The ROMES method for reduced-order-model uncertainty quantification: application to data assimilation

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Data assimilation by Bayesian inference

- Structural health monitoring

Given sensor data, what is the updated knowledge of material properties throughout the aircraft?

- Bayesian inference problem

inputs $\mu \rightarrow \text{high-fidelity model} \rightarrow$ outputs $y$

Given measurements of the outputs, what is the posterior distribution of the inputs?
Bayesian inference

inputs $\mu \rightarrow \text{high-fidelity model} \rightarrow \text{outputs } y$

- Bayes’ theorem

$$P(\mu|\bar{y}) = \frac{P(\bar{y}|\mu)P(\mu)}{P(\bar{y})}$$

- measured outputs $\bar{y} = y(\mu^*) + \varepsilon$ with noise $\varepsilon \sim \mathcal{N}(0, \sigma^2I)$
- posterior $P(\mu|\bar{y})$ is sought
- prior $P(\mu)$ is given
- normalizing factor $P(\bar{y})$ is handled indirectly
- likelihood $P(\bar{y}|\mu) \sim \mathcal{N}(y(\mu), \sigma^2I)$ sampling requires high-fidelity model evaluations

- Objective: numerically sample the posterior distribution
  + achievable in principle, e.g., by MCMC or importance sampling.
  - barrier: sampling requires high-fidelity forward solves
Reduced-order modeling and Bayesian inference

inputs $\mu \rightarrow \text{reduced-order model} \rightarrow \text{outputs } y_{\text{red}}$

- Replace the high-fidelity model with reduced-order model
  - measured outputs $\bar{y} = y(\mu^*) + \epsilon \approx y_{\text{red}}(\mu^*) + \epsilon$
  - likelihood $P(\bar{y}|\mu) \sim \mathcal{N}(y_{\text{red}}(\mu), \sigma^2 I)$ sampling requires 
    reduced-order model evaluations
  - sampling from the posterior becomes tractable

- Problem: neglects reduced-order-model errors

\[
\bar{y} = y(\mu^*) + \epsilon \\
= y_{\text{red}}(\mu^*) + \delta y(\mu^*) + \epsilon
\]  

- “An interesting future research direction is the inclusion of estimates of reduced model error as an additional source of uncertainty in the Bayesian formulation.” [Galbally et al., 2009]

Goal: construct a statistical model of the reduced-order-model error
Strategies for ROM error quantification

1. Rigorous error bounds
   + independent of input-space dimension
   - not amenable to statistical analysis
   - often overestimate the error (i.e., high effectivity)
   - improving effectivity incurs larger costs
     [Huynh et al., 2010, Wirtz et al., 2012] or intrusive reformulation of discretization [Yano et al., 2012]

2. Multifidelity correction [Eldred et al., 2004]

   - surrogate model of low-fidelity error as a function of inputs
   - ‘correct’ low-fidelity outputs with surrogate
   + amenable to statistics
   - curse of dimensionality
   - ROM errors often highly oscillatory in the input space
     [Ng and Eldred, 2012]
Our key observation

- Residual and error bound often correlate with the true error
- **Main idea**: construct a stochastic process that maps error indicators (not inputs $\mu$!) to a distribution of the error
  - independent of input-space dimension
  - amenable to statistics

Reduced-order model error surrogates
- Construct a stochastic process of the ROM error $\tilde{\delta}(\rho)$
- Select a *small number* of error indicators $\rho = \rho(\mu)$ that are
  1. cheaply computable online, and
  2. lead to low variance of the stochastic process.
- First attempt: Gaussian process (GP) such that random variables $(\tilde{\delta}(\rho_1), \tilde{\delta}(\rho_2), \ldots)$ have joint Gaussian distribution
**Definition (Gaussian process)**

A Gaussian process is a collection of random variables, any finite number of which have a joint Gaussian distribution.

\[ \tilde{\delta}(\rho) \sim \mathcal{GP}(m(\rho), k(\rho, \rho')) \]

- mean function \( m(\rho) \); covariance function \( k(\rho, \rho') \)
- given a training set \( \{(\delta_i, \rho_i)\} \), the mean and covariance functions can be inferred via Bayesian analysis
- consider two types of Gaussian processes
  1. kernel regression [Rasmussen and Williams, 2006]
  2. relevance vector machine (RVM) [Tipping, 2001]
**GP #1: Kernel regression**  [Rasmussen and Williams, 2006]

- **prior**: \( \tilde{\delta}(\rho) \sim N(0, K(\rho, \rho) + \sigma^2 I) \)
  - \( k(\rho_i, \rho_j) = \exp \frac{\|\rho_i - \rho_j\|^2}{r^2} \) is a positive definite kernel
  - \( \rho := [\rho_{\text{train}} \rho_{\text{predict}}]^T \)
- **posterior**: \( \tilde{\delta}(\rho_{\text{predict}}) \sim N(m(\rho_{\text{predict}}), \text{cov}(\rho_{\text{predict}})) \)
- infer hyperparameters \( \sigma^2 \) and \( r^2 \)
GP #2: Relevance vector machine [Tipping, 2001]

\[ \tilde{\delta}(\rho) = \sum_{m=1}^{M} w_m \phi_m(\rho) + \varepsilon \]

- fixed basis functions \( \phi_m \) (e.g., polynomials, radial-basis functions)
- stochastic coefficients \( w_m \)
- noise \( \varepsilon \sim \mathcal{N}(0, \sigma^2 I) \)
- prior: \( w \sim \mathcal{N}(0, \text{diag}(\alpha_i)) \)
- posterior: \( w \sim \mathcal{N}(\mathbf{m}, \Sigma) \) leads to posterior dist. of \( \tilde{\delta}(\rho) \)
- infer hyperparameters \( \sigma^2 \) and \( \alpha_i \)
ROMES Algorithm

Offline

1. Populate ROMES database \{((\delta(\mu), \bar{\rho}(\mu)) \mid \mu \in D_{\text{train}}\},
   where \bar{\rho} denotes candidate indicators.

