Density Estimation Framework for Model Error Quantification

Khachik Sargsyan, Xun Huan, Habib Najm

Sandia National Laboratories, Livermore, CA

SIAM UQ
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April 5-8, 2016

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DOE Office of Advanced Scientific Computing Research (ASCR), Scientific Discovery through Advanced Computing (SciDAC)
DOE Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, & Biosciences
DOD, DARPA Enabling Quantification of Uncertainty in Physical Systems (EQUiPS) program

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Outline

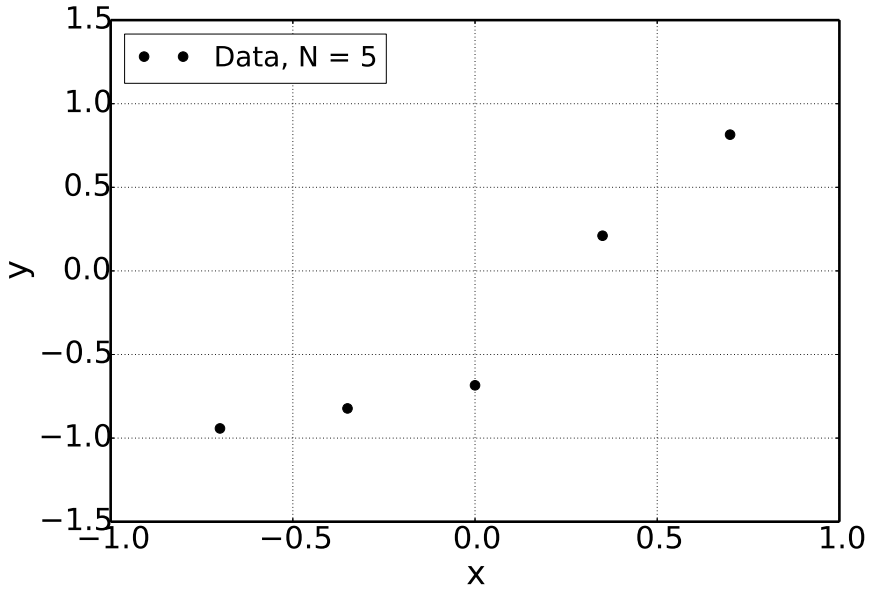
- Motivation: need to quantify and propagate model error
- Issues with current state-of-the-art
- Method
- Toy cases
- Examples
  - Chemistry
  - Atmospheric transport
  - LES computations

Main target

Model error = deviation from 'truth', or from a higher-fidelity model

- Represent and estimate the error associated with
  - Simplifying assumptions, parameterizations
  - Mathematical formulation, theoretical framework
  - Numerical discretization
- ...will be useful for
  - Model validation
  - Model comparison
  - Scientific discovery and model improvement
  - Reliable computational predictions
- Inverse modeling context
  - Given experimental or higher-fidelity model data, estimate the model error

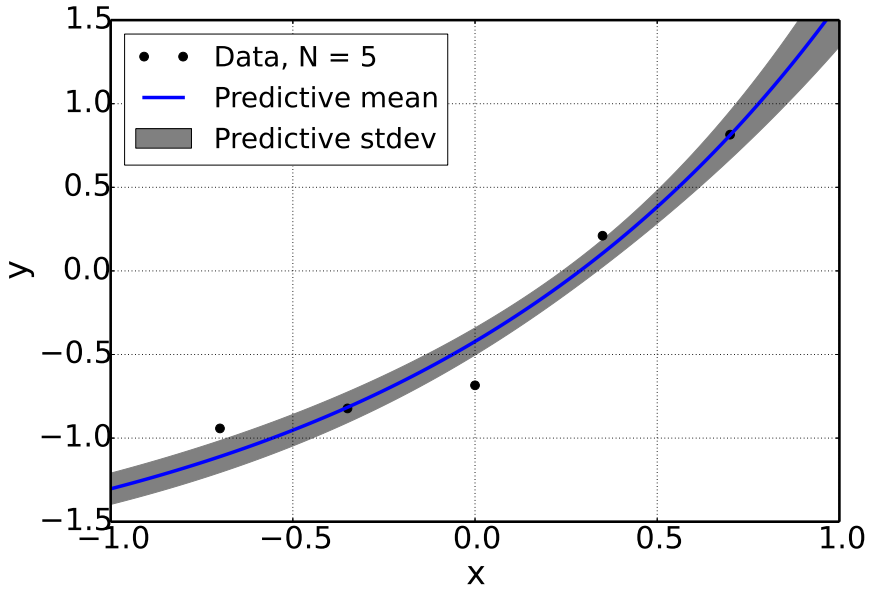
Motivation



Model-data fit

- Given noisy data – Gaussian noise
- $y = g_{\text{true}}(x) + \epsilon$

Motivation



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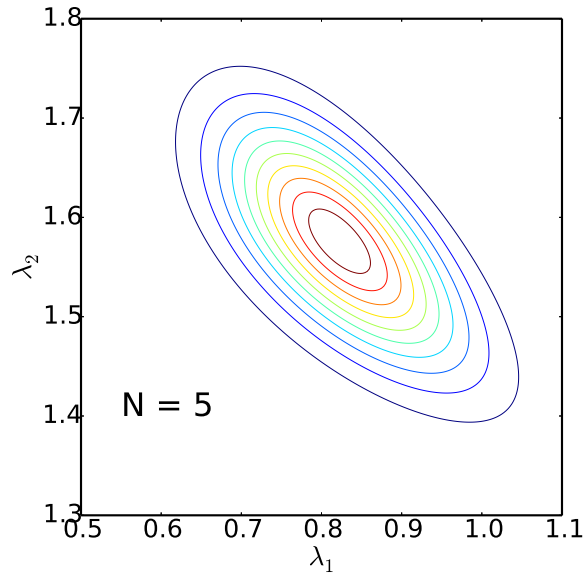
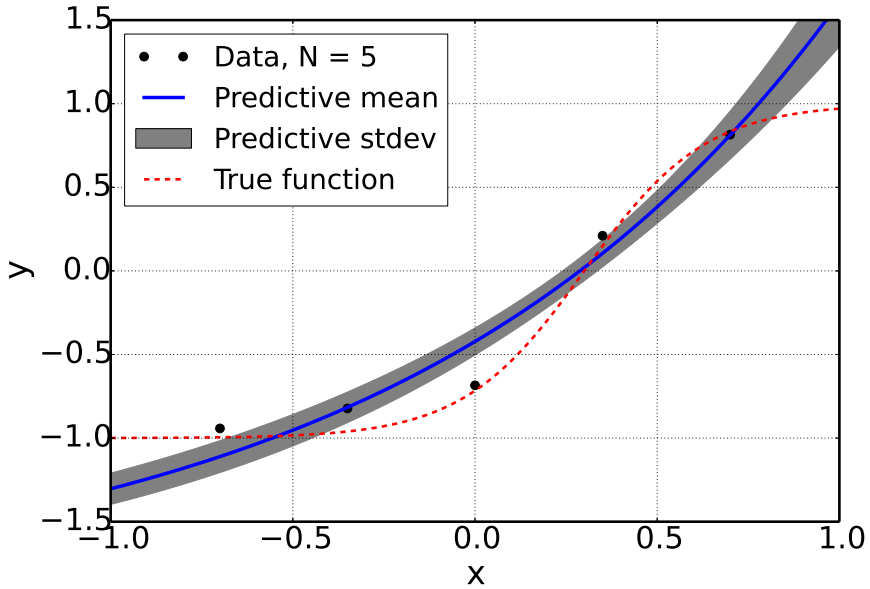


Posterior on parameters

- Employ Bayesian inference to fit an exponential model – $y_{\mathrm{m}} = f(x, \lambda)$
- Discrepancy between data and prediction presumed exclusively due to *i.i.d.* Gaussian data noise – $y = f(x, \lambda) + \epsilon_{\mathrm{d}}$
- Plotted:
  - Posterior density on the parameters
  - Preditive mean and standard deviation

Motivation



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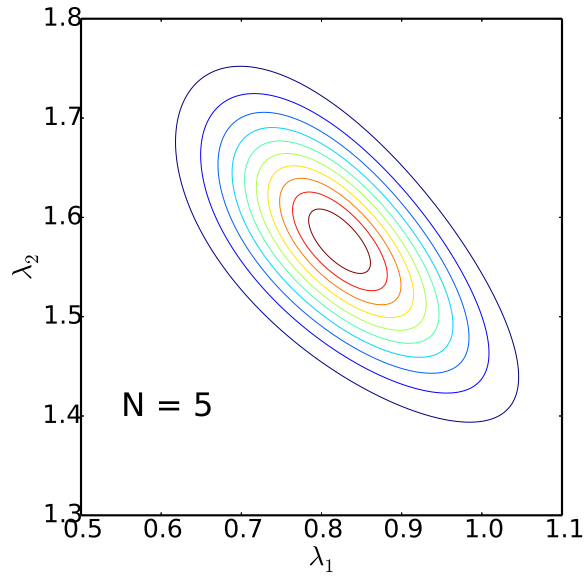

Posterior on parameters

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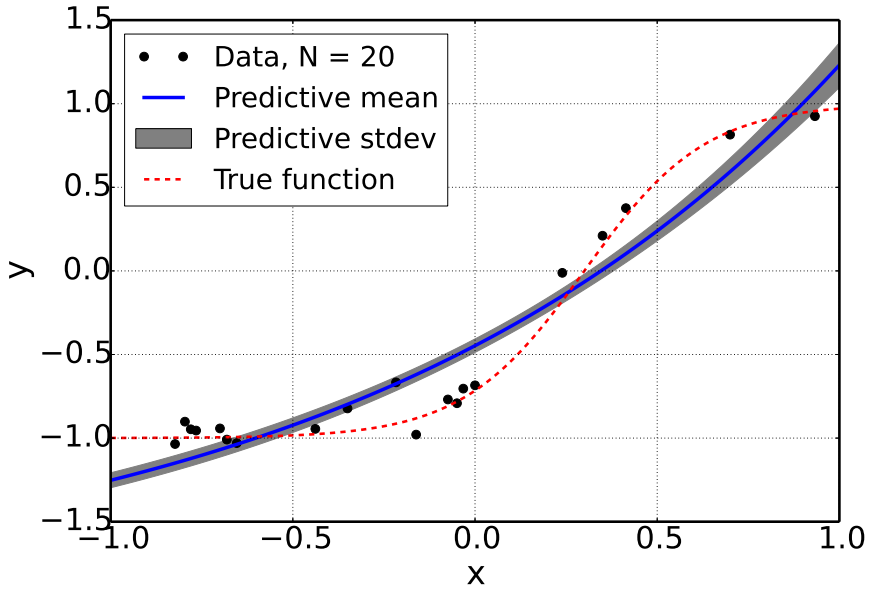
- Discrepancy between data and prediction presumed exclusively due to *i.i.d.* Gaussian data noise – $y = f(x, \lambda) + \epsilon_{\mathrm{d}}$
- True model $g(x)$ – dashed-red – differs from fit model $f(x, \lambda)$
- Actual discrepancy includes both data and model errors

