Overview of Uncertainty Quantification Methods for Complex Models

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EES Modeling PI Meeting
Data, Metrics, and Diagnostics
November 5-9, 2018
Potomac, MD

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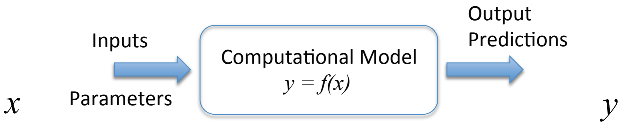
This work was supported in part by:

The Energy Exascale Earth System Model (E3SM) project, funded by the U.S. Department of Energy, Office of Science, Office of Biological and Environmental Research (BER).

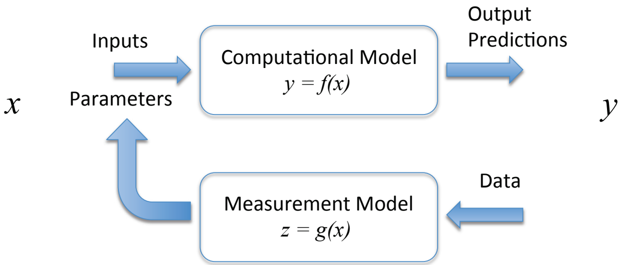
The U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research (ASCR) and Office of Biological and Environmental Research (BER) hrough Advanced Computing (SciDAC) program through the FASTMath Institute and the OSCM project.

Uncertainty Quantification and Computational Science



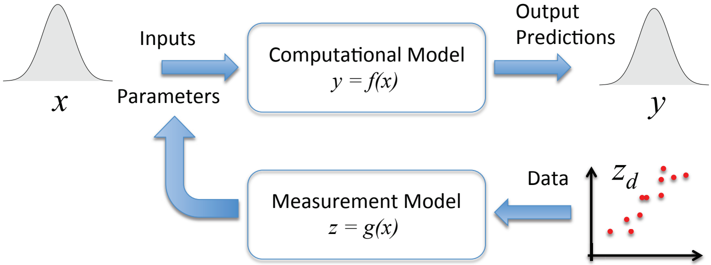
Forward problem

Uncertainty Quantification and Computational Science



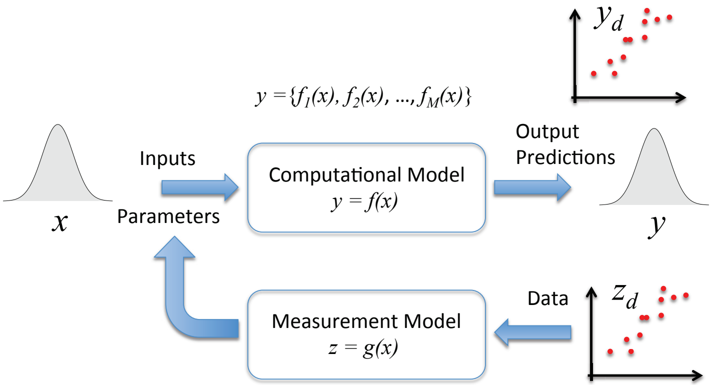
Inverse & Forward problems

Uncertainty Quantification and Computational Science



Inverse & Forward UQ

Uncertainty Quantification and Computational Science



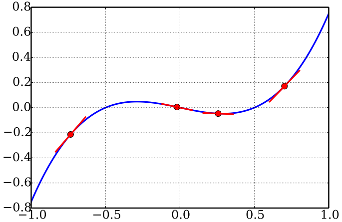
Inverse & Forward UQ

Model validation & comparison, Hypothesis testing

Forward UQ

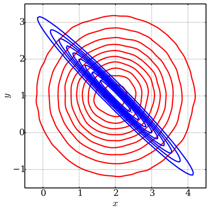
- Local sensitivity analysis and error propagation

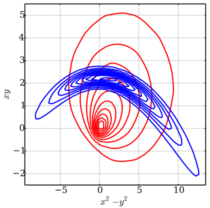
$$\Delta y = \frac{\mathrm{d}f}{\mathrm{d}x}\bigg|_{x_0} \Delta x$$



This is ok for:
  - small uncertainty
  - low degree of non-linearity

- Non-probabilistic methods
  - Evidence theory
  - Fuzzy logic
  - Interval math
  - Misses correlations





