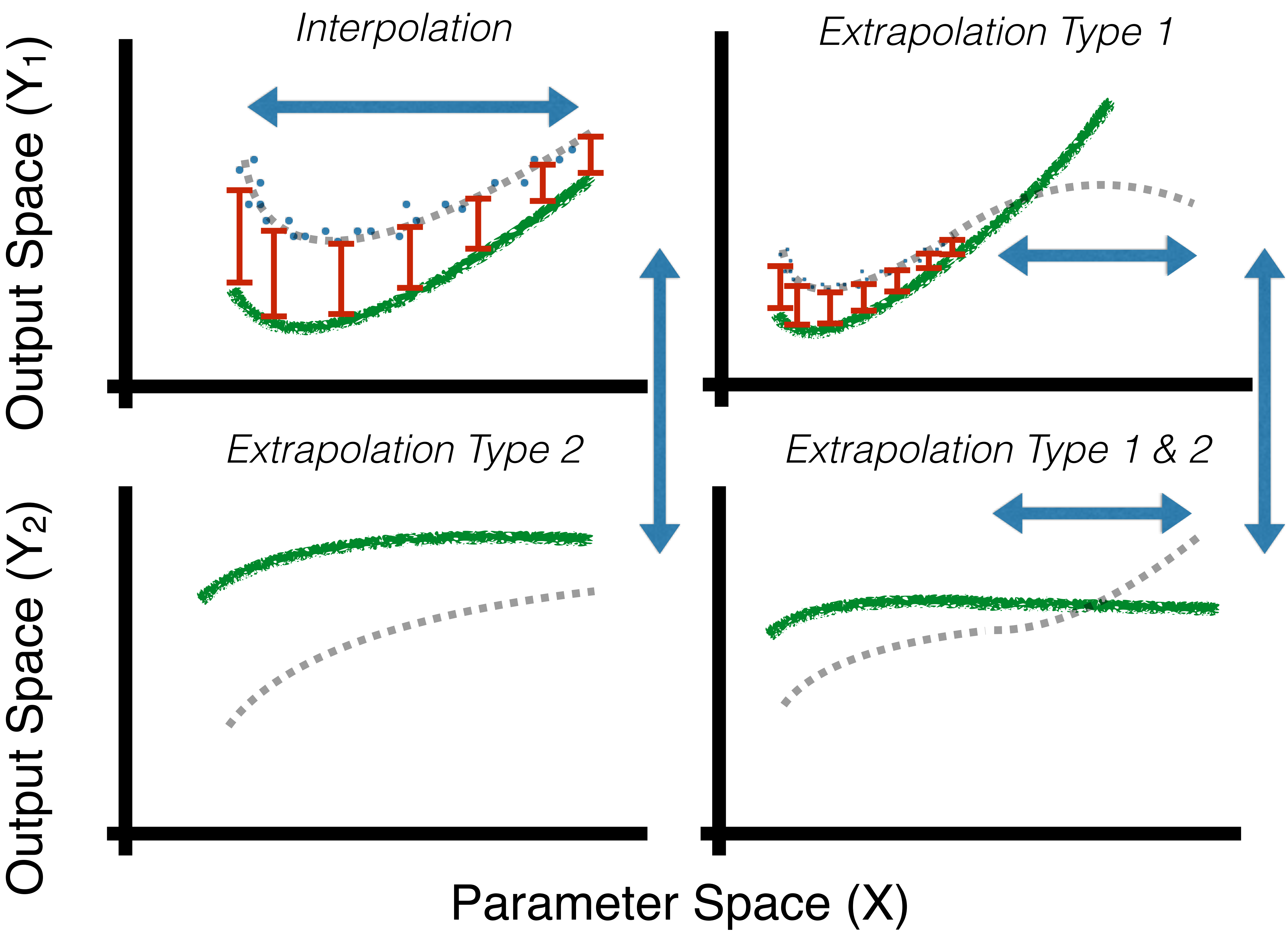


Extrapolation Problem Type 1



Extrapolation Problem Type 2





Interpolation
Extrapolation Type 1
Extrapolation Type 2
Extrapolation Type 1 & 2
Output Space (Y1)
Output Space (Y2)
Parameter Space (X)

