Adaptive approximations of computationally intensive models for uncertainty propagation and inference

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Introduction

- Practical problems in **uncertainty propagation**, **sensitivity analysis**, and **inference** require using computationally expensive forward models, e.g., $f(\mathbf{x})$
- Standard algorithms require an intractable number of evaluations
- Constructing surrogate $\tilde{f}(\mathbf{x})$ can lower the overall cost of the analysis

Part 1: Forward uncertainty propagation

- **Polynomial chaos expansions** (PCEs) are used to approximate functions of known random variables:

$$\tilde{f}(x) = \sum f_i \Psi_i(x)$$

- Ψ are orthonormal polynomials, f_i are Fourier coefficients
- Customizable to various domains and measures
- Extends to higher dimensions via tensor products
- Adaptive Smolyak algorithms allow a flexible and practical construction
- Well-suited to uncertainty propagation

Pseudospectral approximation in one dimension

- We can analytically compute coefficients:

$$f(x) \approx \sum_{i=0}^{\infty} f_i \psi_i^1(x) = \sum_{i=0}^{\infty} \langle f(x), \psi_i^1(x) \rangle \psi_i^1(x)$$

- Pseudospectral approximations use quadrature to compute the integral

$$\mathcal{S}_m^{(1)}(f) = \sum_{i=0}^{q^{(1)}(m)} \mathcal{Q}_m^{(1)}(f\psi_i^{(1)})\psi_i^{(1)}(x)$$

- Choose truncation and quadrature so that every ψ_i^2 is integrated correctly

Smolyak algorithms

- Smolyak approach builds sparse tensor product algorithms from one-dimensional algorithms; good for problems with weak input coupling
- Let

$$\Delta_0^{(i)} = L_0^{(i)} = 0$$
$$\Delta_n^{(i)} = L_n^{(i)} - L_{n-1}^{(i)}$$

- Form the telescoping sum

$$L^{(i)} = \sum_{k_i=0}^{\infty} \Delta_k^{(i)}$$

- Smolyak's algorithm is

$$A(m,d,\vec{L}) := \sum_{\mathbf{k}\in\mathcal{K}} \Delta_{\mathbf{k}_1}^{(1)} \otimes \cdots \otimes \Delta_{\mathbf{k}_d}^{(d)}$$

- or:

$$A(\mathcal{K},d,\vec{L}) = \sum_{\mathbf{k}\in\mathcal{K}} c_{\mathbf{k}} L_{\mathbf{k}_1}^1 \otimes \cdots \otimes L_{\mathbf{k}_d}^d$$

Adaptivity

- Smolyak algorithms are more efficient only if the index set is suited to the problem at hand
- Add indices incrementally, based on empirical local error indicator

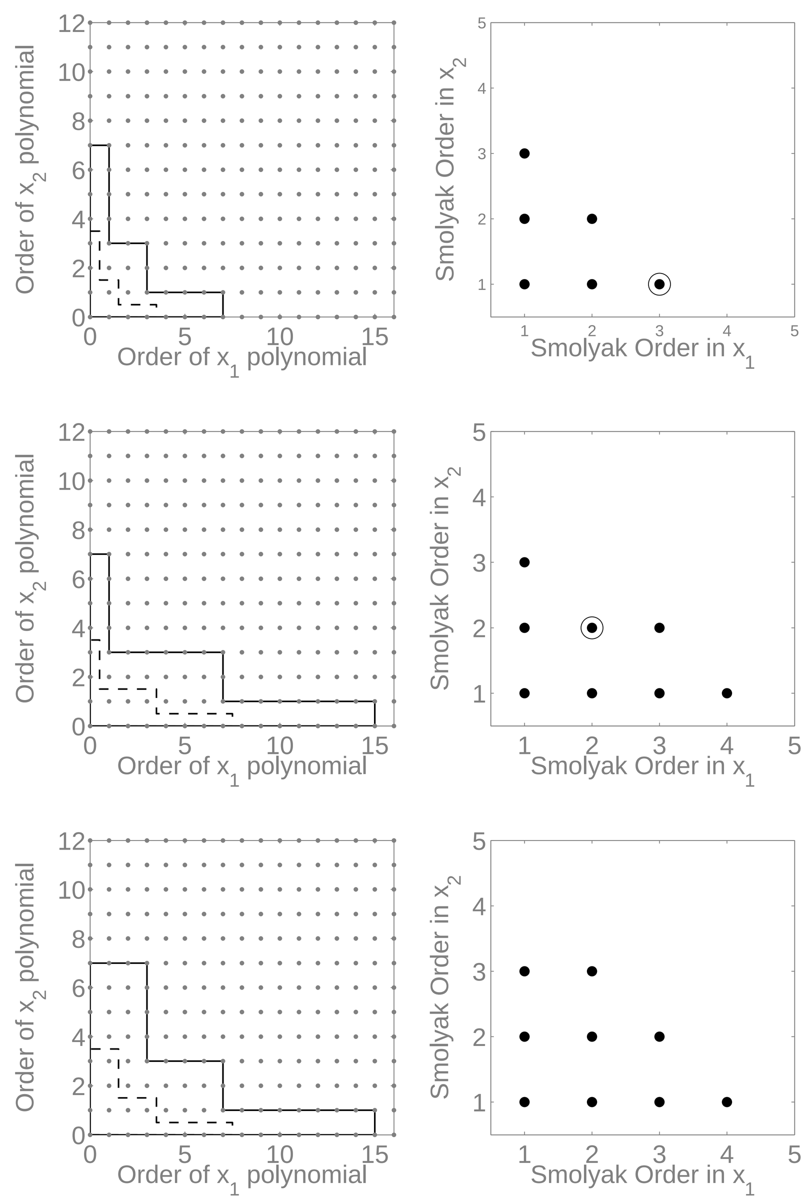
$$\epsilon(\mathbf{k}) := \|\Delta_{\mathbf{k}_1}^1 \otimes \cdots \otimes \Delta_{\mathbf{k}_d}^d\|_2$$