- **Probabilistic methods** – our focus

Probabilistic Forward UQ

- Uncertain inputs/outputs as random variables

$$y = f(\lambda)$$

- Default way - sampling:
  - Random sampling, MC/QMC
  - Generate random samples $\{\lambda_i\}_{i=1}^N$ from the PDF of λ, $p(\lambda)$
  - Evaluate the model $y_i = f(\lambda_i)$, construct $p(y)$ or gather statistics
  - Slow convergence of MC/QMC $\Rightarrow$ infeasibly large N required
- Build a cheap surrogate for $f(\lambda)$, then use MC
  - Collocation – interpolants
  - Regression – fitting
- **Polynomial Chaos (PC)** is a convenient machinery

Polynomial Chaos – functional representation for RVs

$$U \simeq \sum_{k=0}^{p} u_k \psi_k(\xi)$$

- First introduced by Wiener, 1938
- Revitalized by Ghanem and Spanos, 1991
- Think of Fourier-type expansion
- Convergent series if U has finite variance
- Selection of order p is a modeling choice
- Describes a r.v. U with a vector of *PC modes* $(u_0, u_1, \ldots, u_p)$
- Utility
  - Moments: $\mathbb{E}[u] = u_0, \;\; \mathbb{V}[u] = \sum_{k=1}^{K} u_k^2 ||\Psi_k||^2, \;\; \ldots$
  - Global Sensitivities – fractional variances, Sobol' indices
  - Uncertainty propagation
  - Surrogate for forward model

[Wiener, 1938; Ghanem & Spanos, 1991; Xiu & Karniadakis, 2002; Le Maître & Knio, 2010]

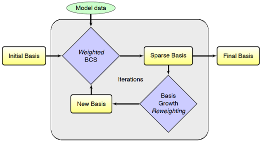
Challenges in Forward UQ

- Large number of input parameters
- Expense of a single model simulation

- Build PC surrogates with regression
  - still relying on an ensemble of simulations, but
  - call it a supervised machine learning, if you wish
  - actually, use Bayesian regression to have uncertainties capturing lack-of-information
- Specific to polynomial bases, employ vast literature on sparse learning [Tipping, 2001]
  - Bayesian compressive sensing [S. et al., 2014; Ricciuto, S., Thornton, 2018]

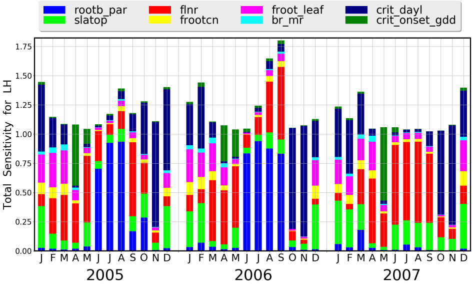
$$Z = f(\boldsymbol{\xi}) \approx \sum_{k=0}^{K} c_k \Psi_k(\boldsymbol{\xi})$$

$$\Psi_k(\xi_1, \xi_2, ..., \xi_d) = \psi_{k_1}(\xi_1)\psi_{k_2}(\xi_2)\cdots\psi_{k_d}(\xi_d)$$



Snapshot of Results

- Main effect sensitivities : rank input parameters
- Joint sensitivities : most influential input couplings
- About 50 input parameters, but ~ 6 contribute to most of the variance,



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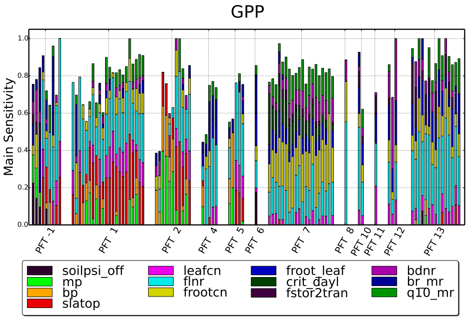

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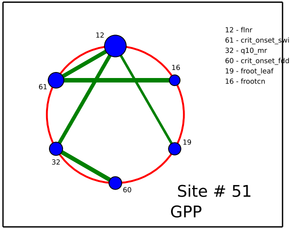

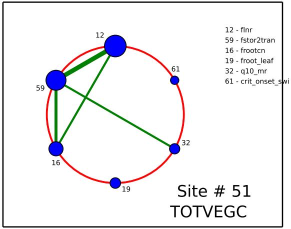

Inverse UQ

- Parameter fitting, tuning
- Statistical inference problem
- Given ...
  - ... model output QoI $y \approx f(x;\lambda)$
  - ... observational data $\{x_i, y_i\}_{i=1}^N$
  - Find model parameters λ

$$\overbrace{p(\lambda|y)}^{\text{Posterior}} = \frac{\overbrace{p(y|\lambda)}^{\text{Likelihood}} \quad \overbrace{p(\lambda)}^{\text{Prior}}}{\underbrace{p(y)}_{\text{Evidence}}}$$