Many Conceptual VUQ Approach Options

propagate uncertainty ➔ validation model ➔ predict

propagate uncertainty ➔ characterize bias ➔ predict

calibrate parameters ➔ predict

calibrate parameters ➔ characterize bias ➔ predict

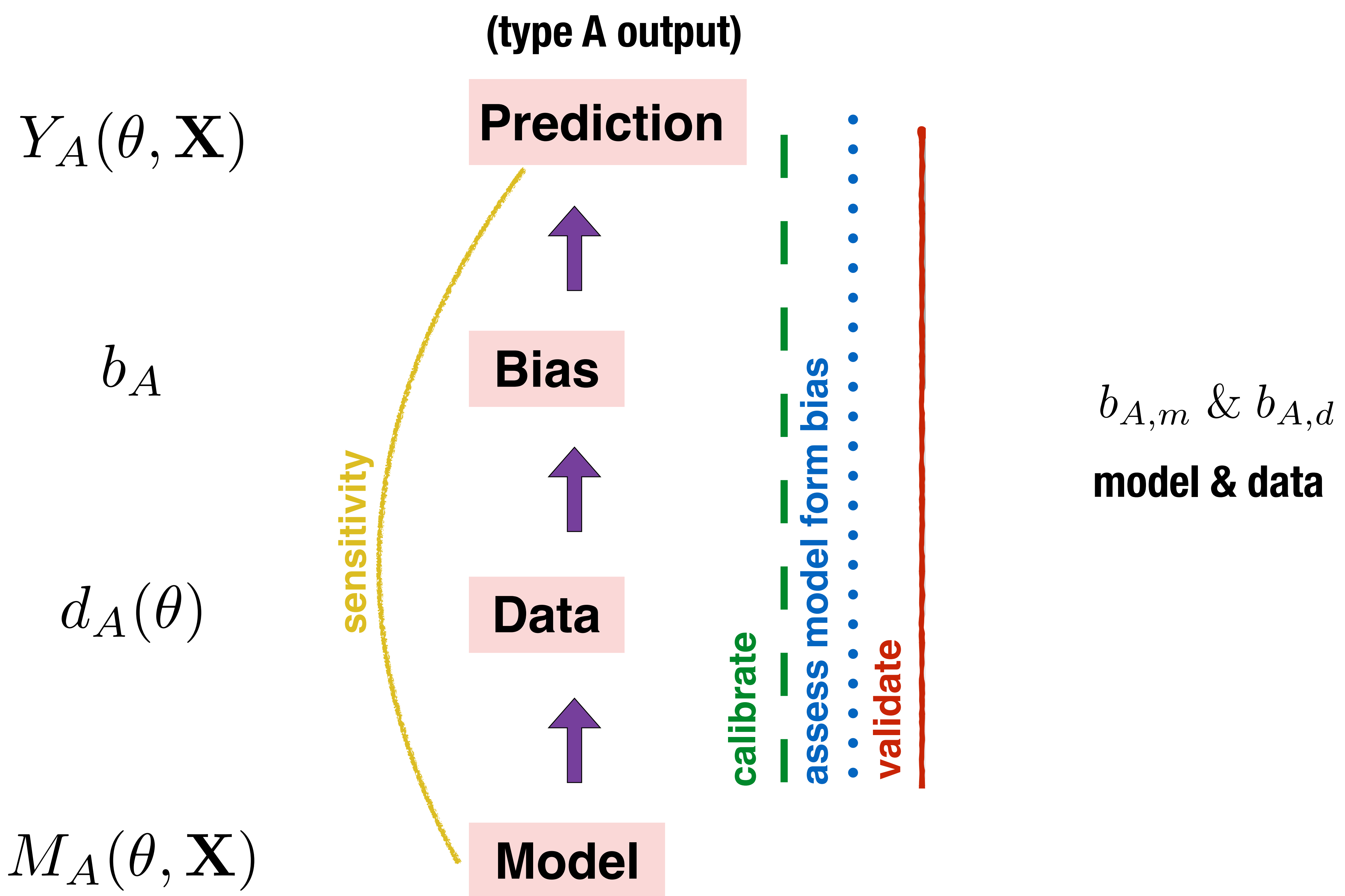
predict

convert datatypes ➔ calibrate parameters ➔ predict

⋮

Overview of Conceptual Approaches

$X \rightarrow$ model parameters $\qquad \theta \rightarrow$ input conditions



modeling $$Y_{A,\text{true}}(\theta) = M_A(\theta, \boldsymbol{X}) + b_{m,A}$$

experiments $$Y_{A,\text{true}}(\theta) = d_A(\theta) + b_{d,A} + \epsilon$$

VUQ basis $$M_A(\theta, \boldsymbol{X}) = d_A(\theta) + b_A + \epsilon$$

$$b_A = b_{m,A} + b_{d,A}$$

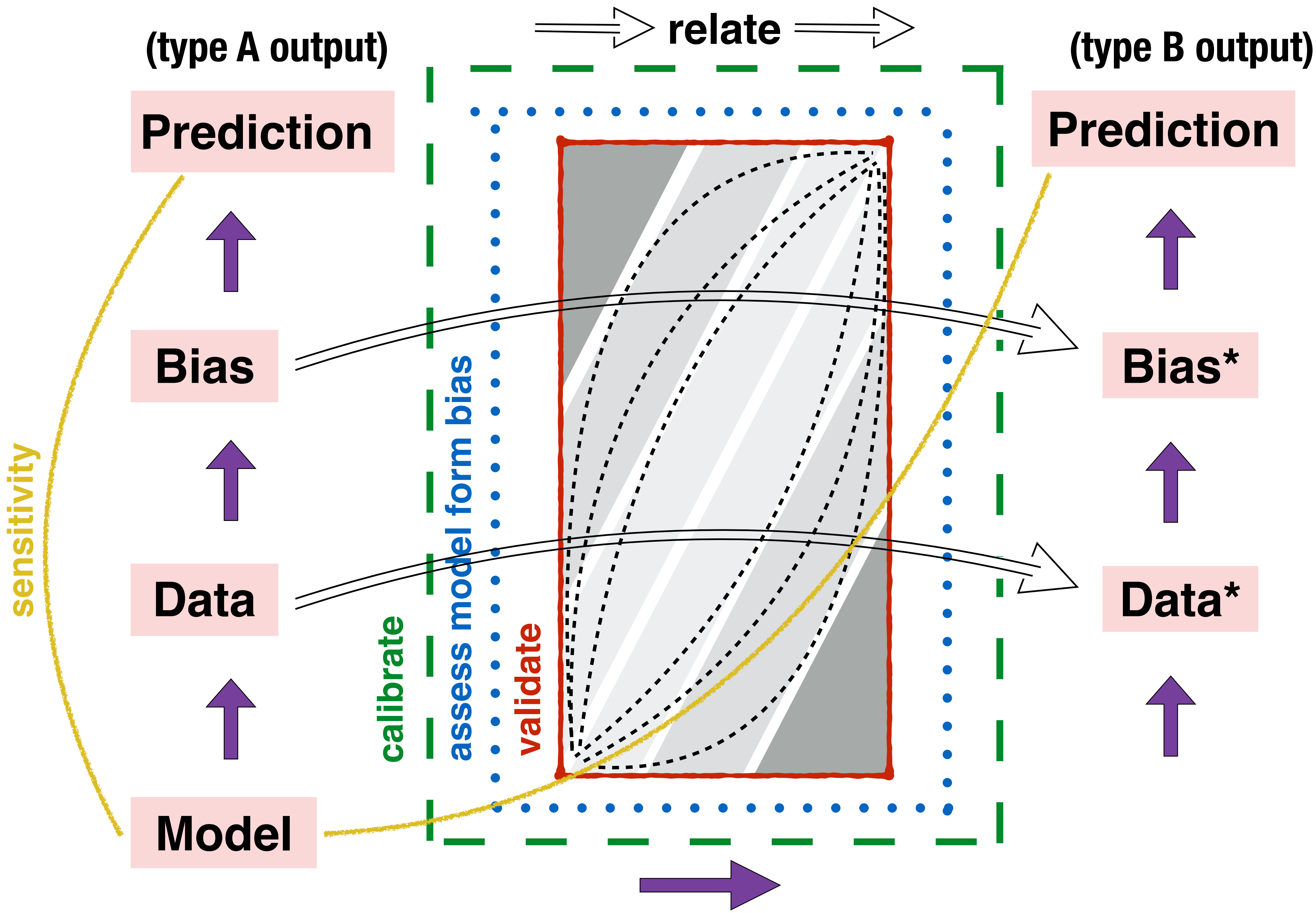
---

calibration $$\min_X \left(M_A(\theta, \boldsymbol{X}) - d_A(\theta) + \epsilon\right)$$

``` with bias $$\min_X \left(M_A(\theta, \boldsymbol{X}) + b_A - d_A(\theta) + \epsilon\right)$$

---

validation $$M_A(\theta, \boldsymbol{X}) - d_A(\theta) = b_A + \epsilon$$

$$|M_A(\theta, \boldsymbol{X}) - d_A(\theta)| < \text{threshold}$$

---

prediction $$Y_{A,\text{pred}}(\theta) = M_A(\theta, \mathbf{X})$$

$$Y_{A,\text{pred}}(\theta) = M_A(\theta, \mathbf{X}_{A,\text{cal.}})$$
```

Overview of Conceptual Approaches

model relation between model outputs to translate between



relation

$$M_B(\theta, \boldsymbol{X}) = f(M_A(\theta, \boldsymbol{X}))$$

VUQ activities

$$\begin{aligned} M_B(\theta, \boldsymbol{X}) &= f(d_A(\theta) + b_A + \epsilon) \\ &= d_B^*(\theta) + b_B^* + \epsilon^* \end{aligned}$$

calibration

⋮

validation

prediction

$$Y_{\mathrm{B,pred}}(\theta) = M_B(\theta, \boldsymbol{X}_{\mathrm{A,val.}})$$

Types of Problems Our Group is Interested in Solving

want quantified uncertainties from models

need to establish model credibility

hierarchy of system complexity / multiple levels of modeling

data poor at top hierarchical levels, expensive validation experiments near space of desired predictions

predictions of quantities outside of measurable conditions

physics models with unknown credibility

Methods of Tackling Problems of Interest: Focusing on Model Form Issues

multiple flavors of Bayesian approaches

- explicit bias/correction term (Kennedy & O`Hagan 2001)
  - calibrate parameters with reduced influence from bias
- rollup into parameter uncertainty based upon validation performance (Sankararaman & Mahadevan 2015)
  - correction of parameter calibration based upon validation

direct application of validation metrics on parameter space to locate validated subspaces