where $\Delta_{\mathbf{k}_1}^1 \otimes \cdots \otimes \Delta_{\mathbf{k}_d}$ is a PCE and $\|\cdot\|_2$ is a L_2 norm over the input space
- Halt adaptation with a global error indicator

$$\epsilon_g := \sum \epsilon_l(\mathbf{k})$$

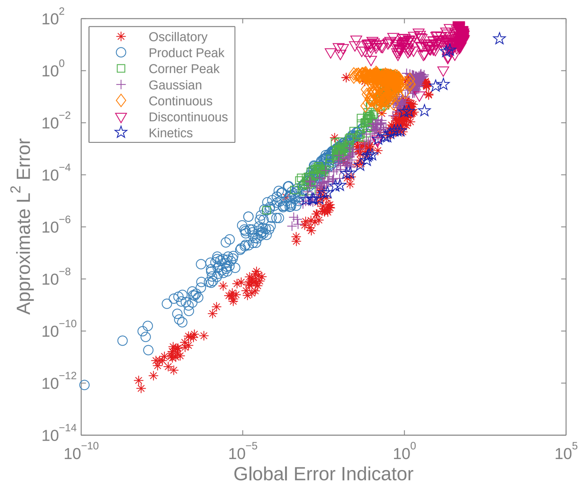
Example of adaptivity

- A fabricated example in an exponential growth Gaussian quadrature setting



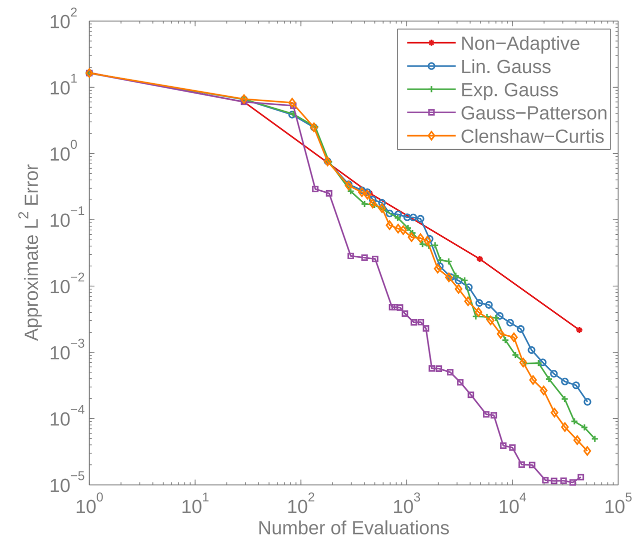
Termination critera

- The global error indicator is typically well-correlated with L^2 error, except for non-smooth functions