Motivation



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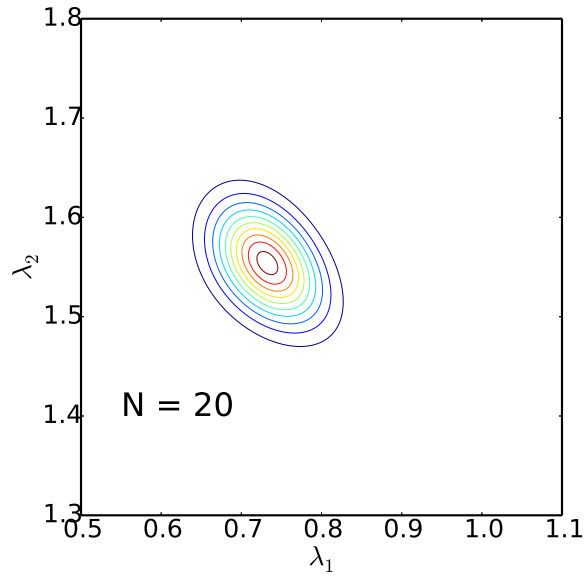
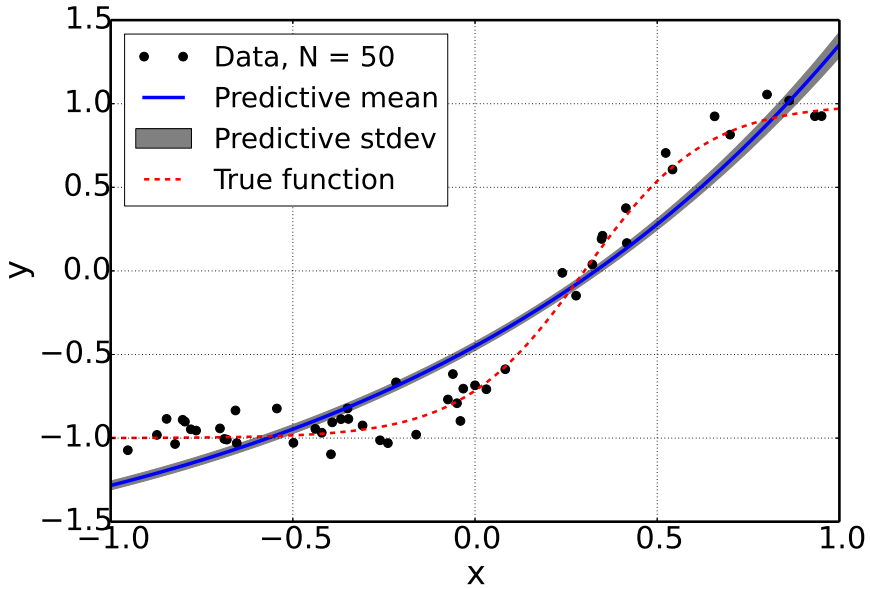


Posterior on parameters

- Increasing number of data points decreases posterior and predictive uncertainty
- We are increasingly sure about predictions based on the *wrong* model

Motivation



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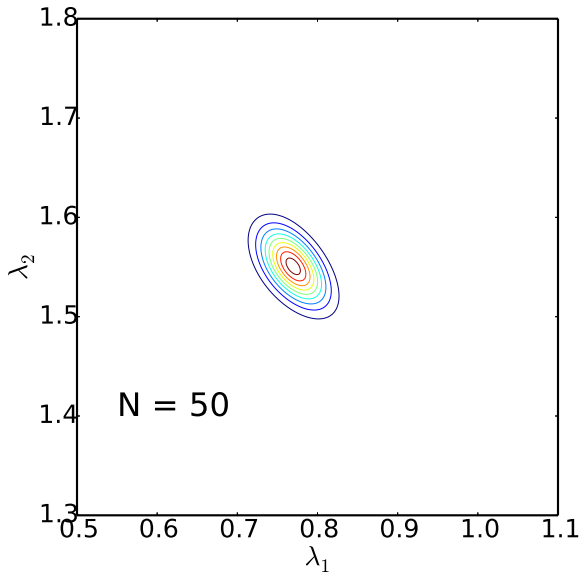

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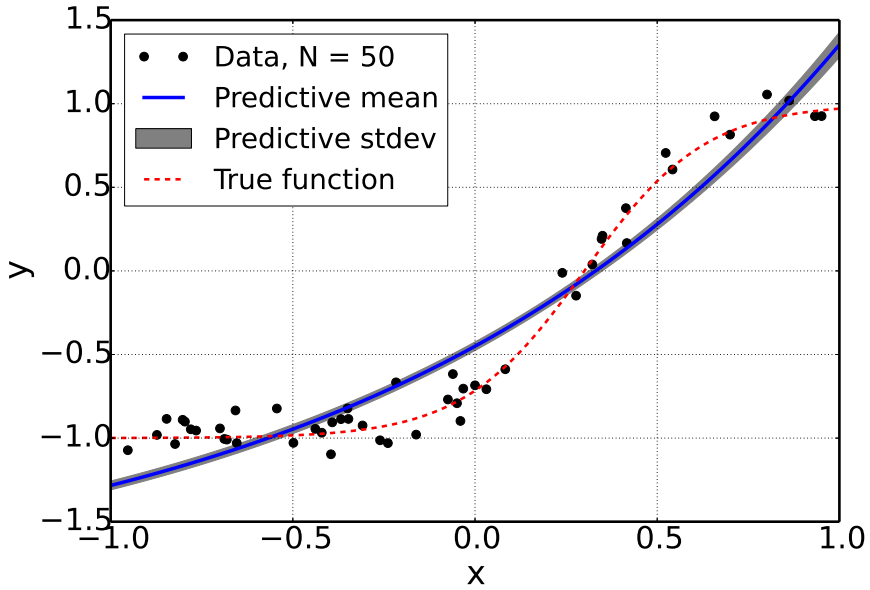

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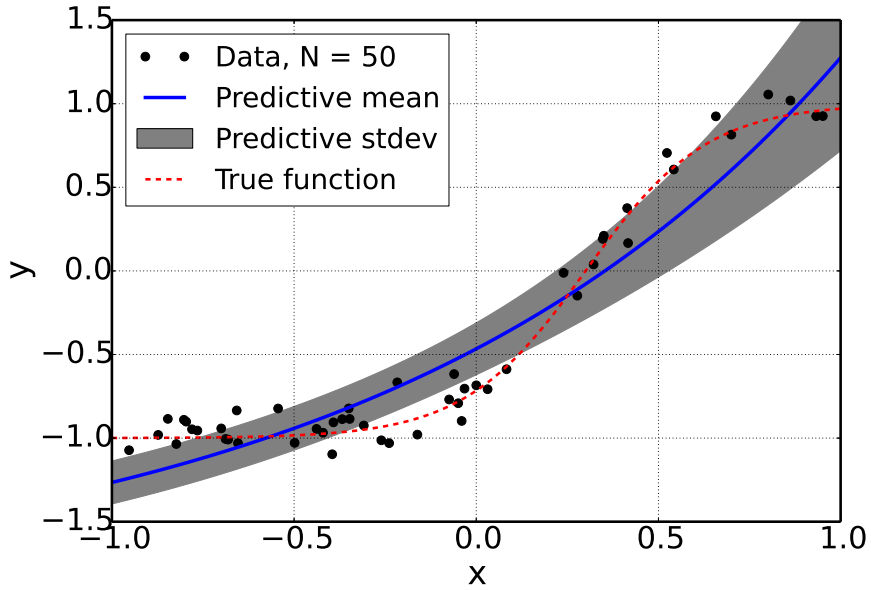


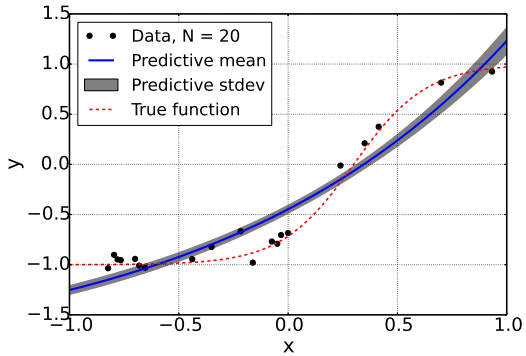
What we want

- If the model has structural uncertainty, more data leads to biased and overconfident results
- We want to quantify model-vs-truth discrepancy in a rigorous and systematic way
  - Cannot ignore model error

Data-Model-Truth

- Measurements

$$\overset{\text{data}}{y_i} = \overset{\text{truth}}{g(x_i)} + \overset{\text{data error}}{\epsilon_i^{\mathrm{d}}}$$



- Model

$$\overset{\text{truth}}{g(x_i)} = \overset{\text{model}}{f(x_i;\lambda)} + \overset{\text{model error}}{\delta(x_i)}$$

- Total error budget

$$y_i = \underbrace{f(x_i;\lambda) + \delta(x_i)}_{\text{truth } g(x_i)} + \epsilon_i^{\mathrm{d}}$$

Explicit statistical modeling of model discrepancy/error $\delta(x)$

Model Error: $\delta(x) \sim \mathrm{GP}(\mu(x), C(x,x'))$

Data Error: $\epsilon_i^{\mathrm{d}} \sim \mathrm{N}(0, \sigma^2)$

Estimate model parameters λ along with those of $\delta(x)$, ϵ_i^{d}

Additive model discrepancy: issues for physical models

$$y_i = \underbrace{f(x_i;\lambda) + \delta(x_i)}_{\text{truth}} + \epsilon_i^{\mathrm{d}}$$

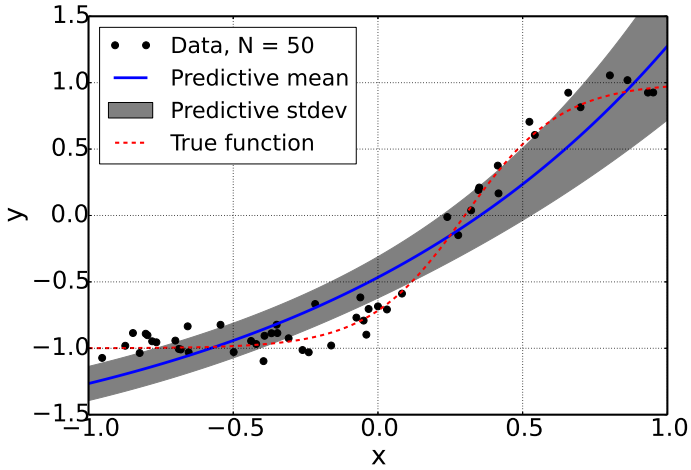
- Explicit additive statistical model for model error $\delta(x)$ Kennedy-O'Hagan (2001).
- Calibrated predictive model: $f(x;\lambda) + \delta(x)$ or $f(x;\lambda)$?