2. Identify a few error indicators \rho \subset \bar{\rho} that lead to low variance in the Gaussian process.

3. Construct the Gaussian process \tilde{\delta}(\rho) \sim \mathcal{GP}(m(\rho), k(\rho, \rho')) by Bayesian inference.

Online (for any \mu^* \in D)

1. compute the ROM solution

2. compute error indicators \rho(\mu^*)

3. obtain \tilde{\delta}(\rho(\mu^*)) \sim \mathcal{N}(m(\rho(\mu^*))), k(\rho(\mu^*), \rho(\mu^*))

4. correct the ROM solution
thermal block  (Parametrically coercive and compliant, affine, linear, elliptic)

\[ \frac{\partial c(x; \mu)}{\partial x} u(x; \mu) = 0 \text{ in } \Omega \quad u(\mu) = 0 \text{ on } \Gamma_D \]
\[ \nabla c(\mu) u(\mu) \cdot n = 0 \text{ on } \Gamma_{N_0} \quad \nabla c(\mu) u(\mu) \cdot n = 1 \text{ on } \Gamma_{N_1} \]

- Inputs \( \mu \in [0.1, 10]^9 \) define diffusivity \( c \) in subdomains
- Output \( y(\mu) = \int_{\Gamma_{N_1}} u(\mu) dx \) is compliant
- ROM constructed via RB–Greedy [Patera and Rozza, 2006]
- Consider two errors: 1) energy norm of state-space error \( \| u(\mu) - u_{\text{red}}(\mu) \| \), 2) output bias \( y(\mu) - y_{\text{red}}(\mu) \)
Error #1: energy norm \[ \| u(\mu) - u_{\text{red}}(\mu) \| \]

- Residual and error bound correlate with error

- ROMES (Kernel, residual indicator) in log-log space promising
Gaussian-process assumptions verified (Kernel, residual indicator)

Observed estimates in predicted interval:

<table>
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<th>$T = 10$</th>
<th>$T = 35$</th>
<th>$T = 65$</th>
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<td>99 %</td>
<td>80.16</td>
<td>94.42</td>
<td>96.26</td>
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</table>
GP variables converge (Kernel GP, residual indicator)

(i) convergence of mean $m$

(ii) convergence of variance $\sigma^2$
Can achieve ‘statistical rigor’ (Kernel GP, residual indicator)

50%-rigorous estimate

90%-rigorous estimate

Mean ± std

Median

Minimum

Maximum

Effectivity (1 = good)

Size of training sample

Frequency of non-rigorous estimations

Size of training sample

Can achieve ‘statistical rigor’ (Kernel GP, residual indicator)
RVM (Legendre-polynomial basis functions): significant uncertainty in mean’s high-order polynomial coefficients
ROMES: Kernel and RVM GP comparison

- **GP structure and confidence intervals verified in both cases**
  - (i) Kernel based GP
  - (ii) RVM based GP

- **Kernel GP produces better effectivity**

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<tr>
<th>c</th>
<th>(i)</th>
<th>(ii)</th>
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<tbody>
<tr>
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</table>
**Error #2: output bias** $y(\mu) - y_{\text{red}}(\mu)$

(i) Indicators mapped to output bias

(ii) Parameters mapped to output bias

+ Residual and error bound are good indicators (ROMES)
- Inputs are poor indicators (Multifidelity correction)
Gaussian-process assumption verification

Residual based GP

Parameter based GP

+ ROMES (Kernel GP, residual indicator) confidence intervals converge.
- Multifidelity correction (Kernel GP, input indicator) confidence intervals do not converge.
Bias improvement

\[
\text{bias reduction} = \frac{E \left( y_{\text{red}}(\mu) + \tilde{y}(\mu) - y(\mu) \right)}{y_{\text{red}}(\mu) - y(\mu)}
\]

(i) Residual based GP

(ii) Parameter based GP

- ROMES reduces bias by roughly an order of magnitude
- Multifidelity correction often increases the bias
Conclusions

ROMES
- combines existing ROM error indicators with supervised machine learning to statistical quantify ROM error
- relies on identifying error indicators that yield low variance
- ‘statistical rigor’ achievable
- outperforms multifidelity correction (inputs are poor error indicators)
- highlights strength of reduced-order models for data assimilation: other surrogates (likely) do not have such powerful error indicators

Future work
- apply to nonlinear, time-dependent problems
- incorporate in likelihood function

\[
\tilde{y} = y_{\text{red}}(\mu^*) + \delta_y(\mu^*) + \varepsilon
\]

where \(\delta_y\) and \(\varepsilon\) may have different distributions
- develop error indicators for this purpose
- automated selection of indicators and Gaussian process
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