- interval predictor models (IPM), random predictor models (RPM), and Bounds to Bounds (B2B)
  - locate parameter subspace enveloping data/uncertainty (Crespo 2014)
  - locate parameter subspace enveloped by data/uncertainty (Feeley 2004)

Methods of Tackling Problems of Interest: Focusing on Model Form Issues

use of partial least squares to create meta-model for predicting uncertainty in prediction space (Hills 2013)

- linear combination of validation results weighted by sensitivity similarity with prediction used to estimate bias
- weighting driven to get same sensitivity as prediction model

explicit propagation of all uncertainties, including bias, to prediction (P-box descriptions) (Roy & Oberkampf 2011)

- no calibration, conservative estimates
- transparent propagation of uncertainties

Distillation of Methods

1. construct bias correction term from validation results
    - identification problem with parameter calibration

2. rollup uncertainty found in validation results into parameter uncertainty
    - poor validation results still mean little confidence in prediction
    - parameter descriptions then model specific

3. use validation results to add uncertainty to predictions
    - conservative answer that may still be wrong

4. locate parameter subspace able to meet validation criteria
    - relies on minimal model form error
    - combine calibration and validation into uncertainty description

Burgers' Equation Example

$$\frac{\partial u}{\partial t} + c\,\frac{\partial u^p}{\partial x} = d\,\frac{\partial^2 u}{\partial x^2}$$

incorrect
-> p=1 is linear conv.-diffus. eqn
correct
-> p=2 is diffusive Burgers' eqn

$u(t,x)$ - velocity distribution over time and space

c, d - advection and diffusion coefficient (uncertain parameters)

p - model form parameter

additional model output - $\text{flux} = cu^p - d\frac{\partial u}{\partial x}$

$$u(x,0) = \begin{cases} 0.5; & x < 1 \\ x - 0.5; & 1 \le x < 2 \\ 1.5; & 2 \le x < 3 \\ 4.5 - x; & 3 \le x < 4 \\ 0.5; & 4 \le x \end{cases}$$

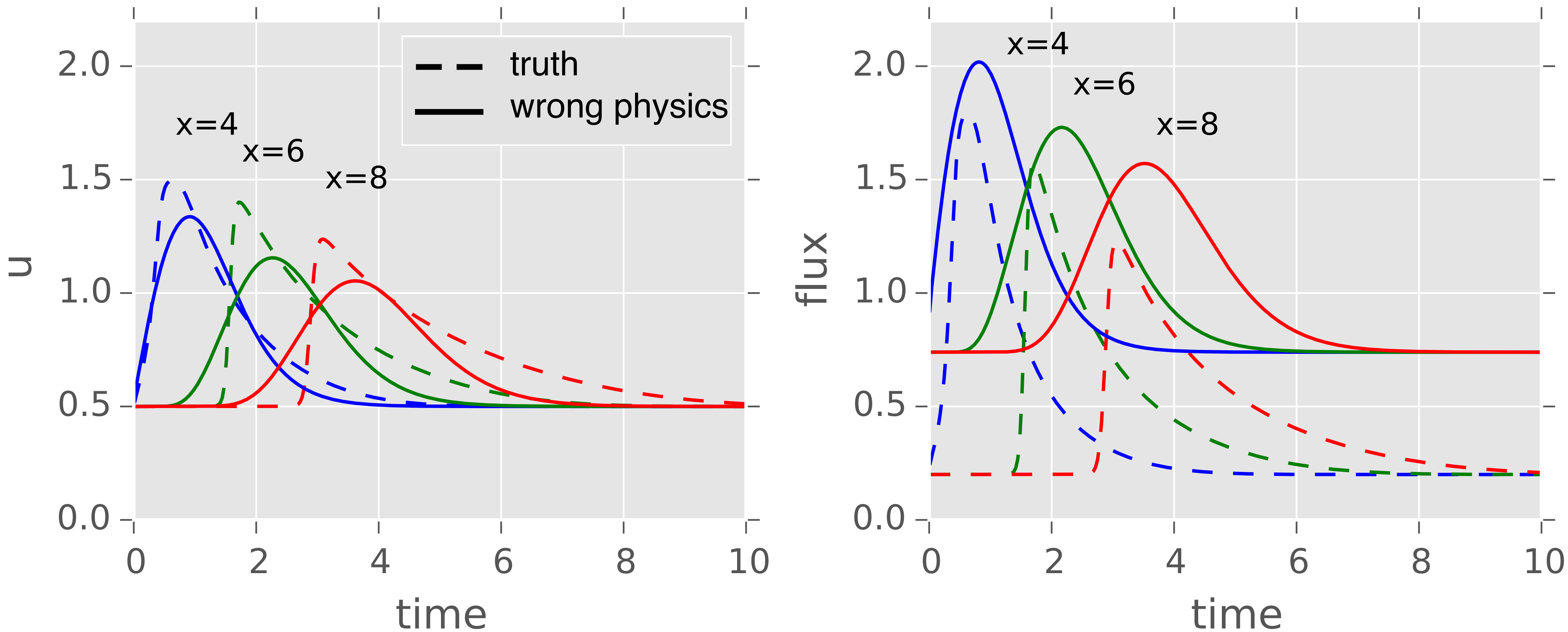
initial conditions

$$u(0) = u(20)$$

boundary conditions

Burgers' Equation Model Form Uncertainty Problems

- incorrect model was fit to data with least squares



Interpolation

can make u(x=6, t) predictions given u(x=4, t) and u(x=8, t)

Type 1 Extrapolation

can make u(x=8, t) predictions given u(x=4, t) and u(x=6, t)

