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Machine-Learning Error Models for Approximate Solutions to Parameterized Systems of Nonlinear Equations

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Outline

- Introduction
- Parameterized Nonlinear Algebraic Equations
- Proposed Approach
- Numerical Experiments
- Summary

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- Introduction
  - Motivation
  - Solution Approximations
  - Uncertainty Quantification
- Parameterized Nonlinear Algebraic Equations
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Motivation

- Many-query problems can impose a formidable computational burden
- **Solution approximations** can exchange fidelity for speed

Solution Approximations

- **Inexact solutions:** When solving nonlinear equations, prematurely end the iterative process
- **Lower-fidelity models:** Neglect physical phenomena, coarsen the mesh, or use lower-order finite differences or elements
- **Reduced-order models:** Decompose the solution into a linear combination of $m_{\mathbf{u}} \ll N_{\mathbf{u}}$ basis functions

Uncertainty Quantification

- Solution approximations require less time than high-fidelity models but introduce an error (i.e. epistemic uncertainty)

- Ultimate task should account for **all sources of uncertainty**

- We quantify the uncertainty by

  1) engineering **features** informative of the error
     - cheaply computable
     - generated by approximate model

  2) applying **machine learning regression** techniques to construct statistical model of the error from these features

- This work matures our previously developed capabilities:
  - Hand-selecting one feature and applying Gaussian process regression

    M. Drohmann and K. Carlberg (2015)
  - Modeling dynamical systems error using machine learning methods

    S. Trehan et al. (2017)

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- Parameterized Nonlinear Algebraic Equations
  - Overview
  - Approximate Solutions
  - Approaches for Error Quantification
- Proposed Approach
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Parameterized Nonlinear Algebraic Equations

Parameterized systems of nonlinear algebraic equations

$$\mathbf{r}_\star(\mathbf{u}(\boldsymbol{\mu}); \boldsymbol{\mu}) = \mathbf{0}$$

- $\mathbf{r}_\star : \mathbb{R}^{N_\mathbf{u}} \times \mathbb{R}^{N_{\boldsymbol{\mu}}} \rightarrow \mathbb{R}^{N_\mathbf{u}}$ residual, nonlinear in at least $\mathbf{u}(\boldsymbol{\mu})$
- $\boldsymbol{\mu} \in \mathcal{D}$ parameters in parameter domain $\mathcal{D} \subseteq \mathbb{R}^{N_{\boldsymbol{\mu}}}$
- $\mathbf{u} : \mathbb{R}^{N_{\boldsymbol{\mu}}} \rightarrow \mathbb{R}^{N_\mathbf{u}}$ state (solution vector)

Quantity of Interest

Scalar-valued quantity of interest

$$s(\boldsymbol{\mu}) \equiv g(\mathbf{u}(\boldsymbol{\mu}))$$

- $s : \mathbb{R}^{N_{\boldsymbol{\mu}}} \rightarrow \mathbb{R}$ quantity of interest
- $g : \mathbb{R}^{N_{\mathbf{u}}} \rightarrow \mathbb{R}$ dependency of the quantity of interest upon the state

Approximate Solutions

- Computing the exact solution $\mathbf{u}(\boldsymbol{\mu})$ can be
  - prohibitively expensive (large $N_{\mathbf{u}}$)
  - unnecessary (inexact solutions suffice for optimization convergence)
- Such cases require an approximate solution $\tilde{\mathbf{u}} : \mathbb{R}^{N_{\boldsymbol{\mu}}} \to \mathbb{R}^{N_{\mathbf{u}}}$
- Approximate solution leads to approximated quantity of interest

$$\tilde{s}(\boldsymbol{\mu}) \equiv g(\tilde{\mathbf{u}}(\boldsymbol{\mu})),$$

where $\tilde{s} : \mathbb{R}^{N_{\boldsymbol{\mu}}} \to \mathbb{R}$

Approximate Solutions (continued)

We consider 3 approaches for computing approximate solutions:

1) Premature termination of nonlinear iterations

2) Lower-fidelity model

3) Model reduction

Inexact Solutions

- Iterative solution to nonlinear equations: sequence of approximations

$$\mathbf{u}^{(k)}, \quad k = 0, \ldots, K$$

- Approximate solution $\mathbf{u}^{(K)}$ can be obtained after iteration K

$$\tilde{\mathbf{u}}(\boldsymbol{\mu}) = \mathbf{u}^{(K)}$$

- K can be determined by
  - satisfying a modest (e.g., $\epsilon = 0.1$) tolerance

$$\|\mathbf{r}_\star(\mathbf{u}^{(K)}; \boldsymbol{\mu})\| / \|\mathbf{r}_\star(\mathbf{0}; \boldsymbol{\mu})\| < \epsilon$$

  - selecting a modest maximum number of iterations (e.g., K=2)

Lower-Fidelity Models

Fidelity reduction approaches

- Neglect physical phenomena
- Reduce spatial accuracy
  - Coarsen the mesh and prolongate (interpolate) the solution:

$$\tilde{\mathbf{u}} = \mathbf{A}\mathbf{u}_{\mathrm{LF}}, \quad \mathbf{A} \in \mathbb{R}^{N_{\mathbf{u}} \times N_{\mathbf{u}_{\mathrm{LF}}}}$$

  - Use lower-order finite differences or elements

Model Reduction

Model reduction restricts approximate solution $\tilde{\mathbf{u}}$ to $m_{\mathbf{u}}$-dimensional affine trial subspace $\bar{\mathbf{u}} + \mathrm{Ran}(\boldsymbol{\Phi}_{\mathbf{u}}) \subseteq \mathbb{R}^{N_{\mathbf{u}}}$ with $m_{\mathbf{u}} \ll N_{\mathbf{u}}$:

$$\tilde{\mathbf{u}}(\boldsymbol{\mu}) = \bar{\mathbf{u}} + \boldsymbol{\Phi}_{\mathbf{u}}\hat{\mathbf{u}}(\boldsymbol{\mu})$$

- $\boldsymbol{\Phi}_{\mathbf{u}} \in \mathbb{R}_{\star}^{N_{\mathbf{u}} \times m_{\mathbf{u}}}$ trial basis, computed using
  - proper orthogonal decomposition (POD)
  - the reduced-basis method
  - variants that employ gradient information
- $\hat{\mathbf{u}} : \mathbb{R}^{N_{\boldsymbol{\mu}}} \to \mathbb{R}^{m_{\mathbf{u}}}$ generalized coordinates of the approx. solution
- $\bar{\mathbf{u}} \in \mathbb{R}^{N_{\mathbf{u}}}$ a reference state

Model Reduction (continued)