- Potential violation of physical constraints
- Disambiguation of model error $\delta(x_i)$ and data error ϵ_i^{d}
- Calibration of model error on measured observable does not impact the quality of model predictions on other QoIs
- Physical scientists are unlikely to augment their model with a statistical model error term on select outputs

Model Error – Challenges with current methods

Total error budget

$$y_i = \underbrace{f(x_i;\lambda) + \delta(x_i)}_{\text{Truth } g(x_i)} + \epsilon_i$$



- Ignoring model error $\delta(x)$ leads to incorrect predictive errors
- Conventional statistical modeling (Kennedy and O'Hagan, 2001)
  - makes it difficult to disambiguate model/data errors
  - may violate physical constraints
  - not meaningful for prediction of other QoIs
- Issue is highlighted in model-to-model calibration ($\epsilon_i = 0$)
  - no a priori knowledge of the statistical structure of the discrepancy

Model error embedding: key idea

Ideally, modelers want predictive *errorbars*:
inserting randomness on the outputs has issues, so...

- Cast input parameters λ as a random variable Λ

  Black-box

  $$y_i = f(x_i; \Lambda) + \epsilon_i^{\mathrm{d}}$$

- Generalize parameter forms,

  Random field

  $$y_i = f(x_i; \Lambda(x_i)) + \epsilon_i^{\mathrm{d}}$$

- More generally, explore additional parameterizations,

  Extra 'physics'

  $$y_i = \tilde{f}(x_i; \lambda, \Theta) + \epsilon_i^{\mathrm{d}}$$

Model error embedding: key idea

Cast input parameters λ as a random variable Λ

$$y_i = f(x_i;\lambda) + \delta(x_i) + \epsilon_i \longrightarrow y_i = f(x_i;\Lambda) + \epsilon_i$$

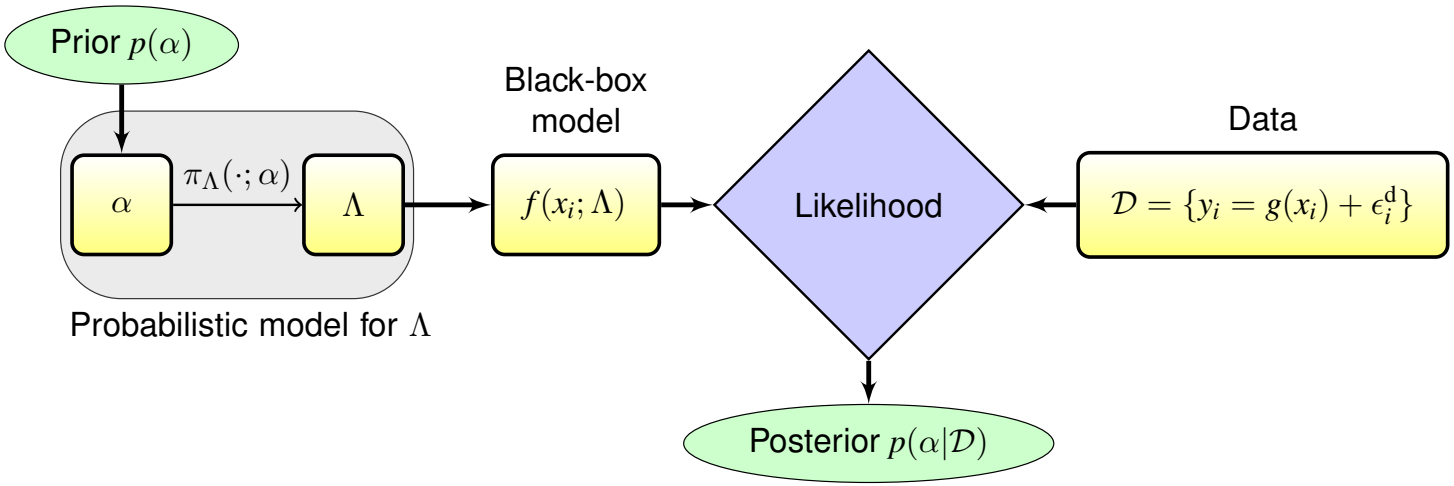
- Embed model error in specific submodel phenomenology
  - a modified transport or constitutive law
  - a modified formulation for a material property
- Allows placement of model error term in locations where key modeling assumptions and approximations are made
  - as a correction or high-order term
  - as a possible alternate phenomenology
- Naturally preserves model structure and physical constraints

Model error embedding: Bayesian formulation

$$y_i = f(x_i; \Lambda) + \epsilon_i^{\mathrm{d}}$$

- Parameter estimation of λ turns into PDF estimation of Λ
- Fixed PDF form $\pi_\Lambda(\cdot;\alpha)$ or Polynomial Chaos $\Lambda = \sum_{k=0}^{K} \alpha_k \Psi_k(\xi)$
- Back to parameter estimation, now for $\alpha = (\alpha_0, \ldots, \alpha_K)$

$$\underbrace{p(\alpha|\mathcal{D})}_{\text{Posterior}} \propto \underbrace{L_{\mathcal{D}}(\alpha)}_{\text{Likelihood}} \underbrace{p(\alpha)}_{\text{Prior}}$$



Model Error – Bayesian density estimation

$$y_i = f(x_i; \Lambda) + \epsilon_i$$

- Parametrize embedded random variable Λ:
  - PDF form $\pi_\Lambda(\cdot; \alpha)$
  - Polynomial Chaos (PC): $\Lambda = \sum_k \alpha_k \Psi_k(\xi)$
  - Multivariate Normal (MVN):

$$\begin{cases} \Lambda_1 = \alpha_{10} + \alpha_{11}\xi_1 \\ \Lambda_2 = \alpha_{20} + \alpha_{21}\xi_1 + \alpha_{22}\xi_2 \\ \quad \vdots \\ \Lambda_d = \alpha_{d0} + \alpha_{d1}\xi_1 + \alpha_{d2}\xi_2 + \cdots + \alpha_{dd}\xi_d \end{cases}$$

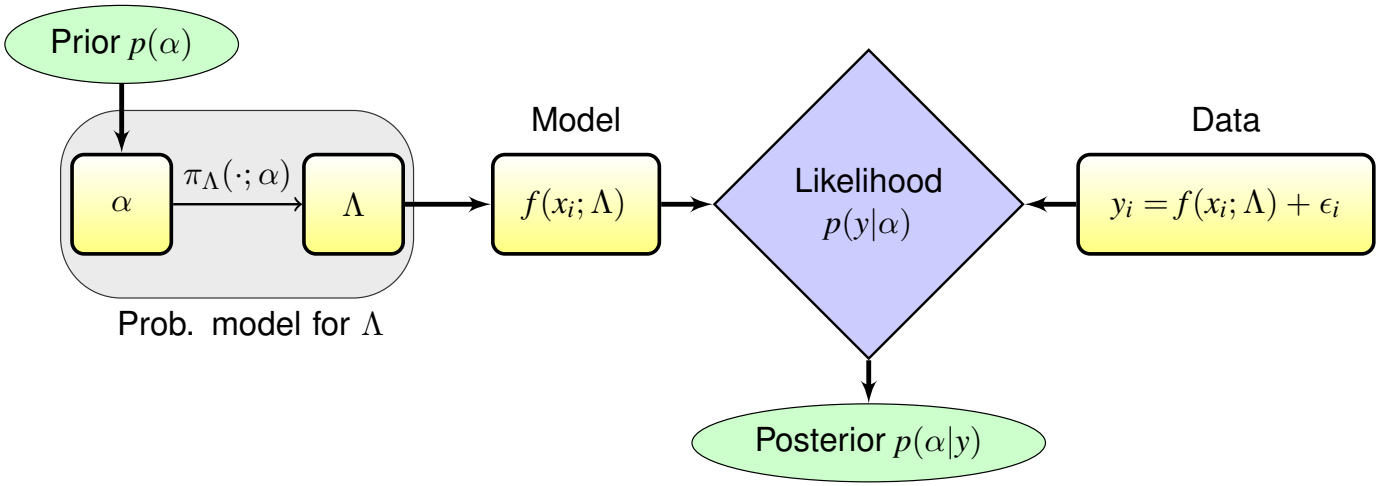
- Inverse modeling context
  - Parameter estimation of $\lambda \Rightarrow$ PDF estimation of $\Lambda \Rightarrow$ parameter estimation of α
- Bayesian formulation

$$\underbrace{p(\alpha|y)}_{\text{Posterior}} \propto \underbrace{L_y(\alpha)}_{\text{Likelihood}} \underbrace{p(\alpha)}_{\text{Prior}}$$

Model Error – Likelihood options

K. Sargsyan, H. Najm, and R. Ghanem, “On the Statistical Calibration of Physical Models”.

International Journal for Chemical Kinetics, 47(4): pp 246–276, 2015.