- Prior $p(\lambda)$: expert knowledge, or uninformative
- Posterior $p(\lambda|y)$: updated 'knowledge' of λ, given data y
- Likelihood $L(\lambda) = p(y|\lambda)$: key, noise/error model, encapsulates assumptions about data collection
- Evidence $p(y)$: not important for parameter (coeff. λ) estimation; crucial for model selection - via Bayes factor (Occam's razor)

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- Posterior sampling via Markov chain Monte Carlo (MCMC)
- Given samples from posterior, one can interrogate it further
  - Estimate PDF with KDE
  - Compute moments
  - Build functional representation, such as PC
  - Pipe it to the next model as an uncertain input

Main target: model *structural* error

deviation from ‘truth’ or from a higher-fidelity model

- Inverse modeling context
  - Given experimental data, estimate the model error

$$y_i \approx f(x_i; \lambda)$$

- Represent and estimate the error associated with
  - Simplifying assumptions, parameterizations
  - Mathematical formulation, theoretical framework
- ...will be useful for
  - Model validation
  - Model comparison
  - Scientific discovery and model improvement
  - Reliable computational predictions
- Ignoring model error leads to overconfident and biased predictions

Model Error – how to correct

Traditional approach: additive correction [Kennedy & O'Hagan, 2001]

$$y_i \approx f(x_i; \lambda) + \delta(x_i) + \epsilon_i$$

- Difficult to distinguish contributions between model and data errors
- No longer guarantees physical constraints in g_i
- Unable to predict other QoIs with model error
- Does not use *a priori* knowledge of discrepancy structure

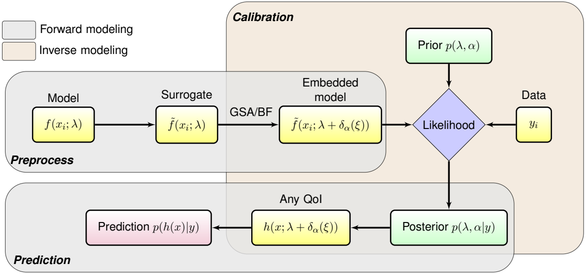
Our approach: embedded model [S., Najm, Ghanem, 2015; S., Huan, Najm, 2018]

$$y_i \approx f(x_i; \lambda + \delta(x_i)) + \epsilon_i$$

- Embeds model error in specific submodel phenomenology
- Allows *targeted* placement of model error term (e.g., in locations where key modeling assumptions and approximations are made)
- Disambiguates model error from data noise
- Inherits model structure and physical constraints

Forward/Inverse UQ workflow

- **Preprocess:** Surrogate construction, GSA, select embedding
- **Calibration:** Prior selection, MCMC
- **Prediction:** Forward PC propagation, possible extrapolation

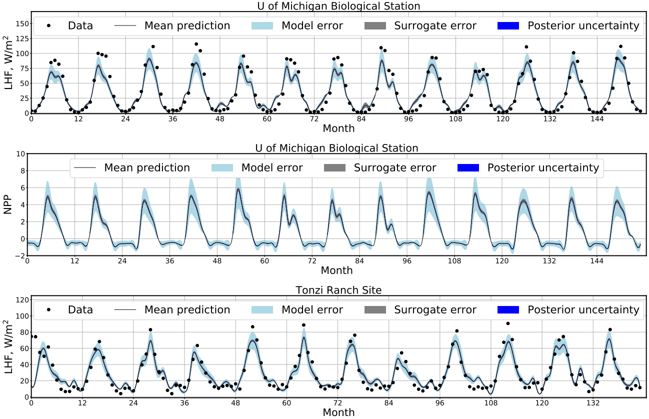


- Predictive uncertainty decomposition: Total Variance =

Parametric uncertainty + Data noise + Model error + Surrogate error

- All developments done within UQTk, lightweight C++/Python library out of SNL-CA (*www.sandia.gov/uqtoolkit*)

Snapshot of Results



- Predictive variance decomposition with model-error component
- Allows meaningful prediction of other QoIs (e.g. no data/observable)
- Allows (a more dangerous) extrapolation to other sites

Literature

General PC

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Challenges and Opportunities