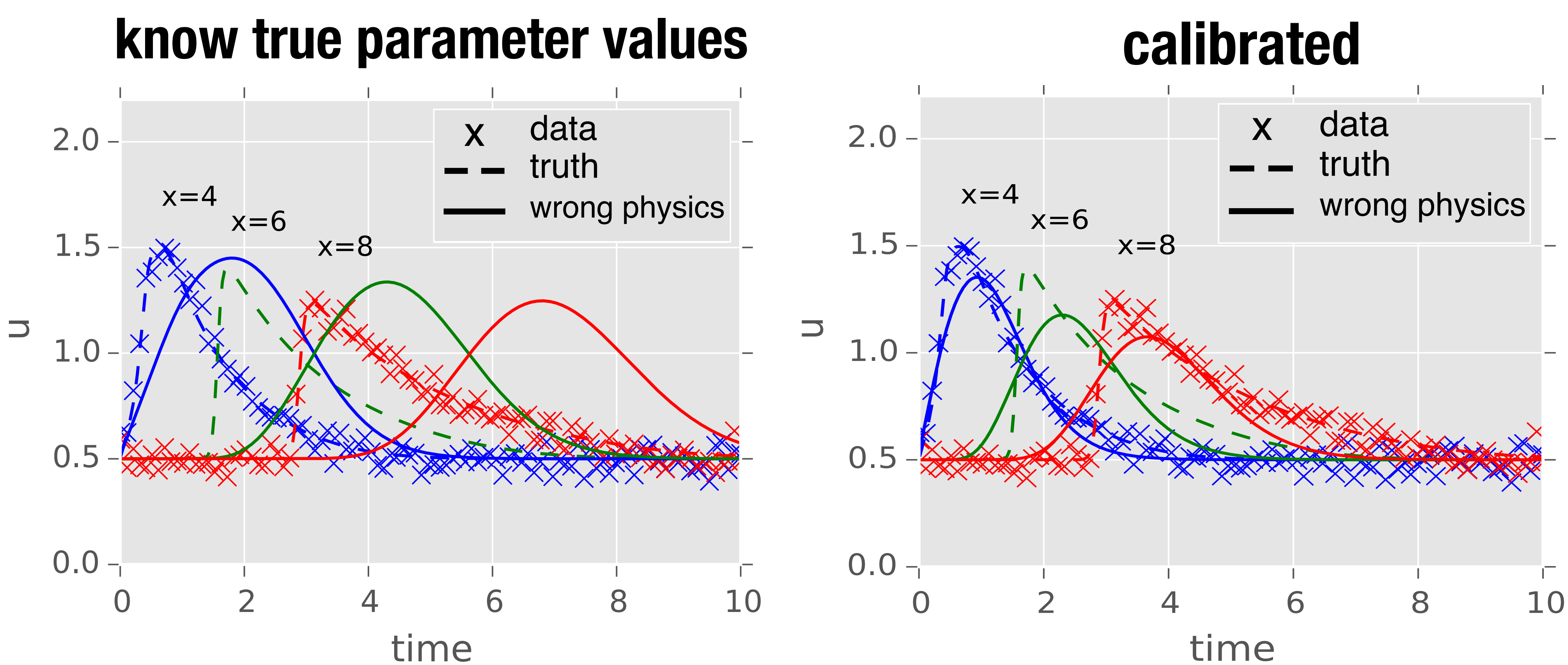
Type 2 Extrapolation

can make flux(x=6, t) predictions given u(x=4, t) and u(x=6, t)

Interpolation

c = 0.8
d = 0.05

c = 1.46
d = 0.20



blue and red are conditions where data exists

green is where prediction is necessary

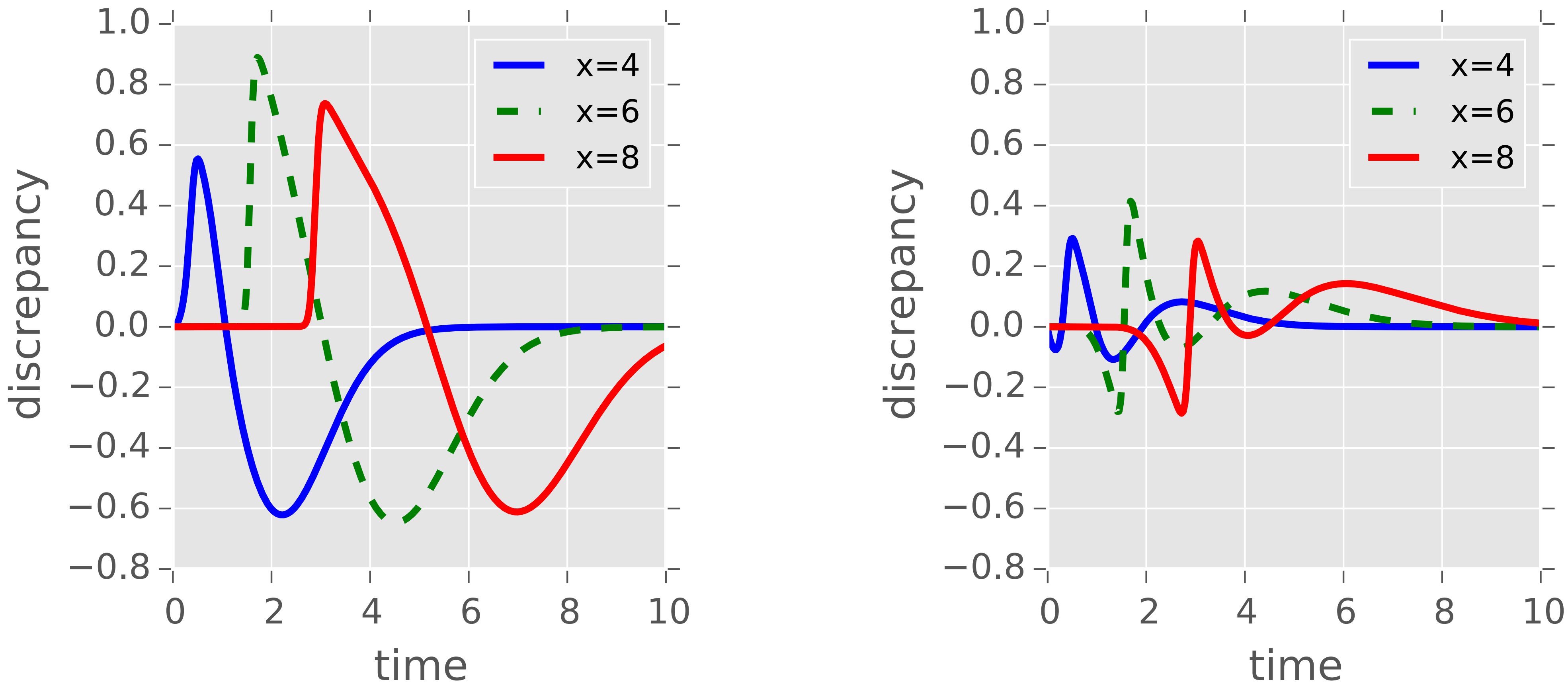
Interpolation

c = 0.8
d = 0.05

know true parameter values

calibrated

c = 1.46
d = 0.20



bias term should allow good interpolation, but calibration may not be physical unless bias form is known a priori

rollup of validation performance into parameter uncertainty or characterizing with error term will be reasonable

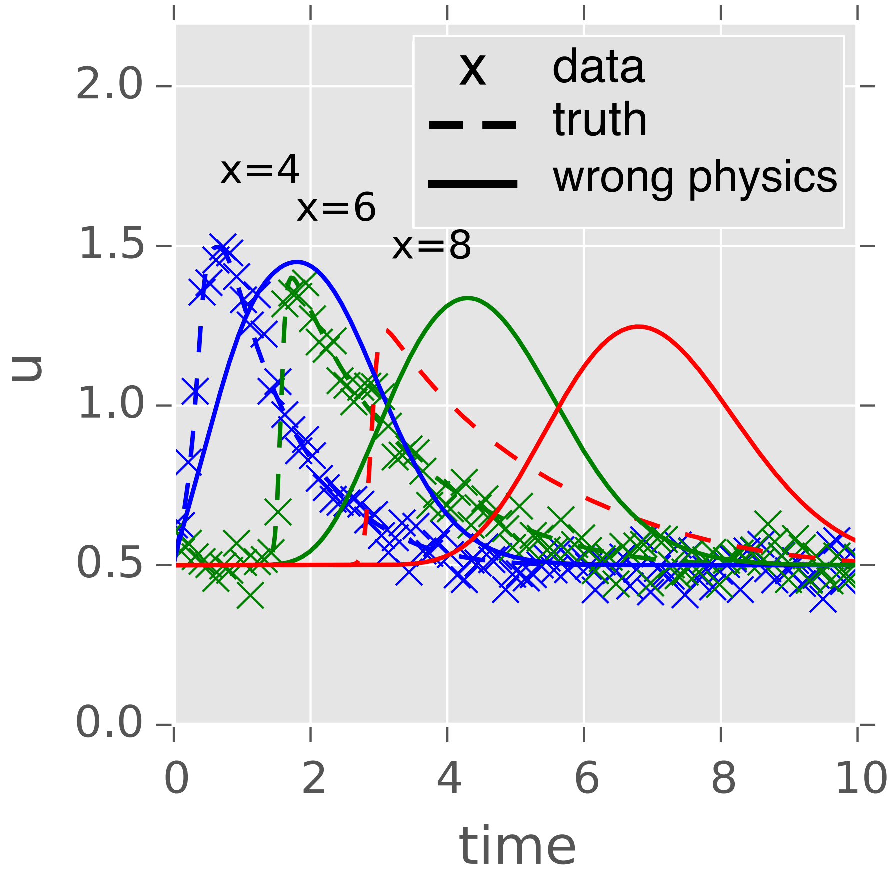
no single set of parameters able to capture data well, but bounding parameter subspace should be able to capture interpolation