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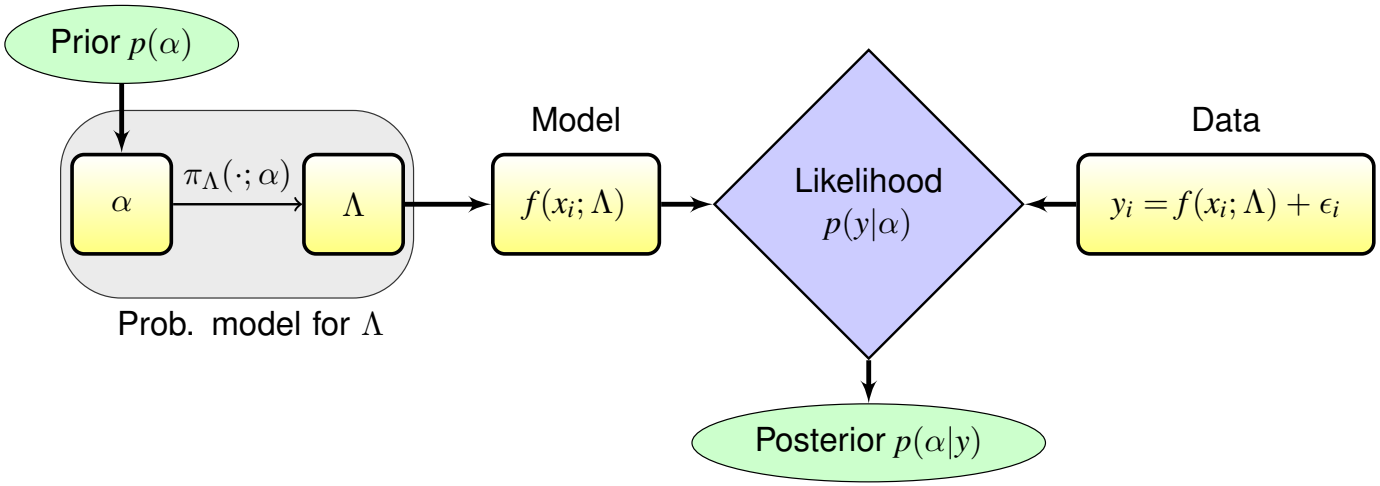

- Full Likelihood: $L(\alpha) = p(y|\alpha) = p(y_1, \ldots, y_N|\alpha) = \pi(y)$
  - Degenerate if no data noise
  - Requires multivariate KDE or high-d integration
  - Gaussian approximation:
    $L(\alpha) \propto \exp\left(-\frac{1}{2}(y-\mu(\alpha))^T\Sigma^{-1}(\alpha)(y-\mu(\alpha))\right)$
  - Non-intrusive spectral projection with Polynomial Chaos relieves the expense and provides easy access to mean $\mu(\alpha)$ and covariance $\Sigma(\alpha)$

Model Error – Likelihood options

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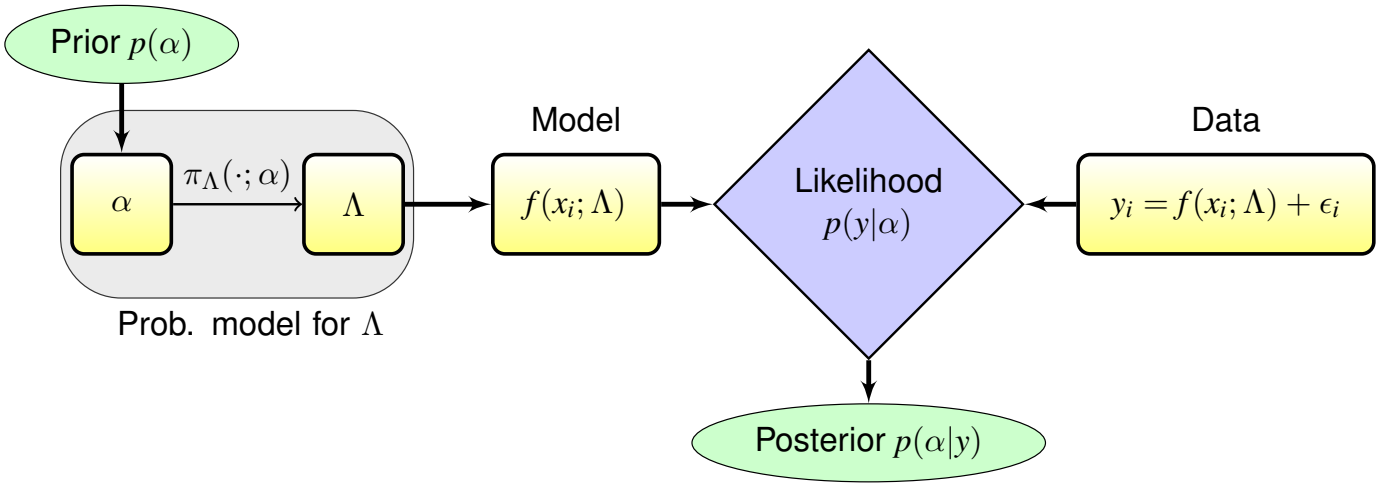

- Marginalized Likelihood:
  $L(\alpha) = p(y|\alpha) \approx \prod_{i=1}^{N} p(y_i|\alpha) = \prod_{i=1}^{N} \pi(y_i)$
  - Requires univariate KDE
  - Neglects built-in correlations
  - Gaussian approximation:
    $L(\alpha) \propto \exp\left(-\frac{1}{2}\sum_{i=1}^{N} \Sigma_{ii}^{-1}(\alpha)(y_i - \mu_i(\alpha))^2\right)$

Model Error – Likelihood options

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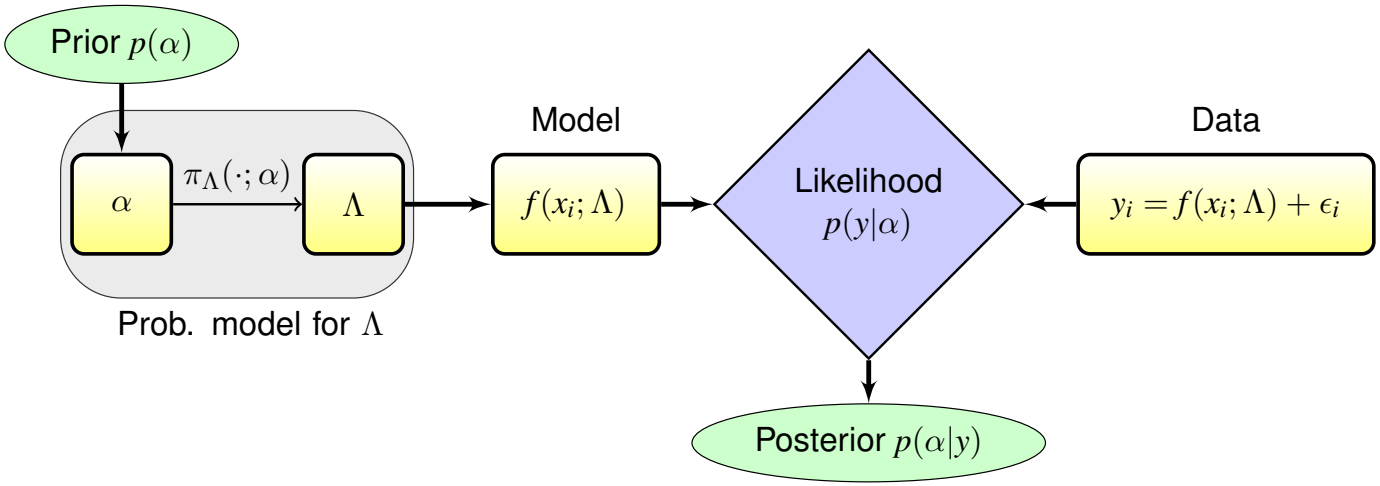

- Approximate Bayesian Computation (ABC): $L(\alpha) = \frac{1}{\epsilon} K\left(\frac{\rho(\mathcal{S}_\mathcal{M},\mathcal{S}_\mathcal{D})}{\epsilon}\right)$
  - Mean of $f(x_i;\Lambda)$ is "centered" on the data
  - The width of the distribution of $f(x_i;\Lambda)$ is consistent with the spread of the data around the nominal model prediction

$$L(\alpha) \propto \exp\left(-\frac{1}{2\epsilon^2}\sum_{i=1}^{N}\left[(\mu_i(\alpha)-y_i)^2 + (\sqrt{\Sigma_{ii}(\alpha)} - \gamma|\mu_i(\alpha)-y_i|)^2\right]\right)$$

Likelihood construction: data model

- Data $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$
- Model $f(x;\Lambda)$
- Model parameters $\Lambda = \lambda(\alpha;\xi) = \sum_k \alpha_k \Psi_k(\xi_1, \ldots, \xi_d)$

- Data generation model; to aid likelihood $p(\mathcal{D}|\hat{\alpha})$ construction

$$
\begin{aligned}
y_i &= f(x_i, \Lambda) + \epsilon_i^{\mathrm{d}} = \\
&= f\left(x_i, \sum_k \alpha_k \Psi_k(\xi_1, \ldots, \xi_d)\right) + \sigma_{\mathcal{D}} \xi_{d+i} = \\
&\overset{NISP}{\approx} \sum_k f_{ik}(\alpha) \Psi_k(\xi_1, \ldots, \xi_d) + \sigma_{\mathcal{D}} \xi_{d+i} = \\
&= h_i(\hat{\xi}; \hat{\alpha})
\end{aligned}
$$

- Infer $\hat{\alpha} = (\alpha, \sigma_{\mathcal{D}})$
- Full PC germ $\hat{\xi} = (\underbrace{\xi_1, \ldots, \xi_d}_{\text{Model error}}, \underbrace{\xi_{d+1}, \ldots, \xi_{d+N}}_{\text{Data noise}})$

Likelihood options

$$y_i = \underbrace{\sum_k f_{ik}(\alpha)\Psi_k(\xi_1, \ldots, \xi_d) + \sigma_{\mathcal{D}}\xi_{d+i}}_{h_i(\hat{\xi};\hat{\alpha})}$$

Note: for each $\hat{\alpha}$,

the data model $\boldsymbol{h}(\hat{\xi};\hat{\alpha})$ is a multivariate random variable with cheap sampling, and easily accessible mean $\boldsymbol{\mu}(\hat{\alpha})$ and covariance $\Sigma(\hat{\alpha})$

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  - Degenerate if no data noise
  - Requires multivariate KDE
  - Gaussian approximation:
    $L(\hat{\alpha}) \propto \exp\left(-\frac{1}{2}(\boldsymbol{y} - \boldsymbol{\mu}(\hat{\alpha}))^T\Sigma^{-1}(\boldsymbol{y} - \boldsymbol{\mu}(\hat{\alpha}))\right)$

Likelihood options

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  - Requires univariate KDE
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Likelihood options

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Calibrated predictions – general x

For fixed α, e.g. Maximum a Posteriori (MAP) value,

Uncertain prediction:

$$y = f(x, \lambda(\alpha; \xi))$$

Mean:

$$\mu(x, \alpha) = \mathbb{E}_\xi[f(x, \lambda(\alpha; \xi))]$$

Variance:

$$\sigma^2(x, \alpha) = \mathbb{V}_\xi[f(x, \lambda(\alpha; \xi))]$$

Average over posterior of α

Posterior predictive (PP):

$$p(f|\mathcal{D}) = \int p(f|\alpha)p(\alpha|\mathcal{D})d\alpha = \mathbb{E}_\alpha[p(f|\alpha)]$$