- $\mathbf{r}_\star(\bar{\mathbf{u}} + \boldsymbol{\Phi}_\mathbf{u}\hat{\mathbf{u}}(\boldsymbol{\mu}); \boldsymbol{\mu}) = \mathbf{0}$ is overdetermined: $N_\mathbf{u}$ equations, $m_\mathbf{u}$ unknowns
- Second step projects residual onto an $m_\mathbf{u}$-dimensional test subspace $\text{Ran}(\boldsymbol{\Psi}_\mathbf{u}) \subseteq \mathbb{R}^{N_\mathbf{u}}$:

$$\boldsymbol{\Psi}_\mathbf{u}^T \mathbf{r}_\star(\bar{\mathbf{u}} + \boldsymbol{\Phi}_\mathbf{u}\hat{\mathbf{u}}(\boldsymbol{\mu}); \boldsymbol{\mu}) = \mathbf{0}$$

- $\boldsymbol{\Psi}_\mathbf{u} \in \mathbb{R}_\star^{N_\mathbf{u} \times m_\mathbf{u}}$ is test basis, common choices include
  - Galerkin projection: $\boldsymbol{\Psi}_\mathbf{u} = \boldsymbol{\Phi}_\mathbf{u}$
  - Least-squares Petrov–Galerkin projection: $\boldsymbol{\Psi}_\mathbf{u} = \dfrac{\partial \mathbf{r}_\star}{\partial \mathbf{u}}(\bar{\mathbf{u}} + \boldsymbol{\Phi}_\mathbf{u}\hat{\mathbf{u}}(\boldsymbol{\mu}); \boldsymbol{\mu})\boldsymbol{\Phi}_\mathbf{u}$

Approaches for Error Quantification

- Regardless of approach, it is essential to quantify error incurred by employing approximate solution $\tilde{\mathbf{u}}$ in lieu of exact solution $\mathbf{u}$

- Existing approaches include
  - Data-fit mapping between parameters and the error
    - Inspired by multifidelity design optimization
  - Reduced-Order Model Error Surrogates (ROMES) method

    M. Drohmann and K. Carlberg, 2015
    - Quantity of interest error approximation using dual-weighted residuals
    - Normed state-space error approx. using residual norm and error bounds

- This work focuses on quantifying two such errors:
  1) Error in quantity of interest: $\delta_s(\boldsymbol{\mu}) \equiv s(\boldsymbol{\mu}) - \tilde{s}(\boldsymbol{\mu})$
  2) Normed state-space error: $\delta_{\mathbf{u}}(\boldsymbol{\mu}) \equiv \|\mathbf{e}(\boldsymbol{\mu})\|_2$, where $\mathbf{e}(\boldsymbol{\mu}) \equiv \mathbf{u}(\boldsymbol{\mu}) - \tilde{\mathbf{u}}(\boldsymbol{\mu})$

State-Space Error

The residual can be approximated about the approximate solution $\tilde{\mathbf{u}}$:

$$\mathbf{r}_\star(\mathbf{u}(\boldsymbol{\mu});\boldsymbol{\mu}) = \mathbf{0} = \mathbf{r}(\boldsymbol{\mu}) + \mathbf{J}(\boldsymbol{\mu})\mathbf{e}(\boldsymbol{\mu}) + \mathcal{O}(\|\mathbf{e}(\boldsymbol{\mu})\|^2)$$

and rearranged to approximate the state-space error:

$$\mathbf{e}(\boldsymbol{\mu}) = -\mathbf{J}(\boldsymbol{\mu})^{-1}\mathbf{r}(\boldsymbol{\mu}) + \mathcal{O}(\|\mathbf{e}(\boldsymbol{\mu})\|^2)$$

- $\mathbf{r}(\boldsymbol{\mu}) \equiv \mathbf{r}_\star(\tilde{\mathbf{u}}(\boldsymbol{\mu});\boldsymbol{\mu})$ residual from approximate solution
- $\mathbf{J}(\boldsymbol{\mu}) \equiv \dfrac{\partial \mathbf{r}_\star}{\partial \mathbf{u}}(\tilde{\mathbf{u}}(\boldsymbol{\mu});\boldsymbol{\mu}) \in \mathbb{R}^{N_\mathbf{u}\times N_\mathbf{u}}$ Jacobian of residual at $\tilde{\mathbf{u}}(\boldsymbol{\mu})$

Error in the Quantity of Interest

The quantity of interest also can be approximated:

$$s(\boldsymbol{\mu}) = \tilde{s}(\boldsymbol{\mu}) + \frac{\partial g}{\partial \mathbf{u}}(\tilde{\mathbf{u}}(\boldsymbol{\mu}))\mathbf{e}(\boldsymbol{\mu}) + \mathcal{O}(\|\mathbf{e}(\boldsymbol{\mu})\|^2)$$

and combined with the state-space error approximation to yield

$$\delta_s(\boldsymbol{\mu}) = \underbrace{-\frac{\partial g}{\partial \mathbf{u}}(\tilde{\mathbf{u}}(\boldsymbol{\mu}))\mathbf{J}(\boldsymbol{\mu})^{-1}}_{\mathbf{y}(\boldsymbol{\mu})^T}\mathbf{r}(\boldsymbol{\mu}) + \mathcal{O}(\|\mathbf{e}(\boldsymbol{\mu})\|^2)$$

- $\mathbf{y}(\boldsymbol{\mu})$ is the dual or adjoint
- dual-weighted residual d is weighted sum of residual elements:

$$d(\boldsymbol{\mu}) \equiv \mathbf{y}(\boldsymbol{\mu})^T\mathbf{r}(\boldsymbol{\mu})$$

Drawbacks to using the Dual-Weighted Residual

- **Computational Cost:** requires solving $N_{\mathbf{u}}$ linear equations
- **Implementation:** requires Jacobian – not always available
- **Uncertainty Quantification:** low-bias error estimate not assured

Nonetheless, construction provides insight into quantity-of-interest error

Normed State-Space Error

- Residual-based bounds commonly used to quantify $\delta_{\mathbf{u}}(\boldsymbol{\mu})$

  A. Buffa et al., 2012; M. A. Grepl and A. T. Patera, 2005; G. Rozza et al., 2008

- Assuming Lipschitz continuity for the residual $\mathbf{r}_{\star}(\cdot;\boldsymbol{\mu})$, then

$$\frac{\|\mathbf{r}(\boldsymbol{\mu})\|_2}{\beta(\boldsymbol{\mu})} \leq \delta_{\mathbf{u}}(\boldsymbol{\mu}) \leq \frac{\|\mathbf{r}(\boldsymbol{\mu})\|_2}{\alpha(\boldsymbol{\mu})},$$

  where α and β are Lipschitz constants

- Drawbacks to using error bounds
  - **Sharpness:** Upper/lower bounds can overpredict/underpredict actual error by several orders of magnitude
  - **Implementation:** Difficult to compute true Lipschitz constants
  - **Uncertainty Quantification:** Do not produce statistical distribution over $\delta_{\mathbf{u}}(\boldsymbol{\mu})$ – cannot quantify epistemic uncertainty

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  - Regression-Function Approximation
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Overview

- We aim to construct statistical models of
  - quantity-of-interest error δ_s
  - normed state-space error $\delta_{\mathbf{u}}$
- We apply high-dimensional regression methods from machine learning
- We use a large number of inexpensive error indicators, resulting in less costly, more accurate error models