The curse of dimensionality

- Models have large number of parameters
- Models are expensive

- Always prebuild a *surrogate* and work with it
- There is room for a lot of 'compression', particularly in spatio-temporal outputs: *Karhunen-Loève expansions* (glorified PCA)
- Certainly go *Bayesian*: allows making sense of any amount of data/simulations and provides uncertainty estimate
- Can we really make sense of the model behavior with 2-3 simulations? – well, getting there: *multi-fidelity* methods for UQ

Model structural errors

- Quantify how wrong the model is
- Just correcting the outputs not good enough - *embed* stochastic terms in the model (or its surrogate)
- *Model selection* needs to be done over ensembles. Again, go *Bayesian*.

Optimal experimental design

- Optimization of Sensor Networks for Improving Climate Model Predictions (OSCM). Joint work with Youssef Marzouk (MIT). PI: Dan Ricciuto

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Potential use cases

- Model fidelity hierarchy
- Prediction under scenario uncertainty
- Uncertain initialization based on observational data
- Model comparison with uncertainties

those that didn't make it

The Case for Uncertainty Quantification

UQ needed for...

- Model predictions
- Model validation and comparison
- Confidence assessment
- Reliability analysis
- Dimensionality reduction
- Optimal design
- Decision support
- (Noisy) data assimilation

Uncertainty Sources

- Model parameters
- Initial/boundary conditions
- Model geometry/structure
- Lack of knowledge
- Data noise
- Intrinsic stochasticity
- Numerical errors, too

PC Postprocessing: global sensitivity information is readily obtained from PCE

$$g(\xi_1, \ldots, \xi_d) = \sum_{k=0}^{P} c_k \Psi_k(\boldsymbol{\xi})$$

- Global sensitivity analysis $\equiv$ Variance decomposition
- Total variance

$$Var[g(\boldsymbol{\xi})] = \sum_{k>0} c_k^2 ||\Psi_k||^2$$

PC Postprocessing: Main Effect and Joint Sensitivity Indices

- Main effect sensitivity indices

$$S_i = \frac{Var[\mathbb{E}(g(\boldsymbol{\xi}|\xi_i)]}{Var[g(\boldsymbol{\xi})]} = \frac{\sum_{k\in\mathbb{I}_i} c_k^2 ||\Psi_k||^2}{\sum_{k>0} c_k^2 ||\Psi_k||^2}$$

  - $\mathbb{I}_i$ is the set of bases with only ξ_i involved
  - S_i is the uncertainty contribution that is due to i-th parameter only
- Joint sensitivity indices

$$S_{ij} = \frac{Var[\mathbb{E}(g(\boldsymbol{\xi}|\xi_i,\xi_j)]}{Var[g(\boldsymbol{\xi})]} - S_i - S_j = \frac{\sum_{k\in\mathbb{I}_{ij}} c_k^2 ||\Psi_k||^2}{\sum_{k>0} c_k^2 ||\Psi_k||^2}$$

  - $\mathbb{I}_{ij}$ is the set of bases with only ξ_i and ξ_j involved
  - S_{ij} is the uncertainty contribution that is due to (i,j) parameter pair

PC Postprocessing: Total Effect Sensitivity Indices

- Total effect sensitivity indices

$$T_i = 1 - \frac{Var[\mathbb{E}(g(\boldsymbol{\xi}|\xi_{-i})]}{Var[g(\boldsymbol{\xi})]} = \frac{\sum_{k\in\mathbb{I}_i^T} c_k^2||\Psi_k||^2}{\sum_{k>0} c_k^2||\Psi_k||^2}$$

  - The notation ξ_{-i} indicates terms that do not have ξ_i in them
  - $\mathbb{I}_i^T$ is the set of bases with ξ_i involved, including all its interactions
  - The sum of all T_i is usually > 1

Sensitivity indices are directly computable from PC

$$g(\boldsymbol{\xi}) = \sum_{k=0}^{P} c_k \Psi_k(\boldsymbol{\xi})$$

Consider dimensionality $d = 3$, total order $p = 2$,
number of PC terms $P + 1 = (d + p)!/(d!p!) = 10$.