PP mean:

$$\mu_{\text{PP}}(x) = \mathbb{E}_\xi \mathbb{E}_\alpha[f(x, \lambda(\alpha; \xi))] = \mathbb{E}_\alpha \mu(x, \alpha)$$

PP variance:

$$\sigma^2_{\text{PP}}(x) = \underbrace{\mathbb{E}_\alpha[\sigma^2(x, \alpha)]}_{\text{model error}} + \underbrace{\mathbb{V}_\alpha[\mu(x, \alpha)]}_{\text{data noise}}$$

Calibrated predictions – compare to data at x_i

For fixed α, e.g. Maximum a Posteriori (MAP) value,
Uncertain prediction:

$$y_i = f(x_i, \lambda(\alpha; \xi)) + \epsilon_i^{\mathrm{d}} \equiv h(x_i, \lambda(\alpha; \xi))$$

Mean:

$$\mu(x_i, \alpha) = \mathbb{E}_\xi[f(x_i, \lambda(\alpha; \xi))]$$

Variance:

$$\sigma^2(x_i, \alpha) = \mathbb{V}_\xi[f(x_i, \lambda(\alpha; \xi))] + \sigma_{\mathcal{D}}^2$$

Average over posterior of α

Posterior predictive (PP):

$$p(h|\mathcal{D}) = \int p(h|\alpha)p(\alpha|\mathcal{D})d\alpha = \mathbb{E}_\alpha[p(h|\alpha)]$$

PP mean:

$$\mu_{\mathrm{PP}}(x_i) = \mathbb{E}_\xi \mathbb{E}_\alpha[f(x_i, \lambda(\alpha; \xi))] = \mathbb{E}_\alpha \mu(x_i, \alpha)$$

PP variance:

$$\sigma_{\mathrm{PP}}^2(x_i) = \underbrace{\mathbb{E}_\alpha[\sigma^2(x_i, \alpha)]}_{\text{model error}} + \underbrace{\mathbb{V}_\alpha[\mu(x_i, \alpha)] + \mathbb{E}_{\sigma_{\mathcal{D}}}[\sigma_{\mathcal{D}}^2]}_{\text{data noise}}$$

Calibrated predictions – compare to data at x_i

For fixed α, e.g. Maximum a Posteriori (MAP) value,
Uncertain prediction:

$$y_i = h(x_i, \lambda(\alpha; \hat{\xi})) = f(x_i, \lambda(\alpha; \xi)) + \sigma_{\mathcal{D}} \xi_{d+i}$$

Mean:

$$\mu(x_i, \alpha) = \mathbb{E}_{\xi}[f(x_i, \lambda(\alpha; \xi))]$$

Variance:

$$\sigma^2(x_i, \alpha) = \mathbb{V}_{\xi}[f(x_i, \lambda(\alpha; \xi))] + \sigma^2_{\mathcal{D}}$$

Average over posterior of α

Pushed-forward posterior:

$$p(h|\mathcal{D}) = \int p(h|\alpha, \sigma_{\mathcal{D}}) p(\alpha, \sigma_{\mathcal{D}}|\mathcal{D}) d\alpha d\sigma_{\mathcal{D}} = \mathbb{E}_{\alpha, \sigma_{\mathcal{D}}}[p(h|\alpha, \sigma_{\mathcal{D}})]$$

Pushed-forward mean:

$$\mu_{\text{PFP}}(x_i) = \mathbb{E}_{\xi}\mathbb{E}_{\alpha}[f(x_i, \lambda(\alpha; \xi))] = \mathbb{E}_{\alpha}\mu(x_i, \alpha)$$

Pushed-forward variance:

$$\sigma^2_{\text{PFP}}(x_i) = \underbrace{\mathbb{E}_{\alpha}[\sigma^2(x_i, \alpha)]}_{\text{model error}} + \underbrace{\mathbb{V}_{\alpha}[\mu(x_i, \alpha)] + \mathbb{E}_{\sigma_{\mathcal{D}}}[\sigma^2_{\mathcal{D}}]}_{\text{data noise}}$$

Model Error – Predictions

$$f(x;\Lambda) = f\left(x;\sum_k \alpha_k \Psi_k(\xi)\right) = \sum_k f_k(x;\alpha)\Psi_k(\xi)$$

- Non-intrusive spectral projection (NISP) will be employed for
  - Likelihood computation
  - Posterior/pushed-forward predictions
  - Easy access to first two moments:

$$\mu(x;\alpha) = f_0(x;\alpha), \qquad \sigma^2(x;\alpha) = \sum_{k>0} f_k^2(x;\alpha)||\Psi_k||^2$$

- Predictive mean

$$\mathbb{E}[y(x) = \mathbb{E}_\alpha[\mu(x;\alpha)]$$

- Decomposition of predictive variance

$$\mathbb{V}[y(x)] = \underbrace{\mathbb{E}_\alpha[\sigma^2(x;\alpha)]}_{\text{Model error}} + \underbrace{\mathbb{V}_\alpha[\mu(x;\alpha)] + \sigma_d^2}_{\text{Poserior/Data error}}$$

Attribution of error components

$$y_i = \underbrace{\sum_k f_{ik}(\alpha)\Psi_k(\xi_1, \ldots, \xi_d) + \sigma_{\mathcal{D}}\xi_{d+i}}_{h_i(\hat{\xi};\hat{\alpha})}$$

Stochastic dimensions:

- Model error $\xi_1, \ldots, \xi_d$
- Measurement error $\xi_{d+1}, \ldots, \xi_{d+N}$
- Posterior uncertainty (α): can be represented via its own PC expansion (using MCMC samples and Rosenblatt transformation)

Full PC expansion: $y_i = \sum f_j \Psi_j(\hat{\hat{\xi}})$

Full stochastic *germ*:

$$\hat{\hat{\xi}} = (\underbrace{\xi_1, \ldots, \xi_d}_{\text{Model error}}, \underbrace{\xi_{d+1}, \ldots, \xi_{d+N}}_{\text{Measurement error}}, \underbrace{\xi_{d+N+1}, \ldots, \xi_{d+N+N_\alpha}}_{\text{Posterior uncertainty}})$$

Posterior predictive variance:

$$\sigma^2_{\text{PP}}(x_i) = \mathbb{E}_\alpha[\sigma^2(x_i, \alpha)] + \mathbb{E}_{\sigma_{\mathcal{D}}}[\sigma^2_{\mathcal{D}}] + \mathbb{V}_\alpha[\mu(x_i, \alpha)]$$

Challenges and Mitigation

- Density estimation is more challenging than parameter estimation
  - Inverse problem is ill-posed or intractable

  $\Rightarrow$ Employ approximate or empirical likelihoods

- Potentially a high-dimensional Bayesian problem
  - Full posterior may be inaccessible...

  $\Rightarrow$ Resort to optimization algorithms in no-noise case
  - ... or hard to sample from

  $\Rightarrow$ Adaptive MCMC algorithms, Likelihood-informed subspaces

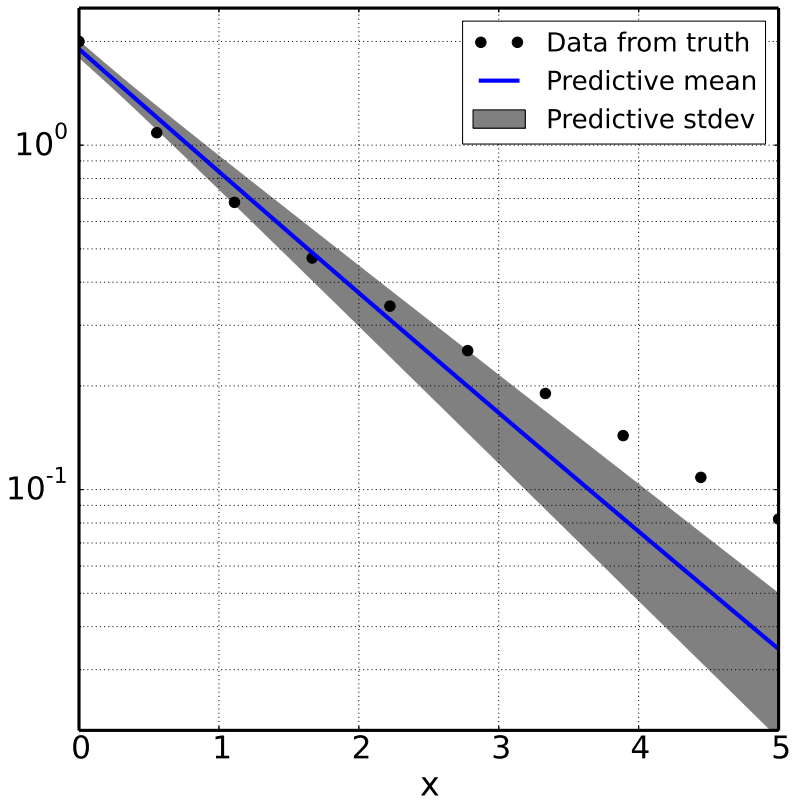
- Sparse data or expensive high-fidelity simulations
  - With low information content, calibration may struggle

  $\Rightarrow$ More informative priors/regularization

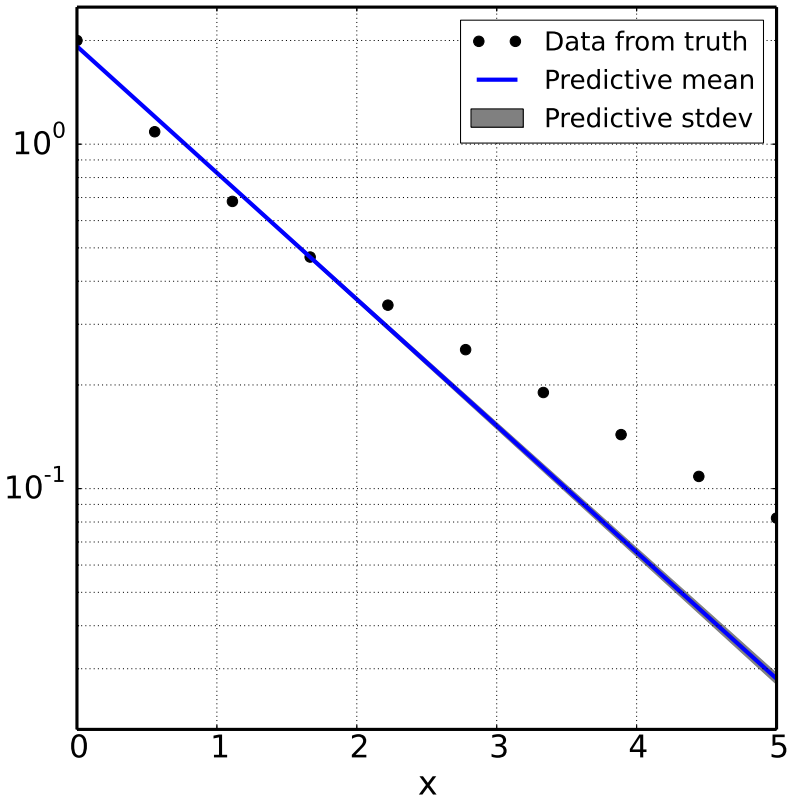
Predictions account for model error

Calibrating single-exponential models
with data from a double exponential model $g(x) = e^{-0.5x} + e^{-2x}$