Combustion model example

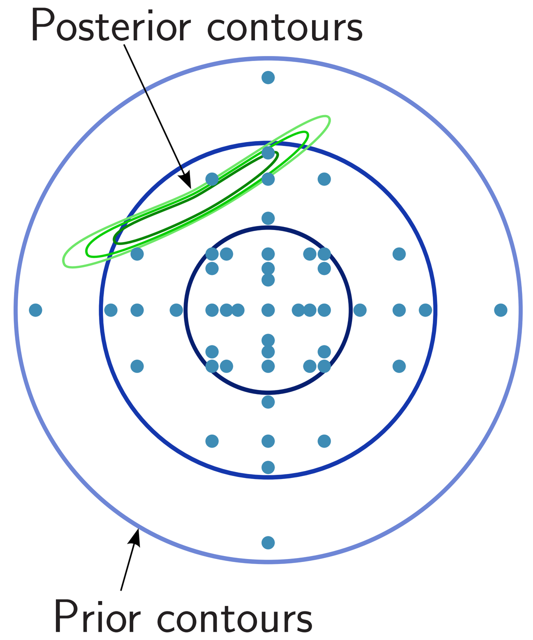
- Model computes the ignition time of a methane/air mixture, based on 14 uncertain input rate parameters
- Testing adaptive and non-adaptive strategies with different growth rules



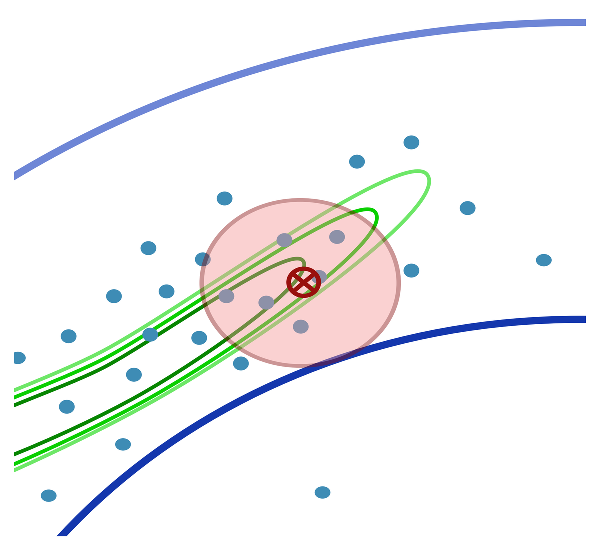
Part 2: Inference and inverse problems

Adaptive local approximations

- When performing inference, it is difficult to efficiently choose distributions for input parameters to build a PCE



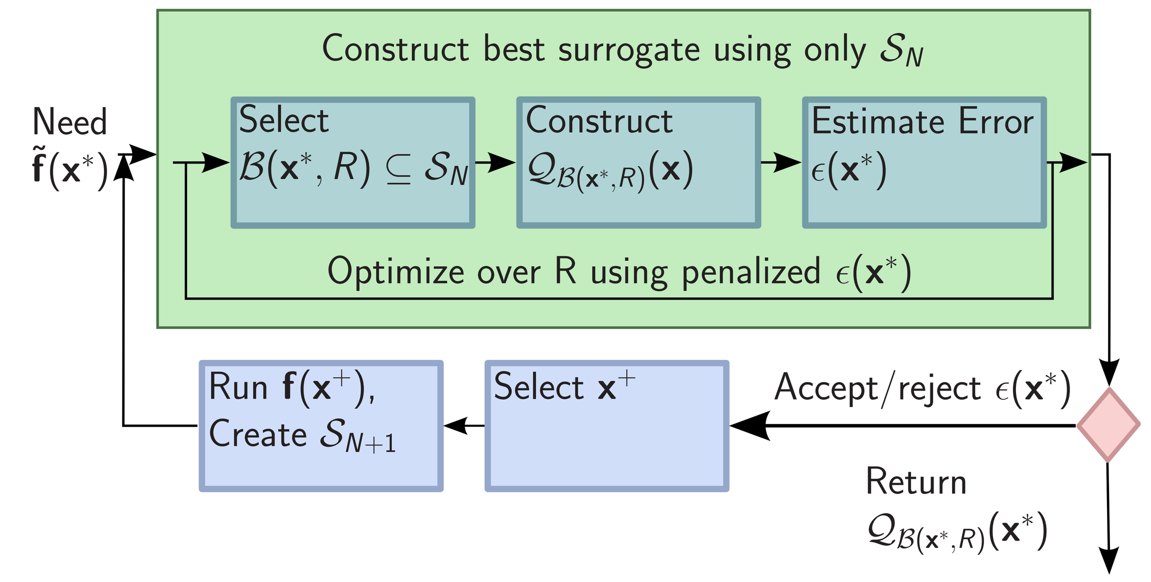
- This example shows how the samples are largely drawn from regions of low posterior mass
- Instead, we aim to build an approximation that is accurate over the posterior