Type 1 Extrapolation : In Parameter Space

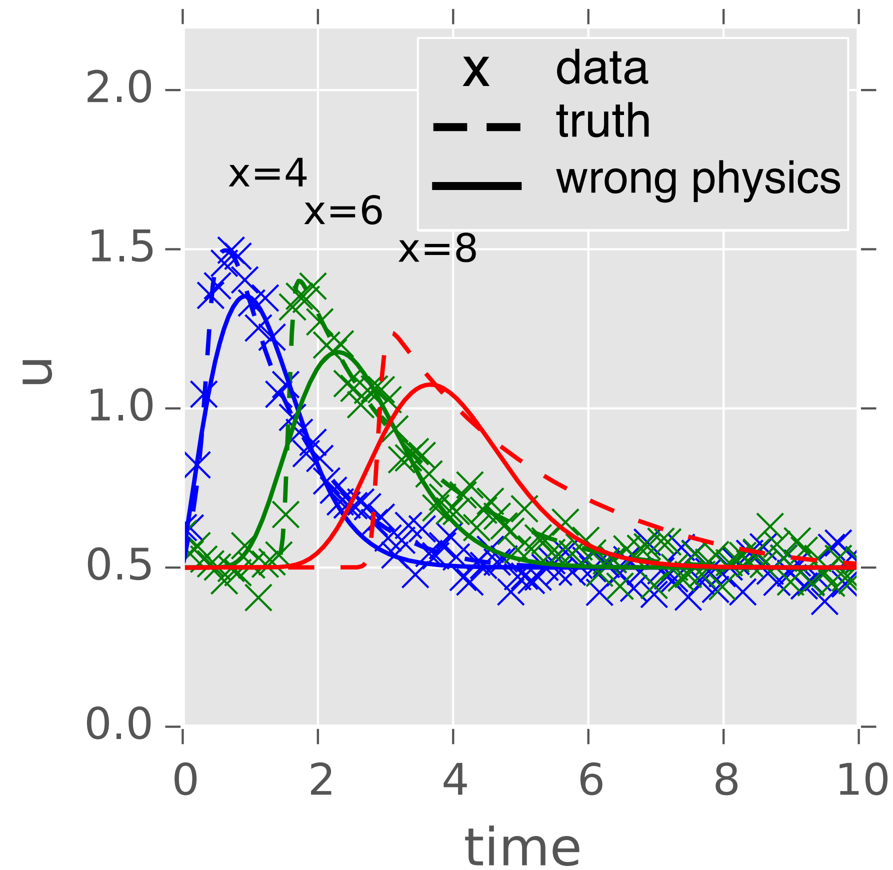
c = 0.8
d = 0.05

c = 1.41
d = 0.19

know true parameter values



calibrated



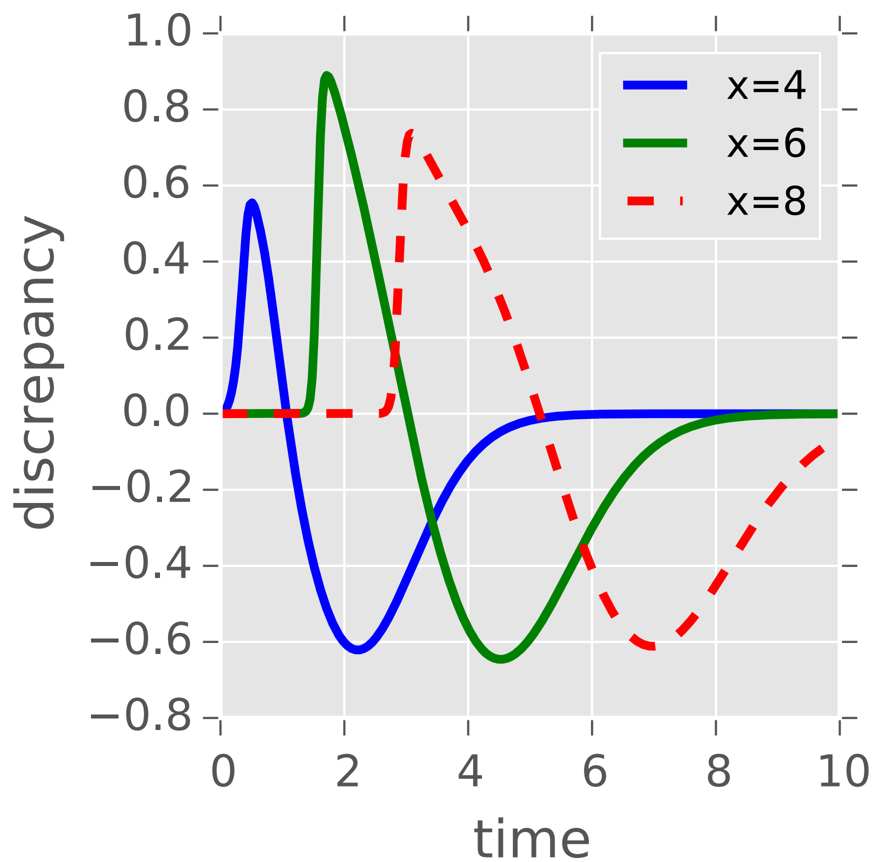
blue and green are conditions where data exists

red is where prediction is necessary

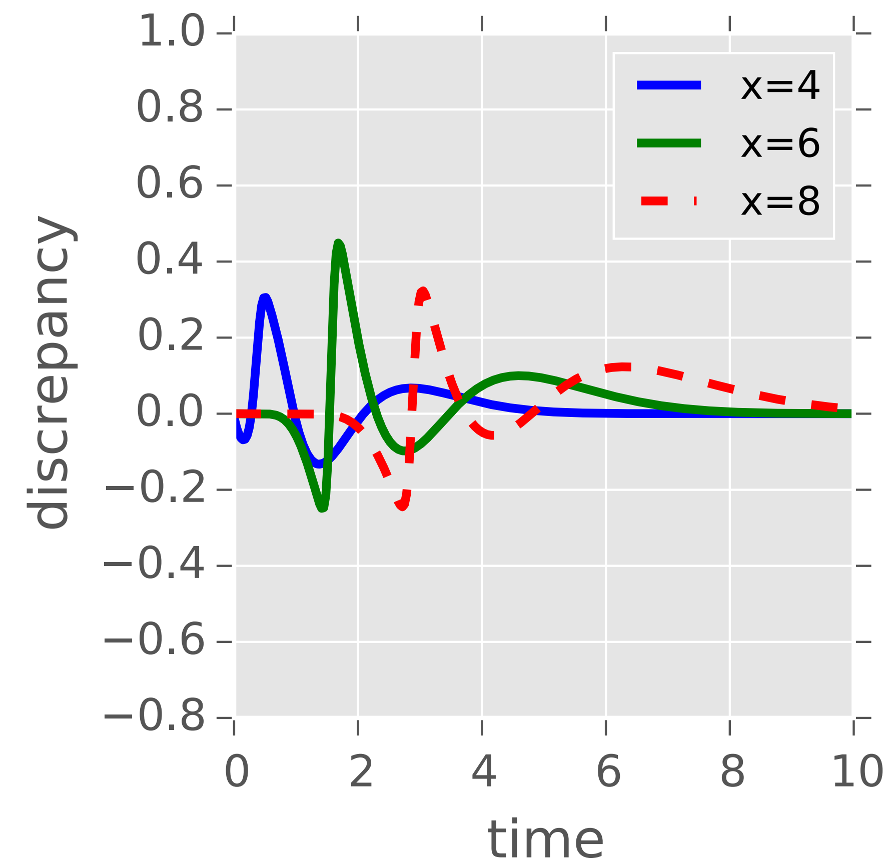
Type 1 Extrapolation : In Parameter Space