Linear-exponential $f(x, \lambda) = e^{\lambda_1 + \lambda_2 x}$



Additive Gaussian error



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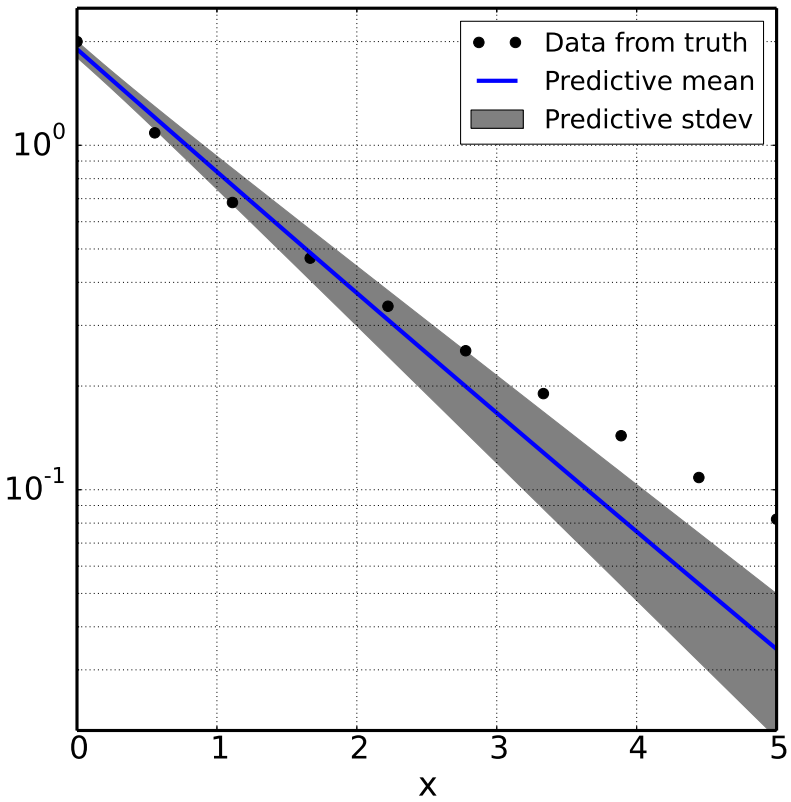
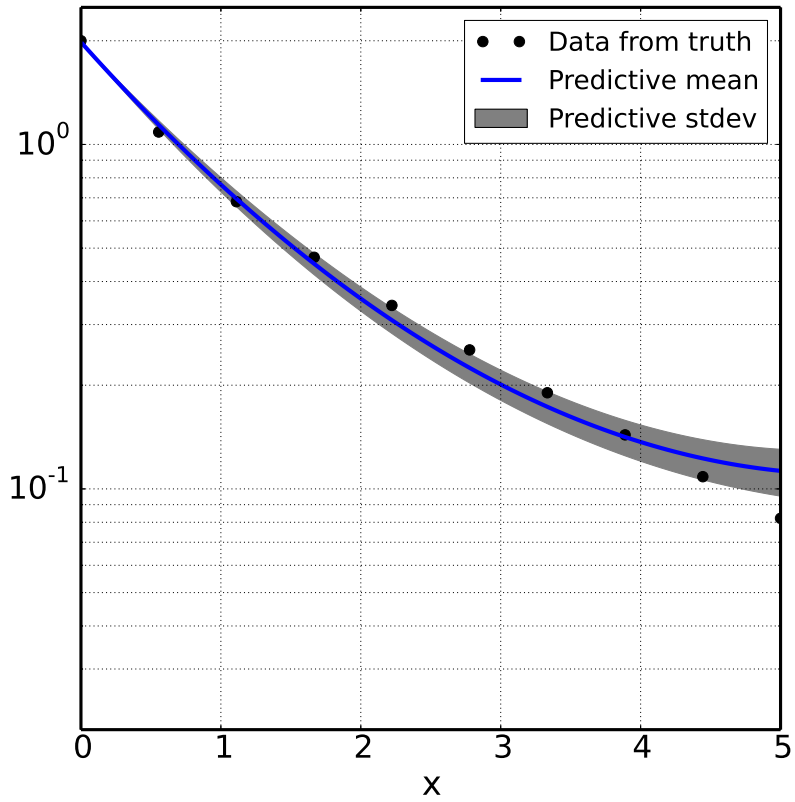
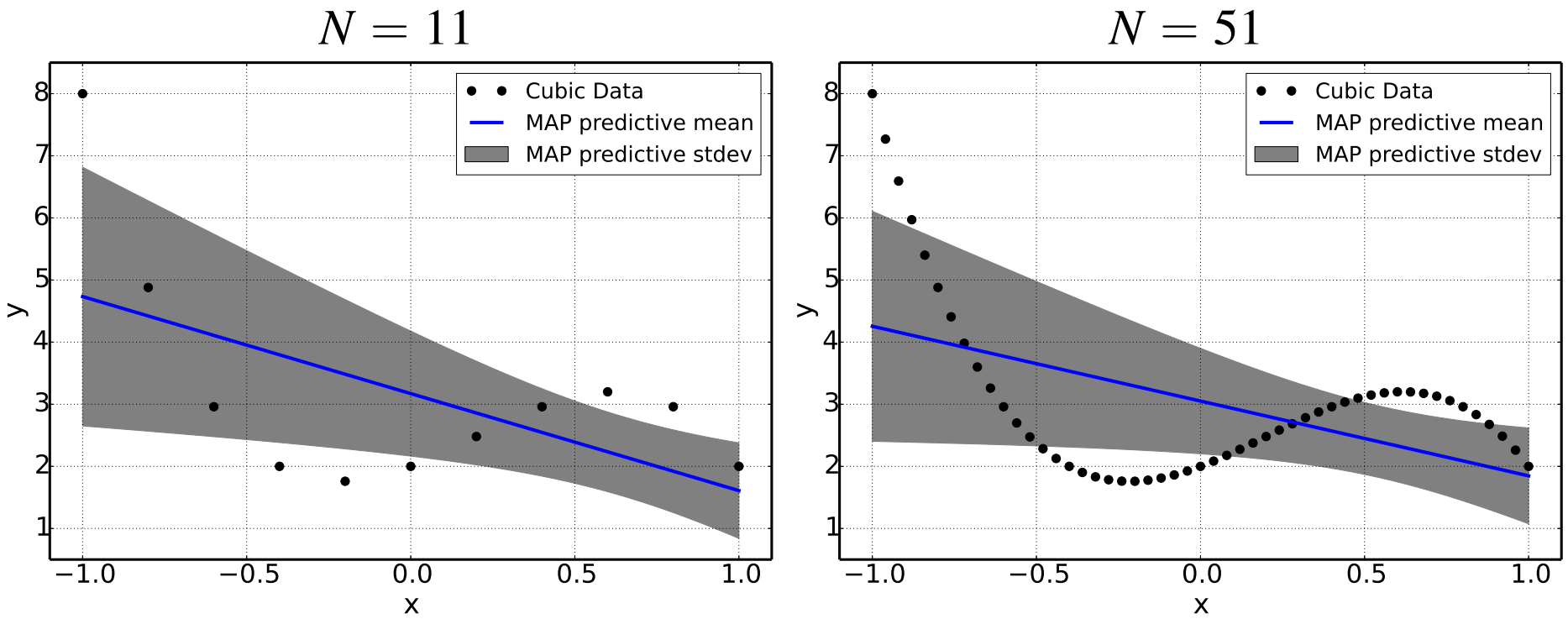


Quadratic-exponential $f_2(x, \lambda) = e^{\lambda_1 + \lambda_2 x + \lambda_3 x^2}$

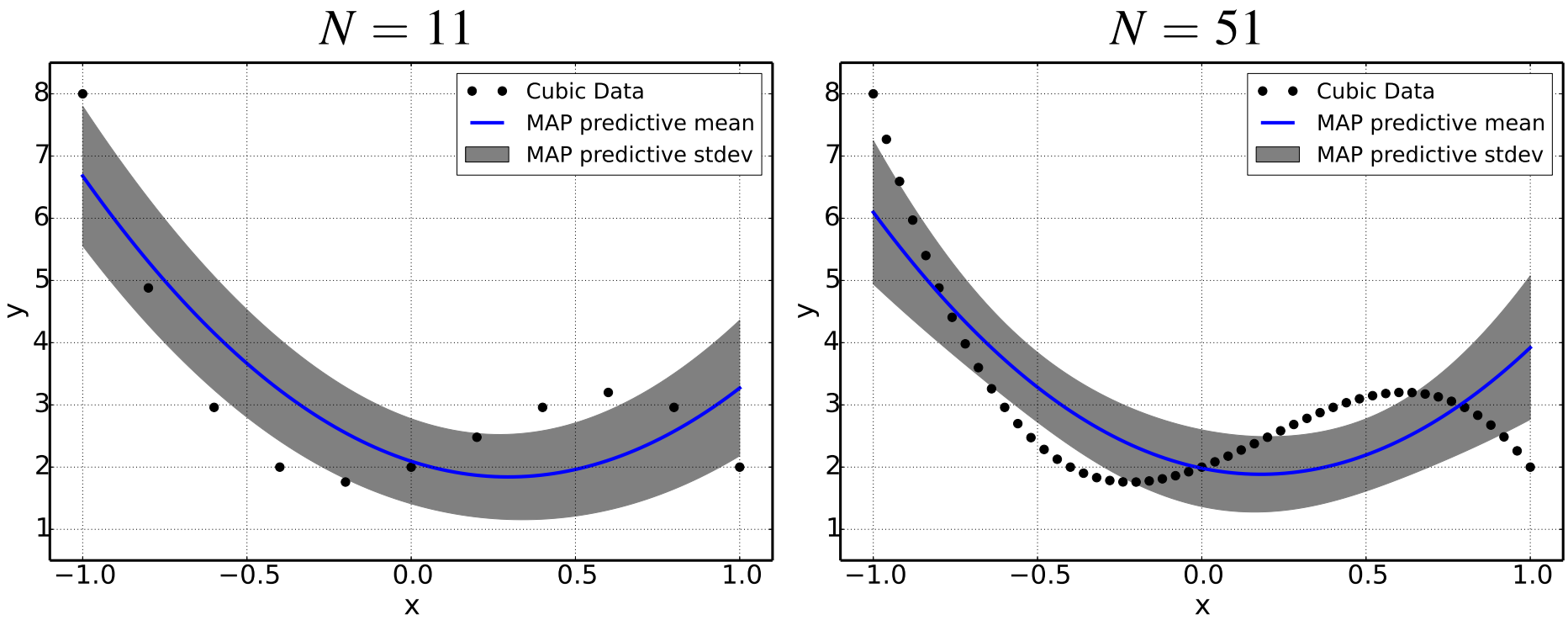


Test problem – Cubic data fit by a line – ABC



- MAP predictive mean centered on data
- MAP predictive standard deviation captures range of discrepancy
- Increasing number of data points has a small effect on both predictive mean and stdev.