Error Model

- Assume there exist $N_{\mathbf{x}}$ *error indicators* or *features* $\mathbf{x}(\boldsymbol{\mu}) \in \mathbb{R}^{N_{\mathbf{x}}}$
  - available from solution approximation
  - cheaply computable
  - informative of the error $\delta(\boldsymbol{\mu}) \in \mathbb{R}$
- We model the nondeterministic mapping $\mathbf{x}(\boldsymbol{\mu}) \mapsto \delta(\boldsymbol{\mu})$

$$\delta(\boldsymbol{\mu}) = f(\mathbf{x}(\boldsymbol{\mu})) + \epsilon(\mathbf{x}(\boldsymbol{\mu}))$$

- f: deterministic regression function
- ϵ: nondeterministic noise
  - Mean-zero random variable
  - Accounts for irreducible error due to missing features
  - Epistemic – additional features can enable zero noise

Regression Model

- Regression function defines conditional expectation of error given the features:

$$\mathrm{E}[\delta(\boldsymbol{\mu}) \mid \mathbf{x}(\boldsymbol{\mu})] = f(\mathbf{x}(\boldsymbol{\mu}))$$

- We construct approximations of
  - deterministic regression function $\hat{f}(\approx f)$
  - nondeterministic noise $\hat{\epsilon}(\approx \epsilon)$,

  which yield a statistical model for the approximate-solution error

$$\hat{\delta}(\boldsymbol{\mu}) = \hat{f}(\mathbf{x}(\boldsymbol{\mu})) + \hat{\epsilon}(\mathbf{x}(\boldsymbol{\mu}))$$

Regression Model Objectives

- **Cheap:** Should employ cheaply computable features $\mathbf{x}$
- **Low Noise Variance:** Should exhibit low noise variance, reduce epistemic uncertainty introduced by approximate solution
- **Numerically Validated:** Empirical distributions of $\hat{\delta}$ and δ should be close on test set **not** used to train model – should not overfit on training data

Regression Model Construction Steps

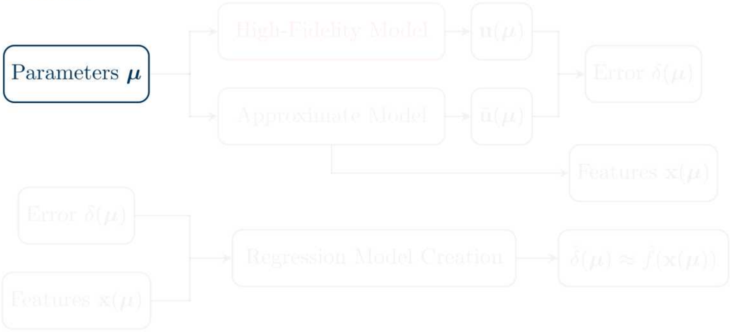
1) **Feature engineering**
   - Cheaply computable features $\mathbf{x}$ from approximate model
   - Informative of the error – construct low-noise-variance model
   - Low dimensional (small $N_{\mathbf{x}}$) such that less training data is needed

2) **Regression-function approximation**
   - Construct $\hat{f}$ using methods from machine learning
   - Approximate mapping from features $\mathbf{x}$ to error δ on a training set

3) **Noise approximation**
   - Mean-zero, constant-variance Gaussian random variable: $\hat{\epsilon} \sim \mathcal{N}(0, \hat{\sigma}^2)$
   - $\hat{\sigma}^2$ is sample variance of regression-model noise on test set (mean squared error on test set)

Summary

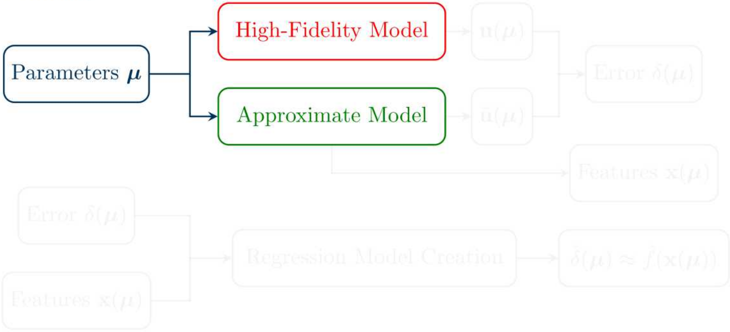
Training



Application

Summary

Training



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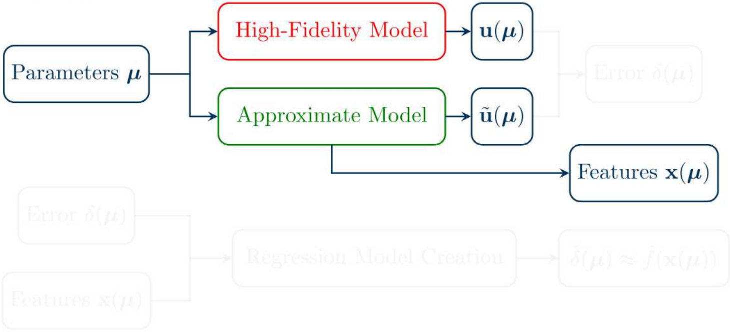

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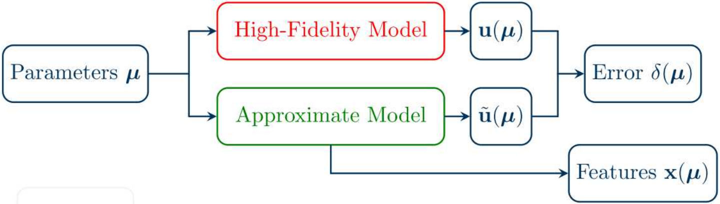

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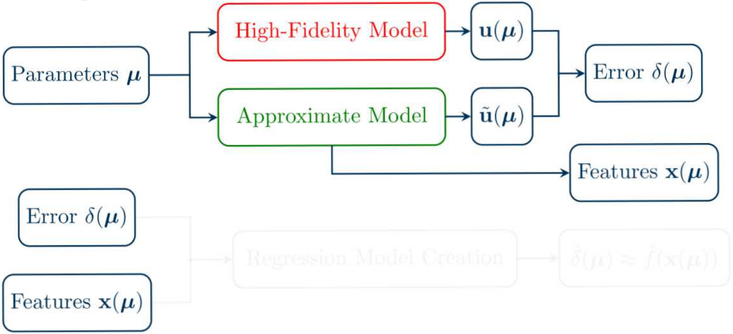