$$g(\xi_1, \xi_2, \xi_3) = c_0 + \; c_1\psi_1(\xi_1) \; + \; c_2\psi_1(\xi_2) \; + \; c_3\psi_1(\xi_3) \; +$$

$$+ \; c_4\psi_2(\xi_1) \; + \; c_5\psi_1(\xi_1)\psi_1(\xi_2) \; + \; c_6\psi_1(\xi_1)\psi_1(\xi_3) \; + \; c_7\psi_2(\xi_2) \; + \; c_8\psi_1(\xi_2)\psi_1(\xi_3) \; + \; c_9\psi_2(\xi_3)$$

Variance contributions

$$Var(g) = 0 + \; c_1^2\langle\psi_1^2\rangle \; + \; c_2^2\langle\psi_1^2\rangle \; + \; c_3^2\langle\psi_1^2\rangle \; +$$

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Main effect sensitivities $\boxed{\xi_1}$ ξ_2 ξ_3

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$$+ \ c_4^2\langle\psi_2^2\rangle \ + \boxed{c_5^2\langle\psi_1^2\rangle\langle\psi_1^2\rangle} + \ c_6^2\langle\psi_1^2\rangle\langle\psi_1^2\rangle \ + \boxed{c_7^2\langle\psi_2^2\rangle} + \boxed{c_8^2\langle\psi_1^2\rangle\langle\psi_1^2\rangle} + \ c_9^2\langle\psi_2^2\rangle$$

Total sensitivities ξ_1 $\boxed{\xi_2}$ ξ_3

Sensitivity indices are directly computable from PC

$$g(\boldsymbol{\xi}) = \sum_{k=0}^{P} c_k \Psi_k(\boldsymbol{\xi})$$

Consider dimensionality $d = 3$, total order $p = 2$,
number of PC terms $P + 1 = (d + p)!/(d!p!) = 10$.

$$g(\xi_1, \xi_2, \xi_3) = c_0 + c_1\psi_1(\xi_1) + c_2\psi_1(\xi_2) + \boxed{c_3\psi_1(\xi_3)} +$$
$$+ c_4\psi_2(\xi_1) + c_5\psi_1(\xi_1)\psi_1(\xi_2) + \boxed{c_6\psi_1(\xi_1)\psi_1(\xi_3)} + c_7\psi_2(\xi_2) + \boxed{c_8\psi_1(\xi_2)\psi_1(\xi_3)} + \boxed{c_9\psi_2(\xi_3)}$$

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Joint sensitivities $\boxed{(\xi_1, \xi_2)}$ (ξ_1, ξ_3) (ξ_2, ξ_3)

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Joint sensitivities (ξ_1, ξ_2) (ξ_1, ξ_3) (ξ_2, ξ_3)

Main target: model *structural* error

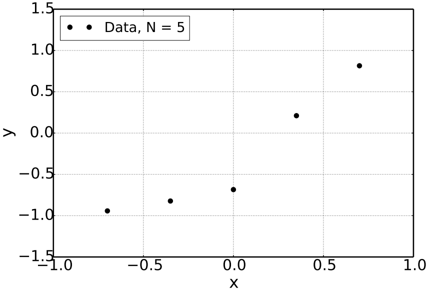
deviation from 'truth' or from a higher-fidelity model

- Inverse modeling context
  - Given experimental or higher-fidelity model data, estimate the model error

---

- Represent and estimate the error associated with
  - Simplifying assumptions, parameterizations
  - Mathematical formulation, theoretical framework
- ...will be useful for
  - Model validation
  - Model comparison
  - Scientific discovery and model improvement
  - Reliable computational predictions

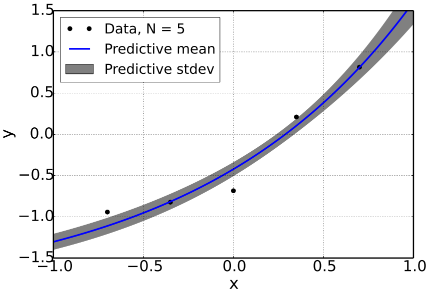
Ignoring model error leads to overconfident and biased predictions