Test problem – Cubic data fit by a quadratic – ABC



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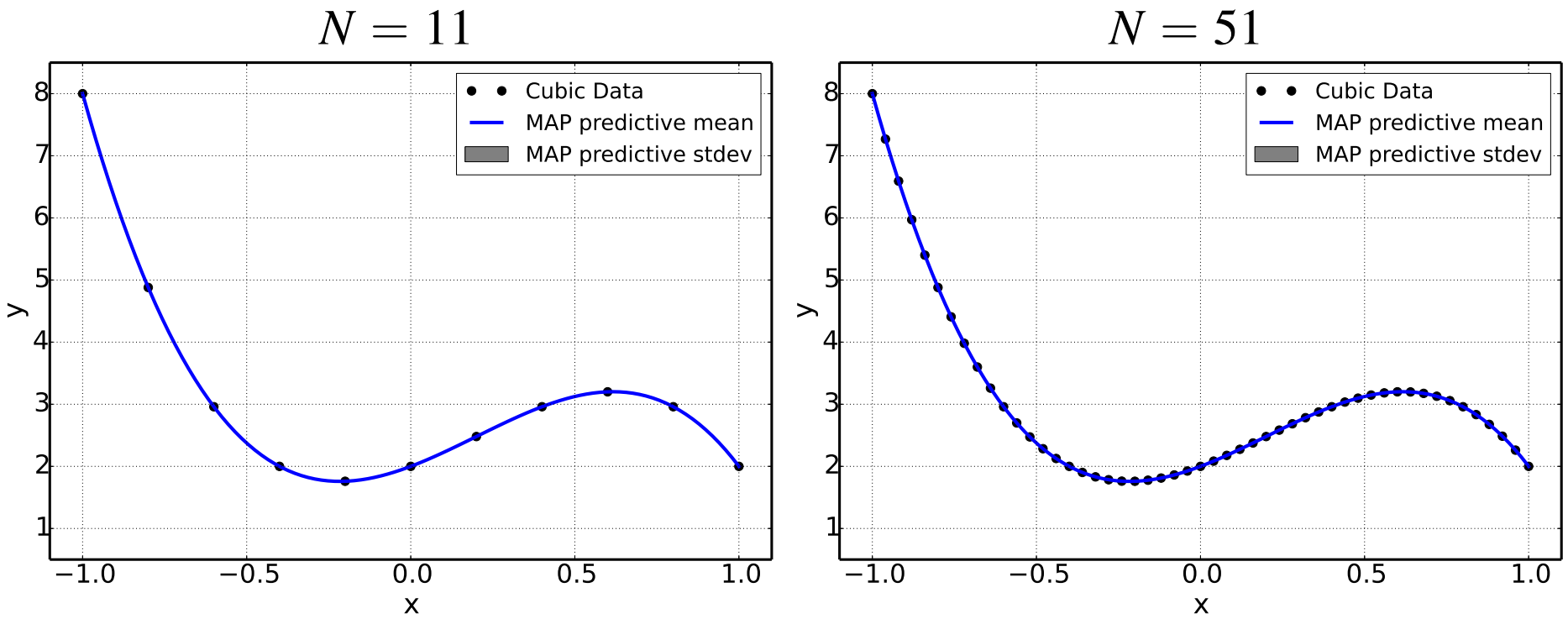
Test problem – Cubic data fit by a cubic – ABC

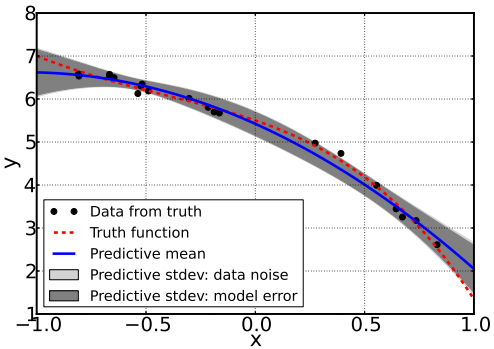


- MAP predictive mean centered on data
- MAP predictive standard deviation captures range of discrepancy
- Increasing number of data points has a small effect on both predictive mean and stdev.

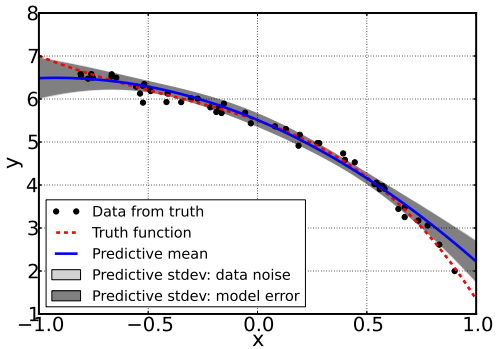
More data leads to 'leftover' model error

Calibrating a quadratic $f(x) = \lambda_0 + \lambda_1 x + \lambda_2 x^2$
w.r.t. 'truth' $g(x) = 6 + x^2 - 0.5(x+1)^{3.5}$ measured with noise $\sigma = 0.1$.

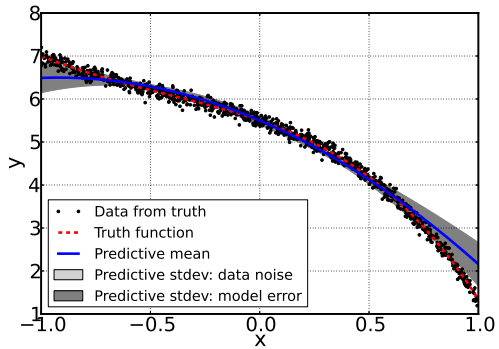
$N = 20$



$N = 50$

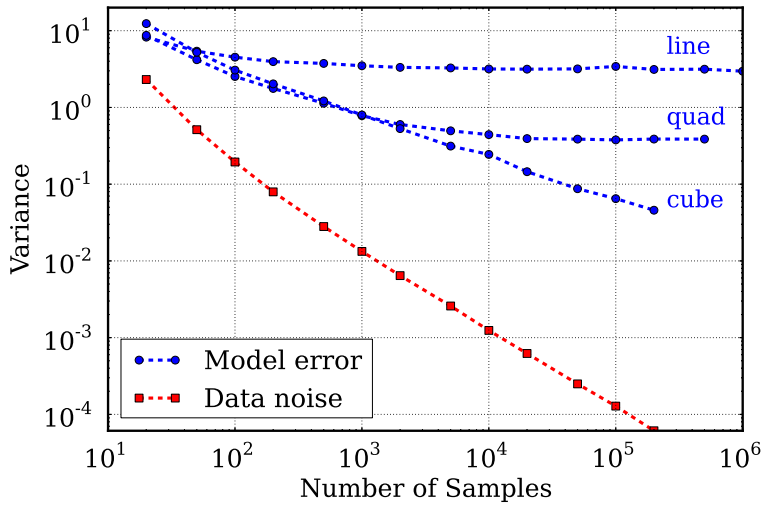


$N = 1000$



Summary of features:

- Well-defined model-to-model calibration
- Model-driven discrepancy correlations
- Respects physical constraints
- Disambiguates model and data errors
- Calibrated predictions of multiple QoIs



Chemistry problem – ABC

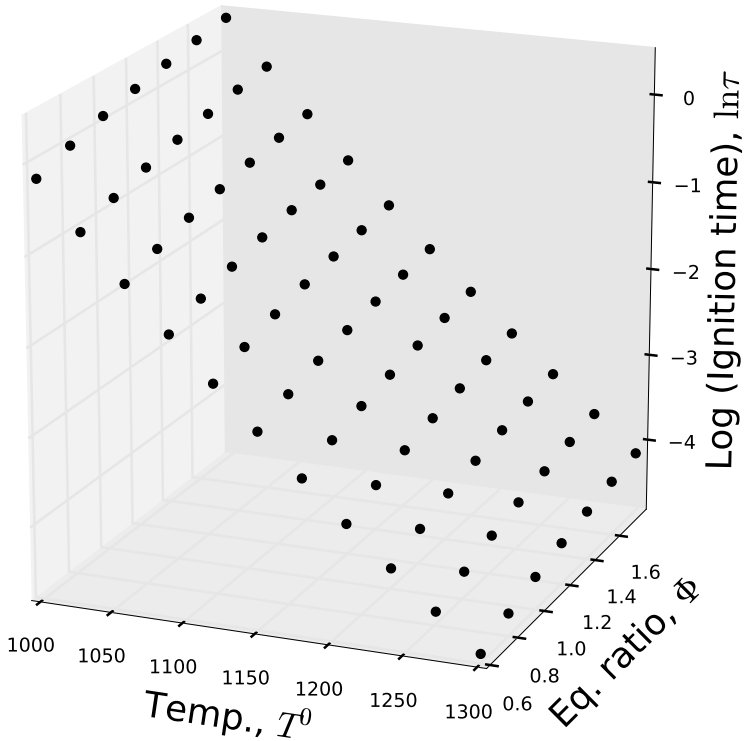
- Homogeneous ignition, methane-air mixture
- Single-step global reaction model calibrated against a detailed chemical kinetic model

- Data: ignition time; range of initial T & equivalence ratio
- Single-step model:

$$\mathrm{CH_4} + 2\mathrm{O_2} \rightarrow \mathrm{CO_2} + 2\mathrm{H_2O}$$

$$\begin{aligned} \mathfrak{R} &= [\mathrm{CH_4}][\mathrm{O_2}]k_f \\ k_f &= A\exp(-E/R^oT) \end{aligned}$$