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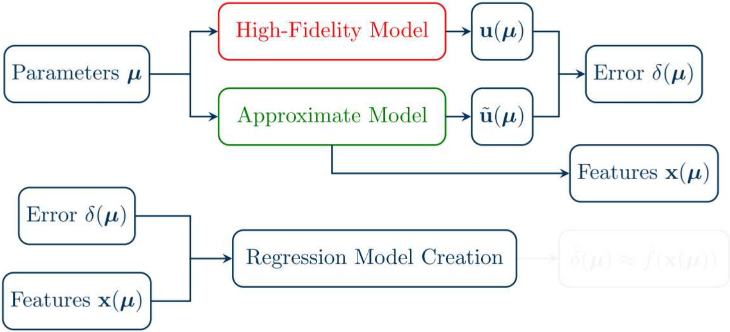

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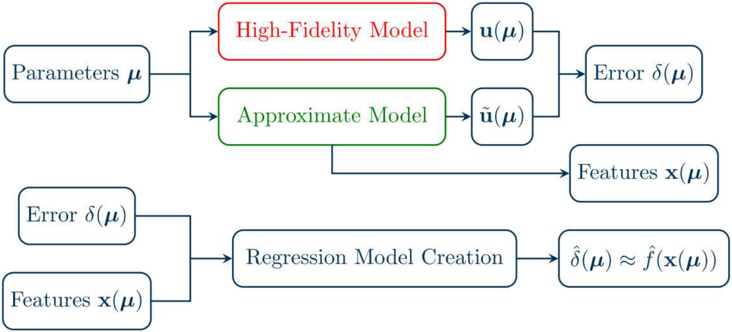

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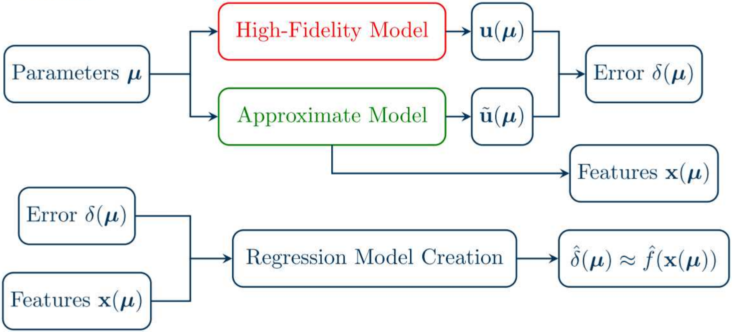

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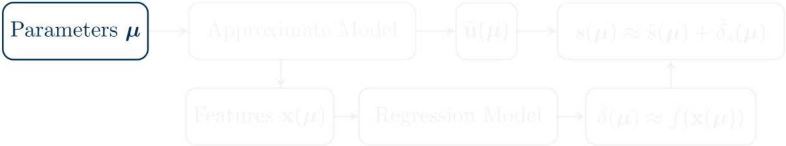

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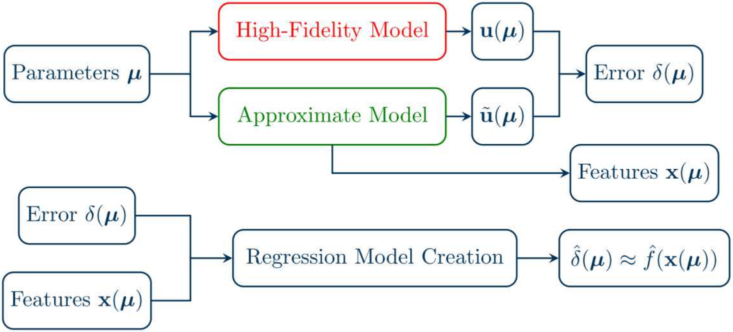

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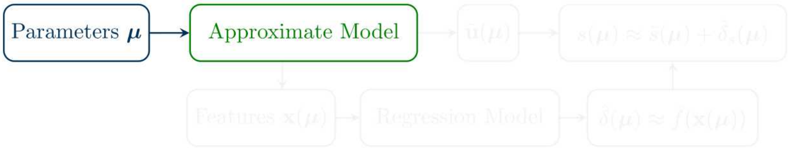

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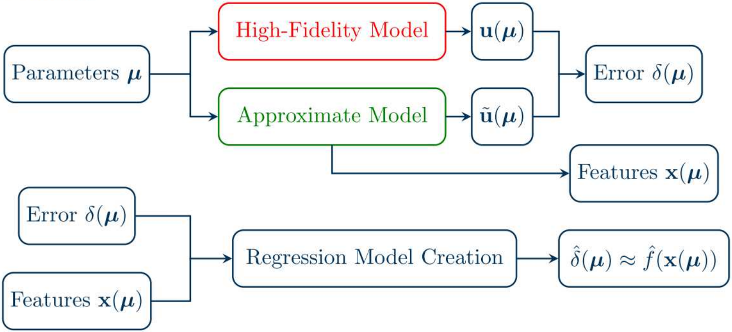

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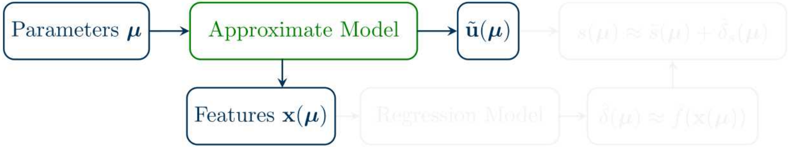

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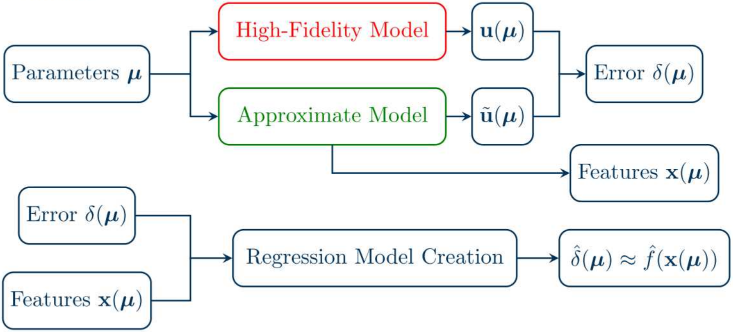

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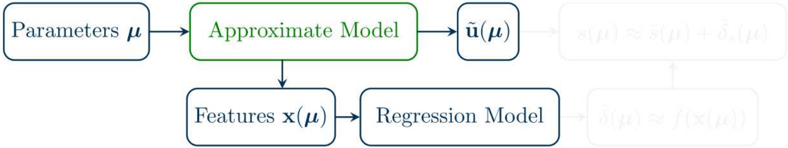

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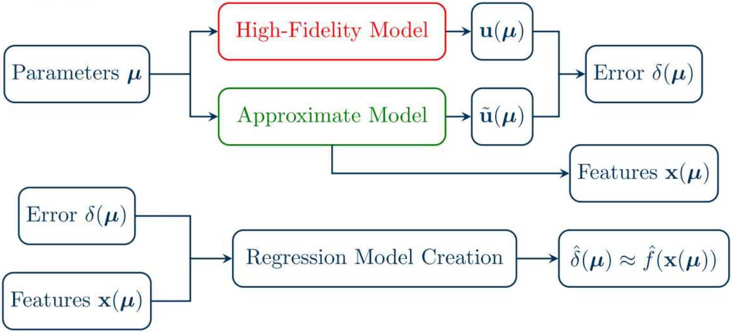