c = 0.8
d = 0.05

know true parameter values



calibrated



c = 1.41
d = 0.19

use of bias term becomes questionable for larger extrapolations

rollup of validation results may not be conservative if discrepancy changes across parameter space

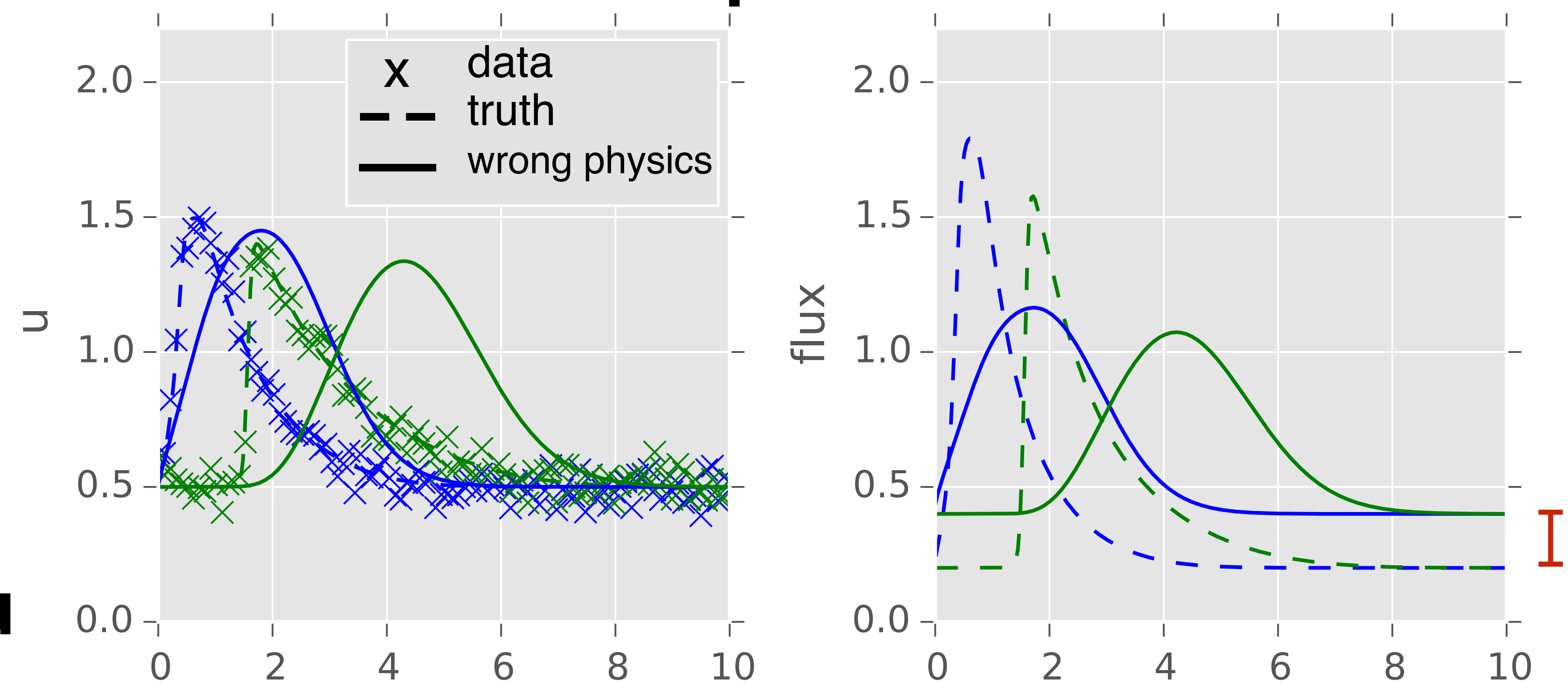
similar issue for characterized validation error