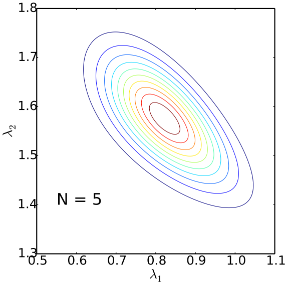
Model-data fit

- Given noisy data, calibrate an exponential model: $g(x) \approx f(x;\lambda)$

Ignoring model error leads to overconfident and biased predictions



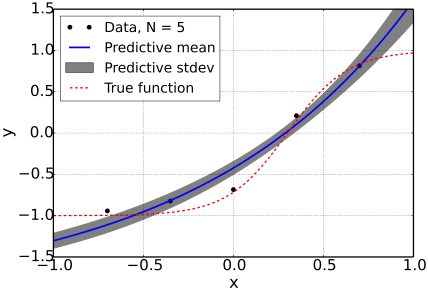
Model-data fit



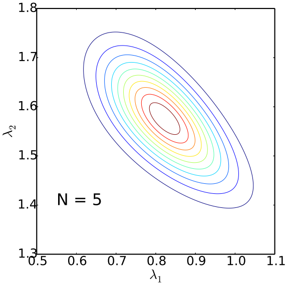
Posterior on parameters

- Given noisy data, calibrate an exponential model: $g(x) \approx f(x;\lambda)$
- Employ Bayesian inference to obtain posterior PDFs on λ

Ignoring model error leads to overconfident and biased predictions



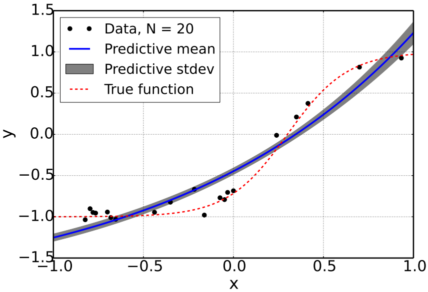
Model-data fit



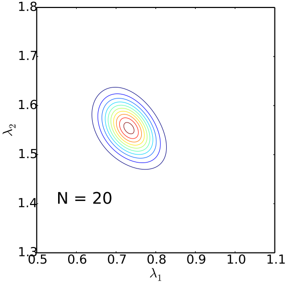
Posterior on parameters

- Given noisy data, calibrate an exponential model: $g(x) \approx f(x;\lambda)$
- Employ Bayesian inference to obtain posterior PDFs on λ
- True model – dashed-red – is *structurally* different from fit model $f(x,\lambda)$

Ignoring model error leads to overconfident and biased predictions



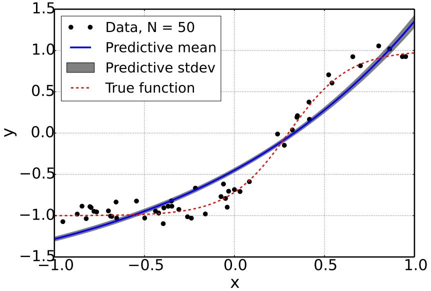
Model-data fit



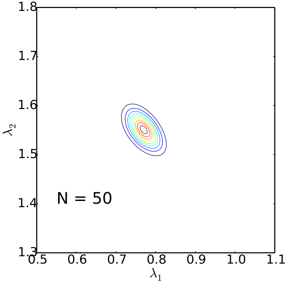
Posterior on parameters

- Given noisy data, calibrate an exponential model: $g(x) \approx f(x; \lambda)$
- Employ Bayesian inference to obtain posterior PDFs on λ
- True model – dashed-red – is *structurally* different from fit model $f(x, \lambda)$
- Higher data amount reduces posterior and predictive uncertainty
  - Increasingly sure about predictions based on the *wrong* model

Ignoring model error leads to overconfident and biased predictions



Model-data fit



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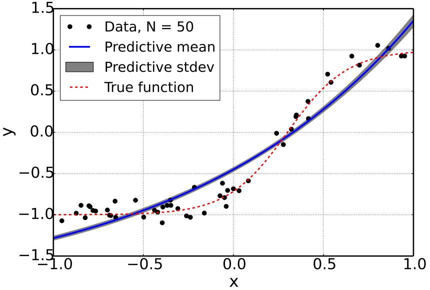
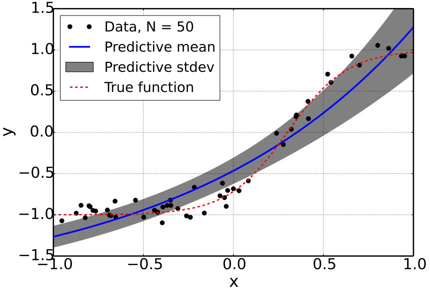


No model error treatment



Model error accounted for

- Given noisy data, calibrate an exponential model: $g(x) \approx f(x; \lambda)$
- Employ Bayesian inference to obtain posterior PDFs on λ
- True model – dashed-red – is *structurally* different from fit model $f(x, \lambda)$
- Accounting for model error allows extra uncertainty component to propagate through predictions