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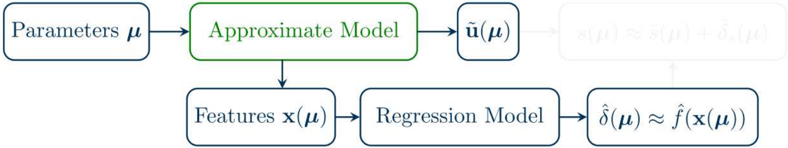

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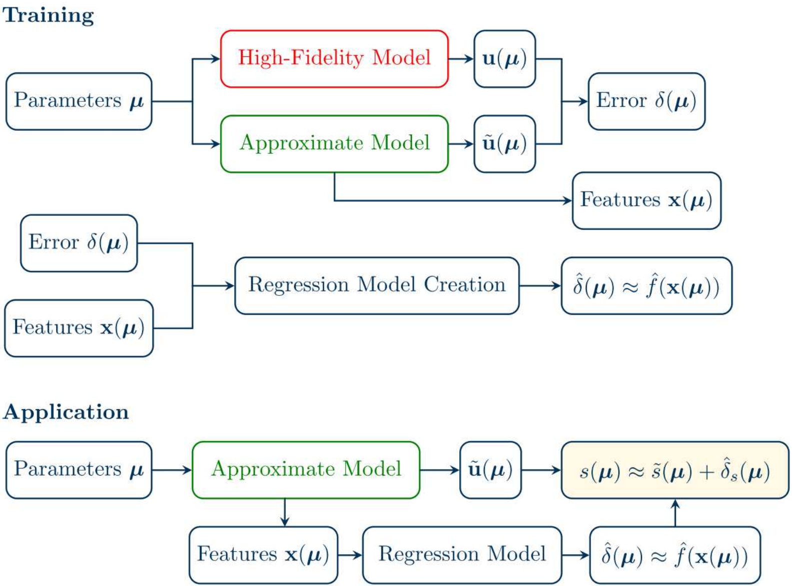
Training
Parameters $\boldsymbol{\mu}$
High-Fidelity Model
Approximate Model
$\mathbf{u}(\boldsymbol{\mu})$
$\tilde{\mathbf{u}}(\boldsymbol{\mu})$
Error $\delta(\boldsymbol{\mu})$
Features $\mathbf{x}(\boldsymbol{\mu})$
Error $\delta(\boldsymbol{\mu})$
Features $\mathbf{x}(\boldsymbol{\mu})$
Regression Model Creation
$\hat{\delta}(\boldsymbol{\mu}) \approx \hat{f}(\mathbf{x}(\boldsymbol{\mu}))$
Application
Parameters $\boldsymbol{\mu}$
Approximate Model
$\tilde{\mathbf{u}}(\boldsymbol{\mu})$
$s(\boldsymbol{\mu}) \approx \tilde{s}(\boldsymbol{\mu}) + \hat{\delta}_s(\boldsymbol{\mu})$
Features $\mathbf{x}(\boldsymbol{\mu})$
Regression Model
$\hat{\delta}(\boldsymbol{\mu}) \approx \hat{f}(\mathbf{x}(\boldsymbol{\mu}))$

Feature Engineering: Parameters

$$\mathbf{x}(\boldsymbol{\mu}) = \boldsymbol{\mu}$$

- The mapping $\boldsymbol{\mu} \mapsto \delta(\boldsymbol{\mu})$ is deterministic, but often complex
  - Can be oscillatory for ROMs since $\delta(\boldsymbol{\mu}) \approx 0$ when $\boldsymbol{\mu} \in \mathcal{D}_{\mathrm{Train}}^{\mathrm{ROM}}$
- Could yield zero noise variance if
  - Large amounts of training data
  - Sufficiently flexible regression model
- Low-quality feature
- Used by 'multifidelity correction' methods for optimization

  Alexandrov et al., 2001; Gano et al., 2005; Eldred et al., 2004

Feature Engineering: Dual-Weighted Residual

$$\mathbf{x}(\boldsymbol{\mu}) = d(\boldsymbol{\mu}) \equiv \mathbf{y}(\boldsymbol{\mu})^T \mathbf{r}(\boldsymbol{\mu})$$

- Second-order-accurate approximation of QoI error $\delta_s(\boldsymbol{\mu})$
- Small number ($N_{\mathbf{x}} = 1$) of high-quality features
- High computational cost and significant implementation effort
- ROMES method uses approximation for dual-weighted residual

  M. Drohmann and K. Carlberg, 2015

Feature Engineering: Parameters and Residual (Approximations)

$$\mathbf{x}(\boldsymbol{\mu}) = [\boldsymbol{\mu}; \mathbf{r}(\boldsymbol{\mu})]$$

- DWR is weighted sum of residual vector elements $d(\boldsymbol{\mu}) \equiv \mathbf{y}(\boldsymbol{\mu})^T \mathbf{r}(\boldsymbol{\mu})$
- Avoids implementation and costs associated with dual vector $\mathbf{y}(\boldsymbol{\mu})$
- Large number ($N_{\mathbf{x}} = N_{\boldsymbol{\mu}} + N_{\mathbf{u}}$) of low-quality features
- Approaches to reduce number of features and improve quality
  - Use $m_{\mathbf{r}} \ll N_{\mathbf{u}}$ principal component coefficients: $\hat{\mathbf{r}}(\boldsymbol{\mu})$
  - Sample $n_{\mathbf{r}} \ll N_{\mathbf{u}}$ elements of residual: $\mathbf{P}\mathbf{r}(\boldsymbol{\mu})$, where $\mathbf{P} \in \{0,1\}^{n_{\mathbf{r}} \times N_{\mathbf{u}}}$
  - Use $m_{\mathbf{r}} \ll N_{\mathbf{u}}$ gappy principal component coefficients: $\hat{\mathbf{r}}_{\mathrm{g}}(\boldsymbol{\mu})$

Feature Engineering: Residual Norm with/without Parameters

$$\mathbf{x}(\boldsymbol{\mu}) = \|\mathbf{r}(\boldsymbol{\mu})\|_2 \quad \text{or} \quad \mathbf{x}(\boldsymbol{\mu}) = [\boldsymbol{\mu};\ \|\mathbf{r}(\boldsymbol{\mu})\|_2]$$

- DWR can be bounded using the Cauchy–Schwarz inequality:

$$|d(\boldsymbol{\mu})| \leq \|\mathbf{y}(\boldsymbol{\mu})\|_2 \|\mathbf{r}(\boldsymbol{\mu})\|_2$$

- Normed state-space error $\delta_{\mathbf{u}}(\boldsymbol{\mu})$ can be bounded:

  M. Drohmann and K. Carlberg, 2015

$$\frac{\|\mathbf{r}(\boldsymbol{\mu})\|_2}{\beta(\boldsymbol{\mu})} \leq \delta_{\mathbf{u}}(\boldsymbol{\mu}) \leq \frac{\|\mathbf{r}(\boldsymbol{\mu})\|_2}{\alpha(\boldsymbol{\mu})}$$

- $\boldsymbol{\mu}$ can be omitted ($\mathbf{x}(\boldsymbol{\mu}) = \|\mathbf{r}(\boldsymbol{\mu})\|_2$) if
  - $\boldsymbol{\mu}$ is not indicative of error
  - $N_{\boldsymbol{\mu}}$ is too large relative to training data
- Requires computing entire residual vector $\mathbf{r}(\boldsymbol{\mu})$
- Small number of potentially low-quality features

Regression-Function Approximation

We consider several different regression models

- Ordinary least squares (OLS)
  - Linear (OLS: Linear)
  - Quadratic expansion of features (OLS: Quadratic)
- Support vector regression (SVR)
  - Linear kernel (SVR: Linear)
  - Gaussian (radial basis function) kernel (SVR: RBF)
- Random forest (RF)
- k-nearest neighbors (k-NN)
- Artificial neural network / multilayer perceptron (MLP)

Training and Test Data

Training Data

- Consists of parameter $\boldsymbol{\mu}$ subset from parameter space $\mathcal{D}$
- High-fidelity and approximate solutions train regression models
- Cross-validated to tune regression model hyper-parameters
- Used to compute principal components of residuals

Test Data

- Consists of parameter $\boldsymbol{\mu}$ choices **not** used for training data
- Used to assess regression models and quantify nondeterministic noise

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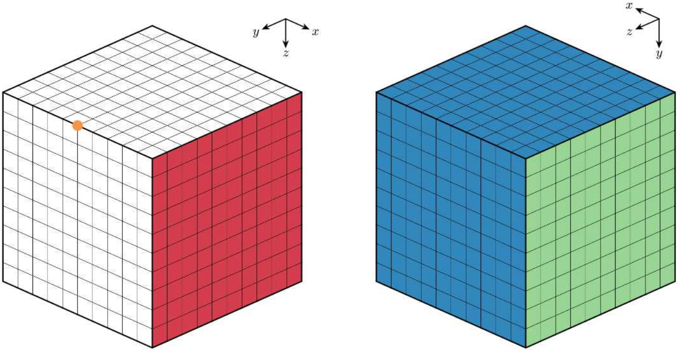
  - Cube: Reduced-Order Modeling
  - PCAP: Reduced-Order Modeling
  - Burgers' Equation: Unconverged Iterations and Coarse Solution Prolongation
- Summary

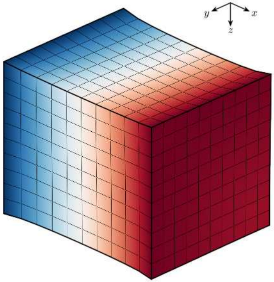
Cube: Reduced-Order Modeling

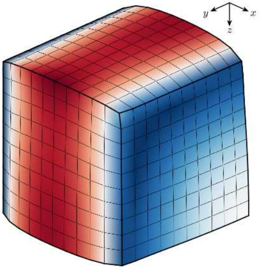


- Applied traction (Neumann boundary condition)
- Planar constraint (Dirichlet boundary condition)
- Complete constraint (Dirichlet boundary condition)
- Node of interest

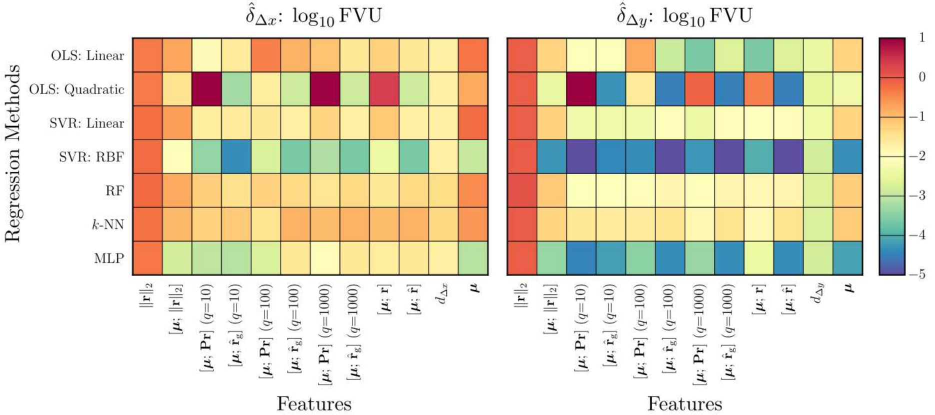
Cube: Overview

- $N_{\mathbf{u}} = 3993$ – deliberately small to calculate $d(\boldsymbol{\mu})$ and use $\mathbf{r}(\boldsymbol{\mu})$
- $N_{\boldsymbol{\mu}} = 3$ parameters: $\boldsymbol{\mu} = [E; \nu; t]$
  - $E \in [75, 125]$ GPa, $\nu \in [0.20, 0.35]$, $t \in [40, 60]$ GPa
- 8 HF runs $\rightarrow$ up to $m_{\mathbf{u}} = 8$ ROM basis functions (2 used – 99.25%)





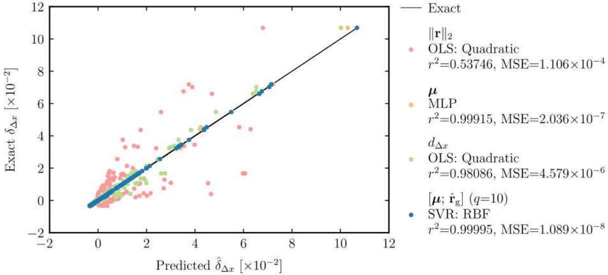
Cube: FVU for QoI Error Prediction

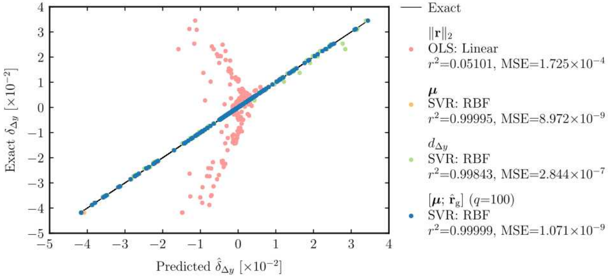


Fraction of variance unexplained (FVU) is $1 - r^2$ (r^2 is coefficient of determination)

- SVR: RBF and MLP perform the best
- $[\boldsymbol{\mu}; \hat{\mathbf{r}}_g]$ and $[\boldsymbol{\mu}; \mathbf{Pr}]$ well with only $q = 10$ samples (compared to $N_{\mathbf{u}} = 3443$)