- Samples might be allocated as shown, drawn with density similar to the posterior density
- These samples may be used to construct local linear or quadratic approximations

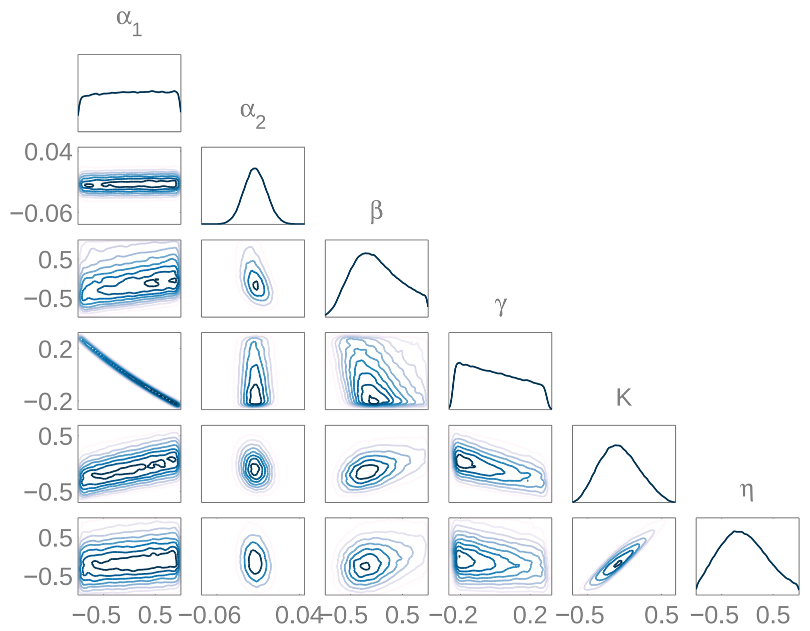
Algorithm outline

- On each iteration, when Markov chain Monte Carlo needs to evaluate the approximate forward model, construct/update the approximation as follows

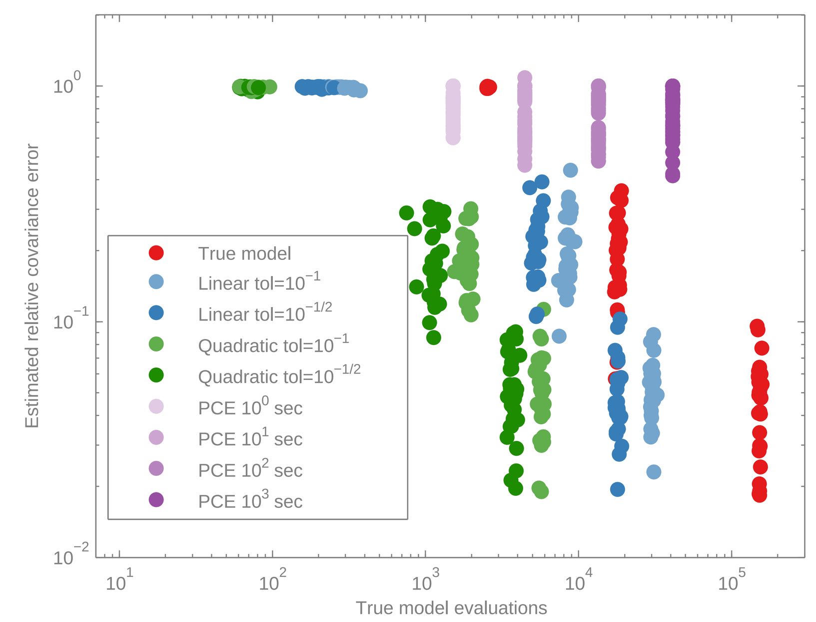


Genetic toggle switch

- Infer six parameters of a kinetic model simulating a genetic toggle switch



- Test performance by performing inference repeatedly, with or without approximations



Conclusions

- Uncertainty quantification tasks can be made tractable with surrogates
- Adaptive polynomial approximations are well-suited to uncertainty propagation
- Novel surrogates can exploit the structure of inference problems

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