bounded parameter subspace may not capture extrapolations

Type 2 Extrapolation : New QoI

c = 0.8
d = 0.05

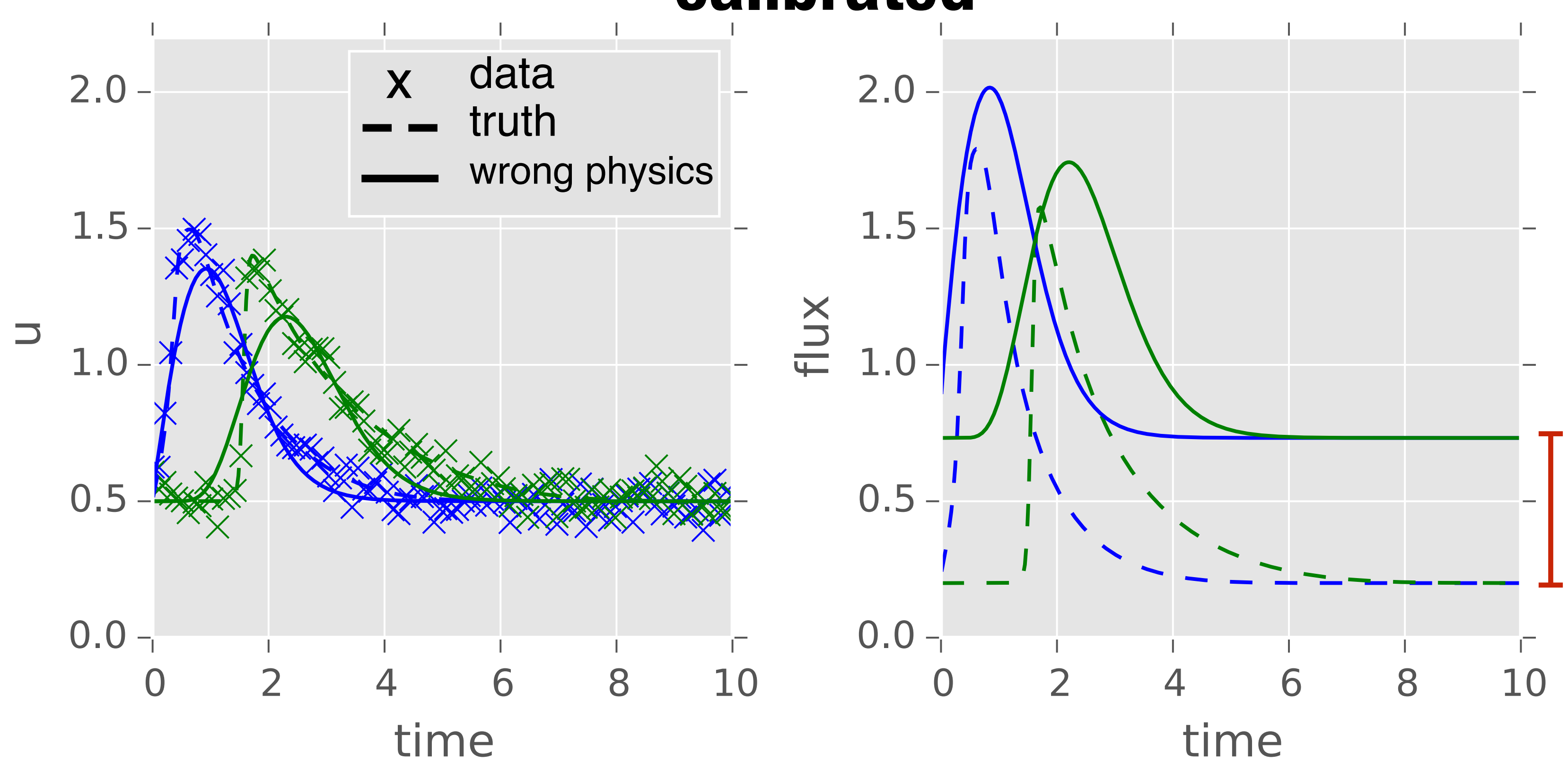
know true parameter values



blue and green data exists for u

model form issue causes gap

calibrated



no data exists for flux

c = 1.46
d = 0.20

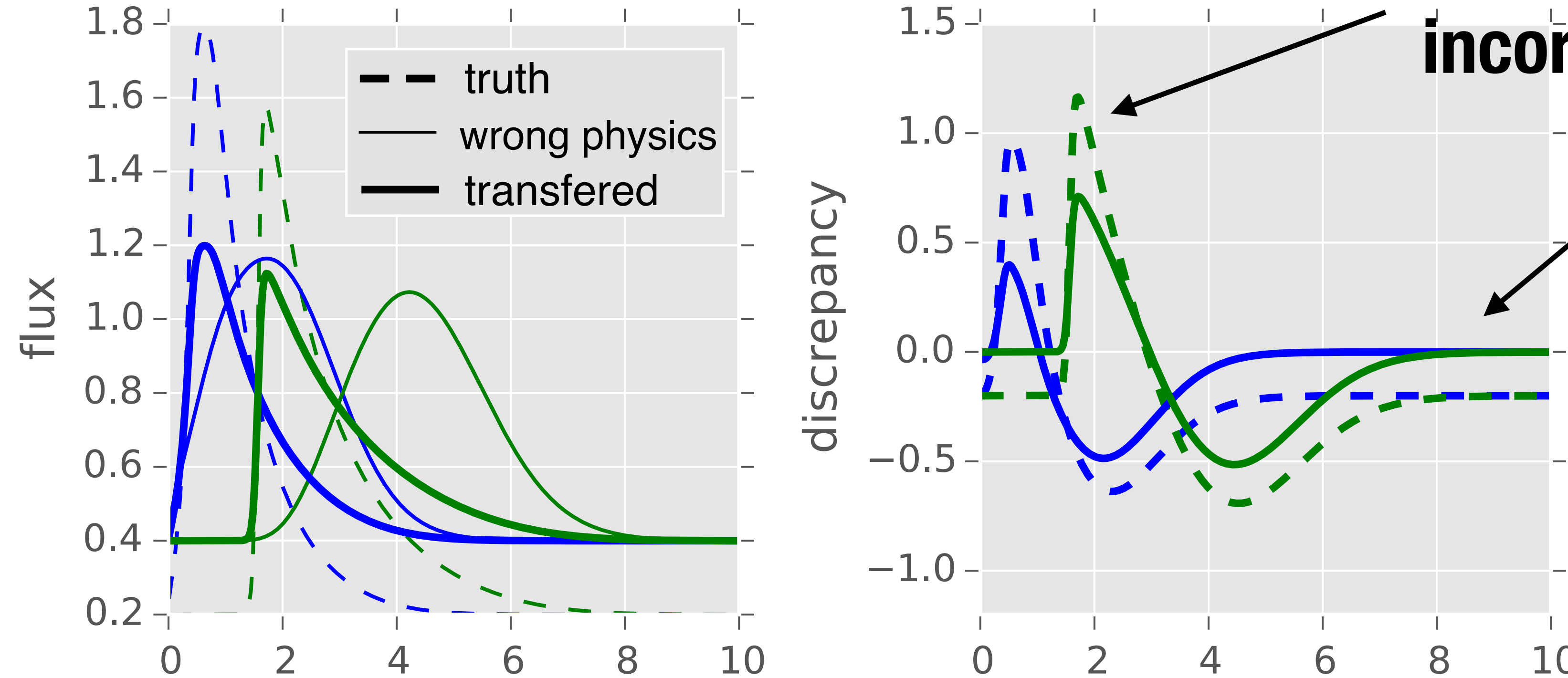
Type 2 Extrapolation : New QoI

c = 0.8
d = 0.05

know true parameter values

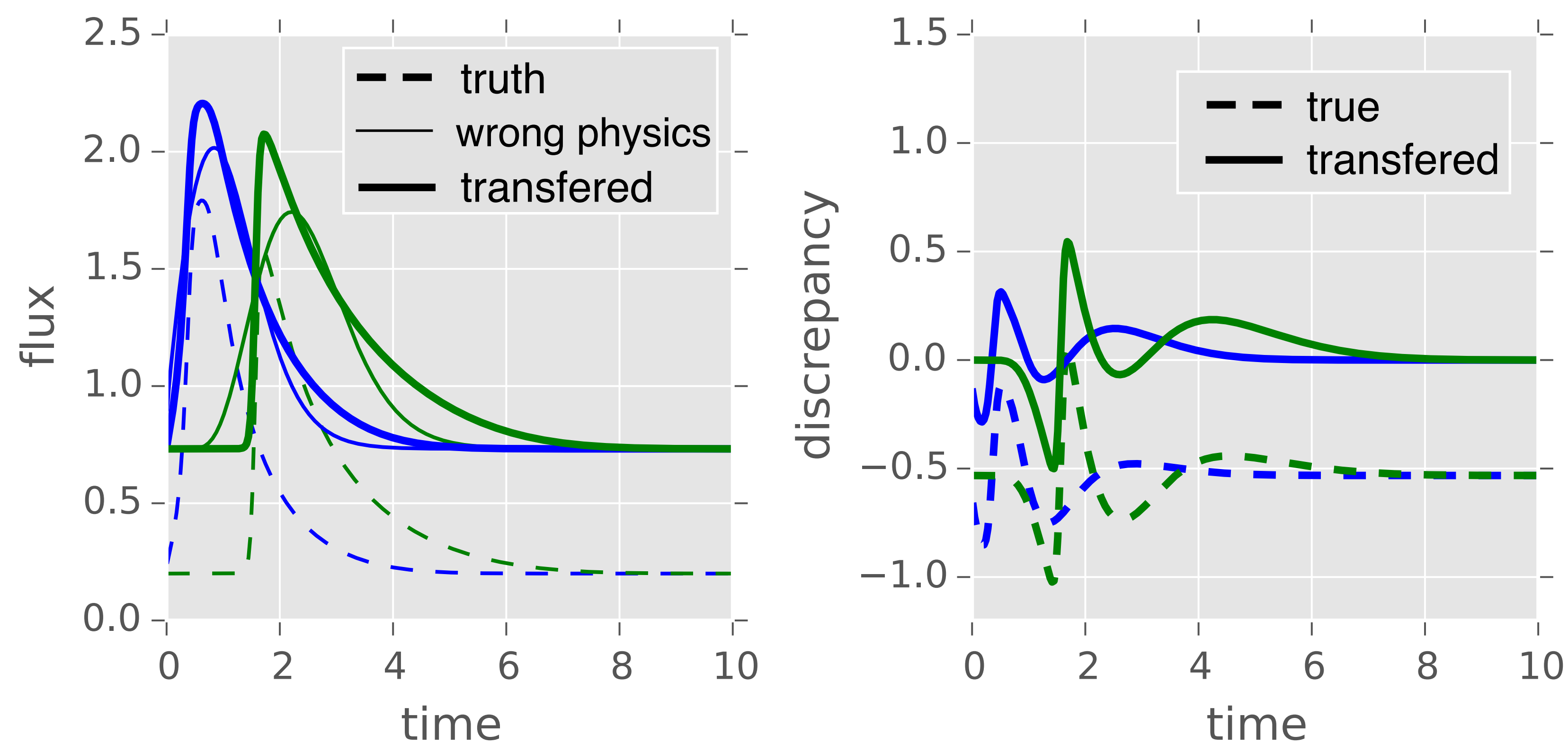
difference between incorrect model and truth