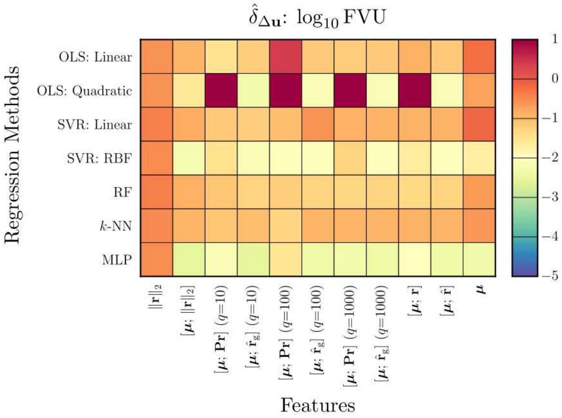
Cube: QoI Error Predictions





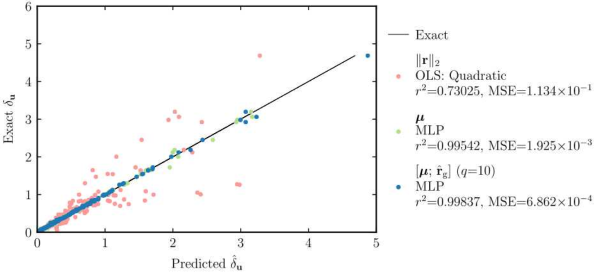
- Our methods beat previous state-of-the-art methods with $r^2 > 0.9999$ in both cases

Cube: FVU for Normed State-Space Error Prediction



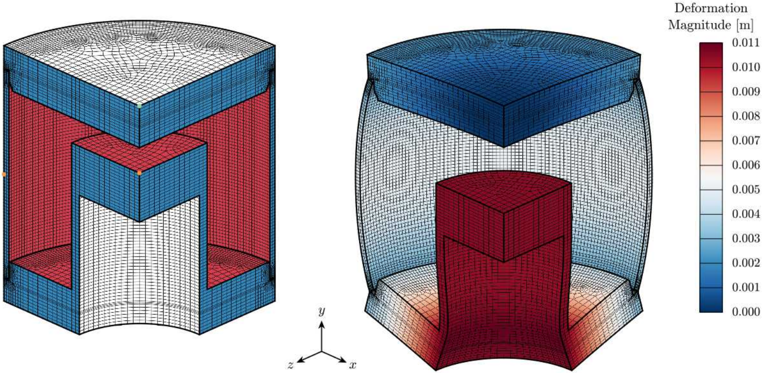
- SVR: RBF and MLP perform the best
- $[\boldsymbol{\mu}; \hat{\mathbf{r}}_{\mathrm{g}}]$ and $[\boldsymbol{\mu}; \mathbf{Pr}]$ perform well with only $q = 10$ samples (compared to $N_{\mathbf{u}} = 3443$)

Cube: Normed State-Space Error Predictions



- Our methods beat previous state-of-the-art methods with $r^2 > 0.998$

Predictive Capability Assessment Project: Reduced-Order Modeling

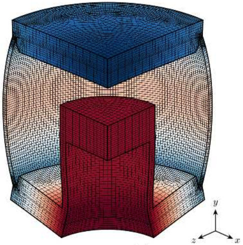


- Applied pressure (Neumann boundary condition)
- Planar constraint (Dirichlet boundary condition)
- Complete constraint (Dirichlet boundary condition)
- Nodes of interest

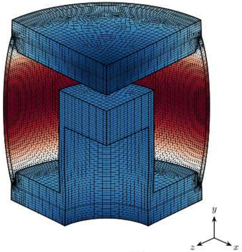
PCAP: Overview

- $N_{\mathbf{u}} = 278,301$ for quarter of domain
- $N_{\boldsymbol{\mu}} = 3$ parameters: $\boldsymbol{\mu} = [E;\, \nu;\, t]$
  - $E \in [50,\, 100]$ GPa, $\nu \in [0.20,\, 0.35]$, $p \in [6,\, 10]$ GPa
- 8 HF runs $\rightarrow$ up to $m_{\mathbf{u}} = 8$ ROM basis functions (5 used – 99.90%)
- 30 training runs for regression model

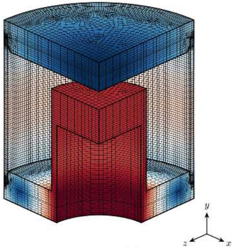
PCAP: Basis Functions



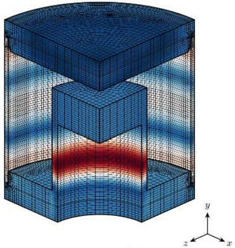
1: 85.03%



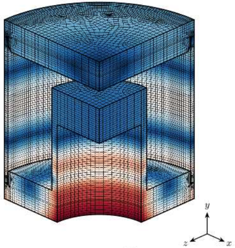
2: 95.69%



3: 99.35%

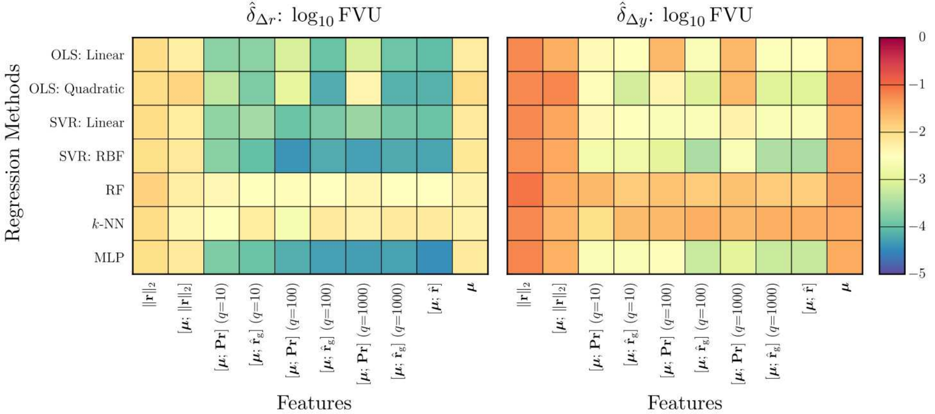


4: 99.77%



5: 99.90%

PCAP: FVU for QoI Error Prediction

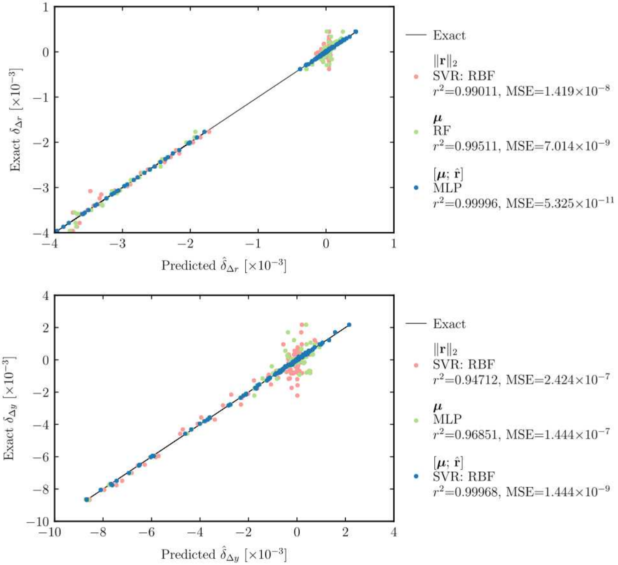


Fraction of variance unexplained (FVU) is $1 - r^2$ (r^2 is coefficient of determination)

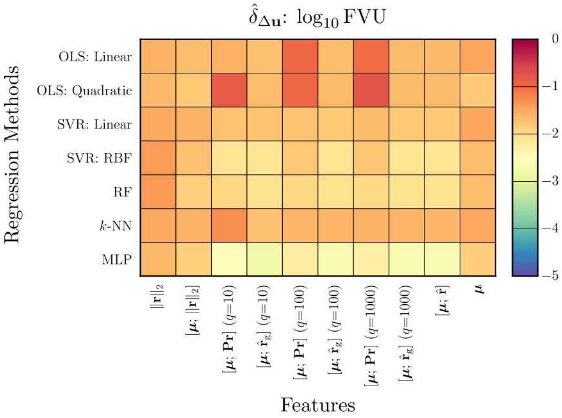
- SVR: RBF and MLP perform the best
- $[\boldsymbol{\mu}; \hat{\mathbf{r}}_{\mathrm{g}}]$ and $[\boldsymbol{\mu}; \mathbf{Pr}]$ well with only $q = 100$ samples (compared to $N_{\mathbf{u}} = 278,301$)

PCAP: QoI Error Predictions

- Our methods beat previous state-of-the-art methods with $r^2 > 0.9996$ in both cases

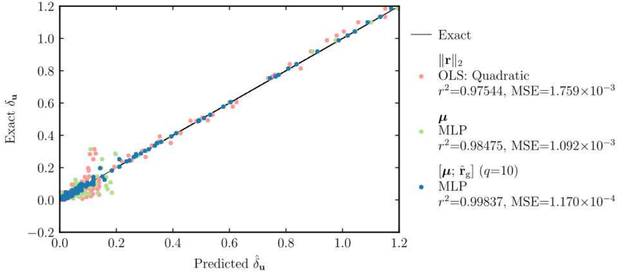


PCAP: FVU for Normed State-Space Error Prediction



- MLP performs the best
- $[\boldsymbol{\mu}; \hat{\mathbf{r}}_{\mathrm{g}}]$ and $[\boldsymbol{\mu}; \mathbf{Pr}]$ perform well with only $q = 10$ samples (compared to $N_{\mathbf{u}} = 278,301$)

PCAP: Normed State-Space Error Predictions

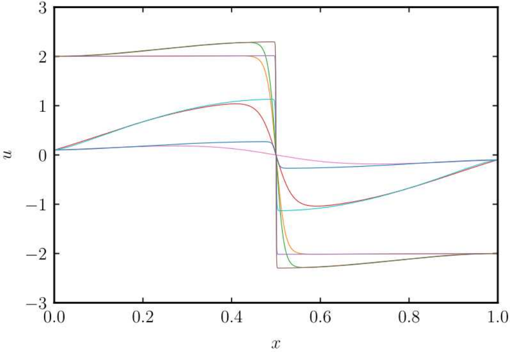


- Our methods beat previous state-of-the-art methods with $r^2 > 0.998$

Burgers' Equation: Unconverged Iterations and Coarse Solution Prolongation

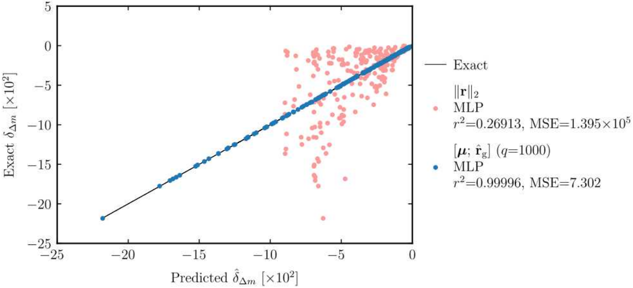
$$uu_x - \frac{1}{R}u_{xx} = \alpha \sin 2\pi x$$

$$u(0) = u_a, \quad u(1) = -u_a$$



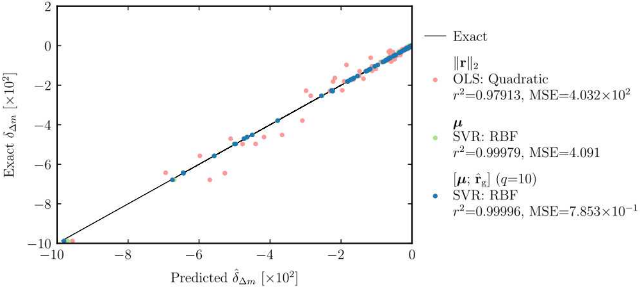
- $N_{\mathbf{u}} = 2001$
- $N_{\boldsymbol{\mu}} = 3$ parameters: $\boldsymbol{\mu} = [\alpha;\, u_a;\, R]$
  - $\alpha \in [0.1,\, 2.0]$, $u_a \in [0.1,\, 2.0]$, $R \in [50,\, 1000]$
- Quantity of interest s is the slope m at $x = \frac{1}{2}$
- $K = 1$ and $K = 2$ or $N_{\mathbf{u}_{\mathrm{LF}}} = 501$ and $N_{\mathbf{u}_{\mathrm{LF}}} = 1001$

Burgers' Equation, Unconverged Iterations: QoI Error Predictions



- Our methods beat previous state-of-the-art method with $r^2 > 0.9999$

Burgers' Equation, Coarse Mesh Prolongation: QoI Error Predictions



- Our methods beat previous state-of-the-art methods with $r^2 > 0.9999$
- Only $q = 10$ samples (compared to $N_{\mathbf{u}} = 2001$)

Outline

- Introduction
- Parameterized Nonlinear Algebraic Equations
- Proposed Approach
- Numerical Experiments
- Summary
  - Feature Choices
  - Feature Reduction

Feature Choices

- Norm of the residual, $\|\mathbf{r}\|_2$
  - Low-quality single feature
  - Expensive to compute and performs poorly
- Dual-weighted residual, d
  - High-quality single feature
  - Performs well for small amounts of training data
  - Very expensive to compute
- Parameters $\boldsymbol{\mu}$
  - Only perform well with SVR: RBF or MLP
  - Do not perform well with OLS: Linear
- Parameters and gappy principal componenets of residual, $[\boldsymbol{\mu}; \hat{\mathbf{r}}_{\mathrm{g}}]$
  - Performs the best with $r^2 > 0.998$ for each experiment
  - Only requires about 13 features

Feature Reduction

- Gappy PCA more effective than directly sampling the residual
- Little benefit to using $q \geq 100$ samples; more samples are more expensive and do not perform much better
- Often, only $q = 10$ samples are necessary to get accurate prediction

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Questions?

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