difference between transferred data and truth

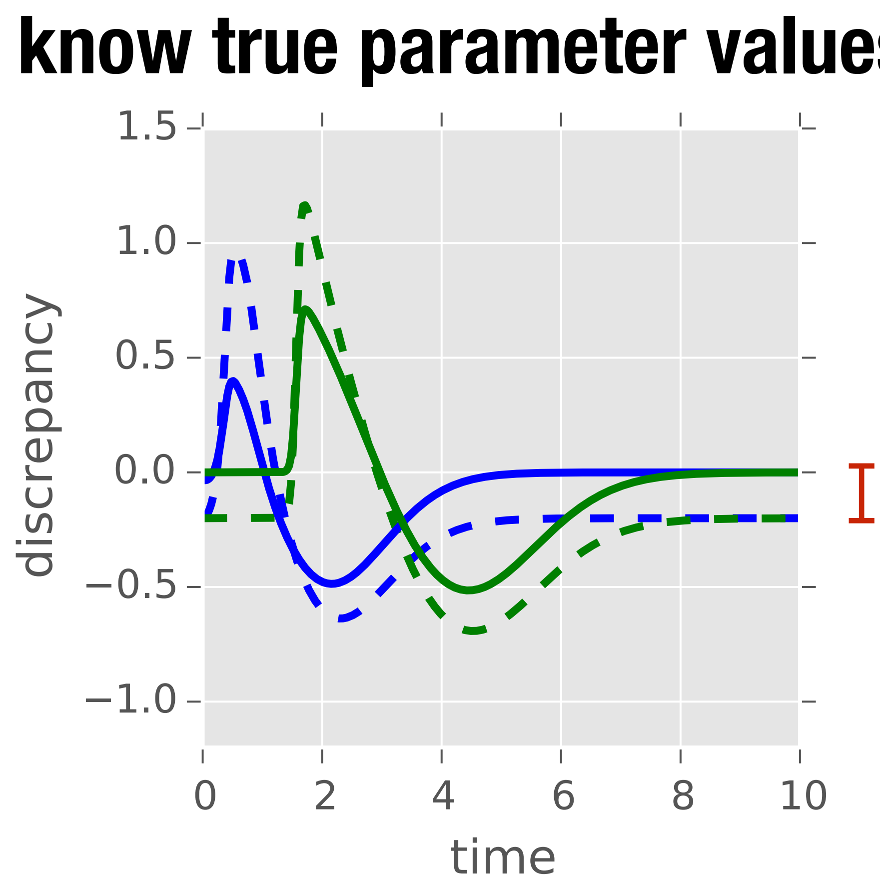


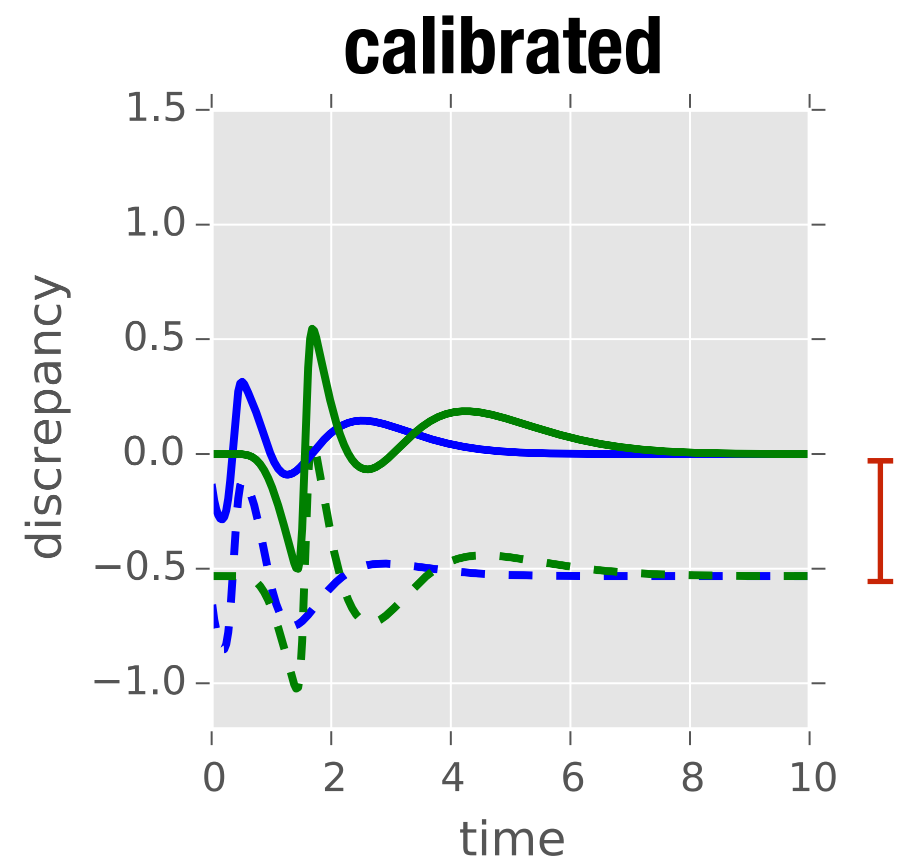
calibrated

c = 1.46
d = 0.20



Type 2 Extrapolation : New QoI





translation of bias to flux has issues due to baseline discrepancy not present in velocity, but captures trends

rollup of validation may have issues with extent of model form error

quantified validation error will perform better if good initial parameter uncertainty

mixed calibration/validation will not translate well to new QoI

Current Hypothesis from Analysis

if converting datatype, parameters should be validated in initial datatype space at a minimum

construct and characterize bias term for interpolations

simultaneously calibrate bias and parameters if bias form known

shy away from constructing bias term for extrapolations in parameter space unless bias form well known

converting bias to new datatype may work if the datatype relation is believed to be well characterized/understood

identifiability issue may cause validation only or validation inclusive schemes to be more sound (safe and conservative)

combining calibration and validation may be unsuccessful when significant model form issues are present

Ongoing Work

- considering how methods of rolling up uncertainty and dealing with model form uncertainty impact resource allocation decisions

- comparing differences in interpretation of methods results

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Questions