- $(\ln A, E) = \sum_k \boldsymbol{\alpha}_k \Psi_k(\xi)$

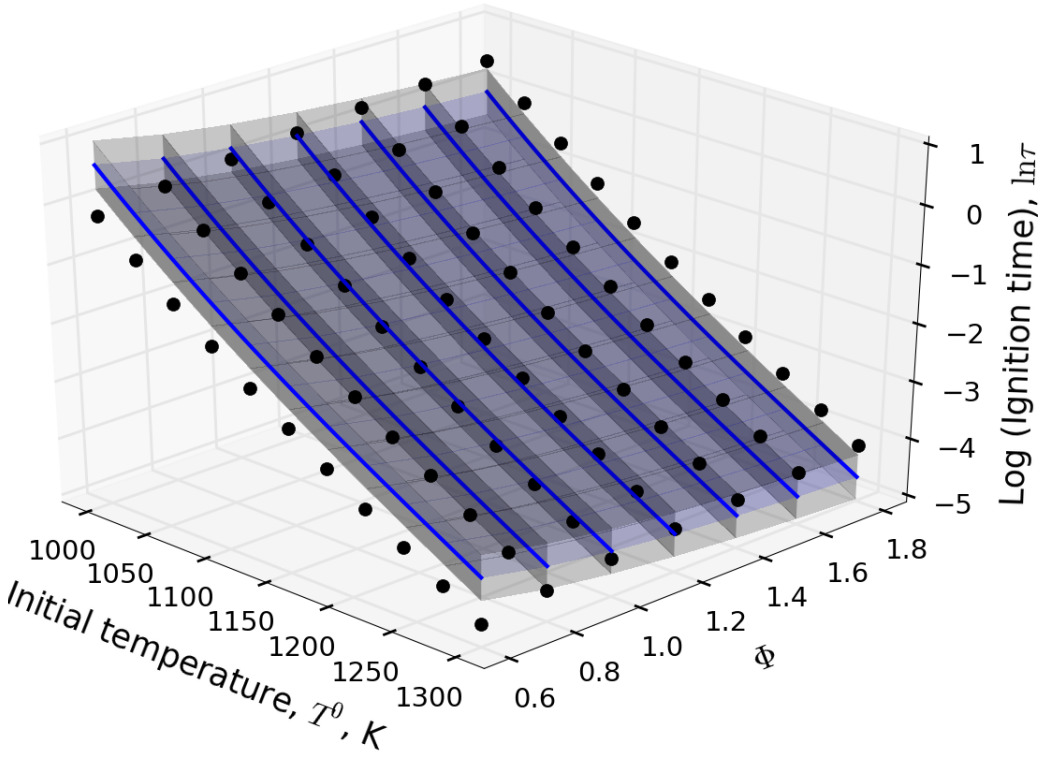


Quality of Uncertain Calibrated Model Predictions

Calibrated uncertain fit model is consistent with the detailed-model data.

Over the range of (T^0, Φ):

- MAP predictive mean ignition-time is centered on the data
- MAP predictive stdv is consistent with the scatter of the data



K. Sargsyan, H.N. Najm, and R. Ghanem
"On the Statistical Calibration of Physical Models"
Int. J. Chem. Kin., 47(4): 246-276, 2015

TransCom3 Experiment of CO_2 Flux Inversion

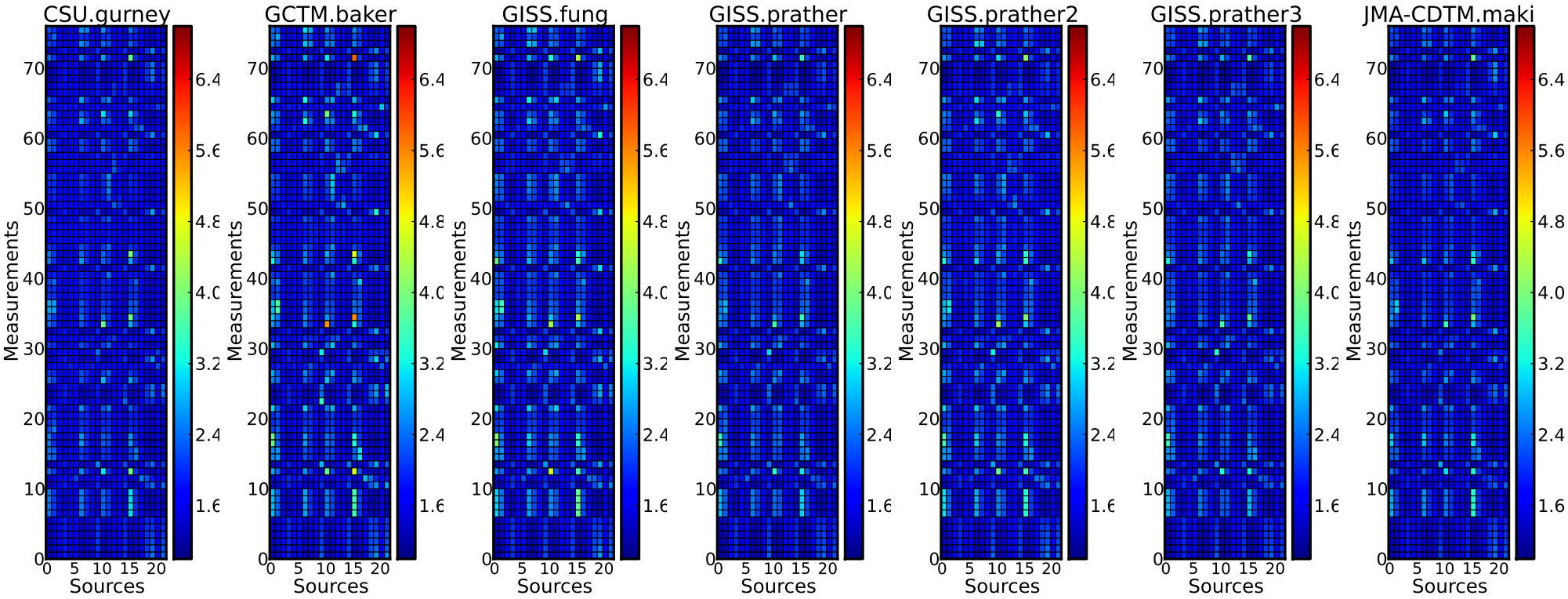
[Gurney *et al.*, Tellus B, 2003]

- Observations $\mathbf{d}$ at $N = 77$ sites around the world
- Inverse problem: find fluxes $\mathbf{s}$ at $M = 22$ locations
- Linearized 'response' model $\mathbf{R}$, such that $\mathbf{d} \approx \mathbf{Rs}$

$$\mathbf{d} = \mathbf{Rs} + \boldsymbol{\epsilon}_\mathbf{d}$$

- Model $\mathbf{R}$ is never perfect thus contaminating the inversion
- The inferred values of $\mathbf{s}$ compensate for model deficiencies
- $\boldsymbol{\epsilon}_\mathbf{d}$ is meant to capture data errors, but is 'entangled' with model errors

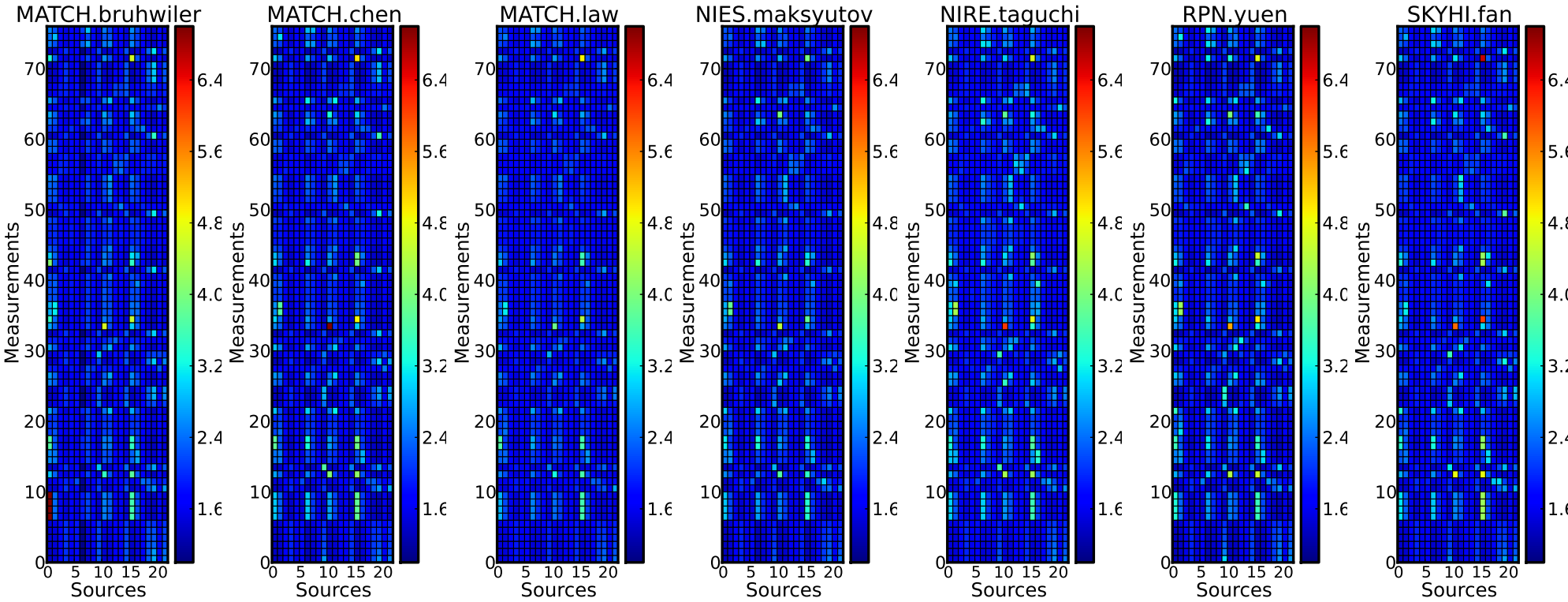
Consider 14 different response models $\mathbf{R}$



Infer fluxes $\mathbf{s}$, given measurements $\mathbf{d}$ to satisfy $\mathbf{d} \approx \mathbf{Rs}$

- Conventional additive Gaussian error (least-squares): $\mathbf{d} = \mathbf{Rs} + \xi$
- Embed probabilistic model for fluxes s: $\mathbf{d} = \mathbf{R}(\mu_{\mathbf{s}} + \mathbf{C}_{\mathbf{s}}\xi)$

Consider 14 different response models $\mathbf{R}$



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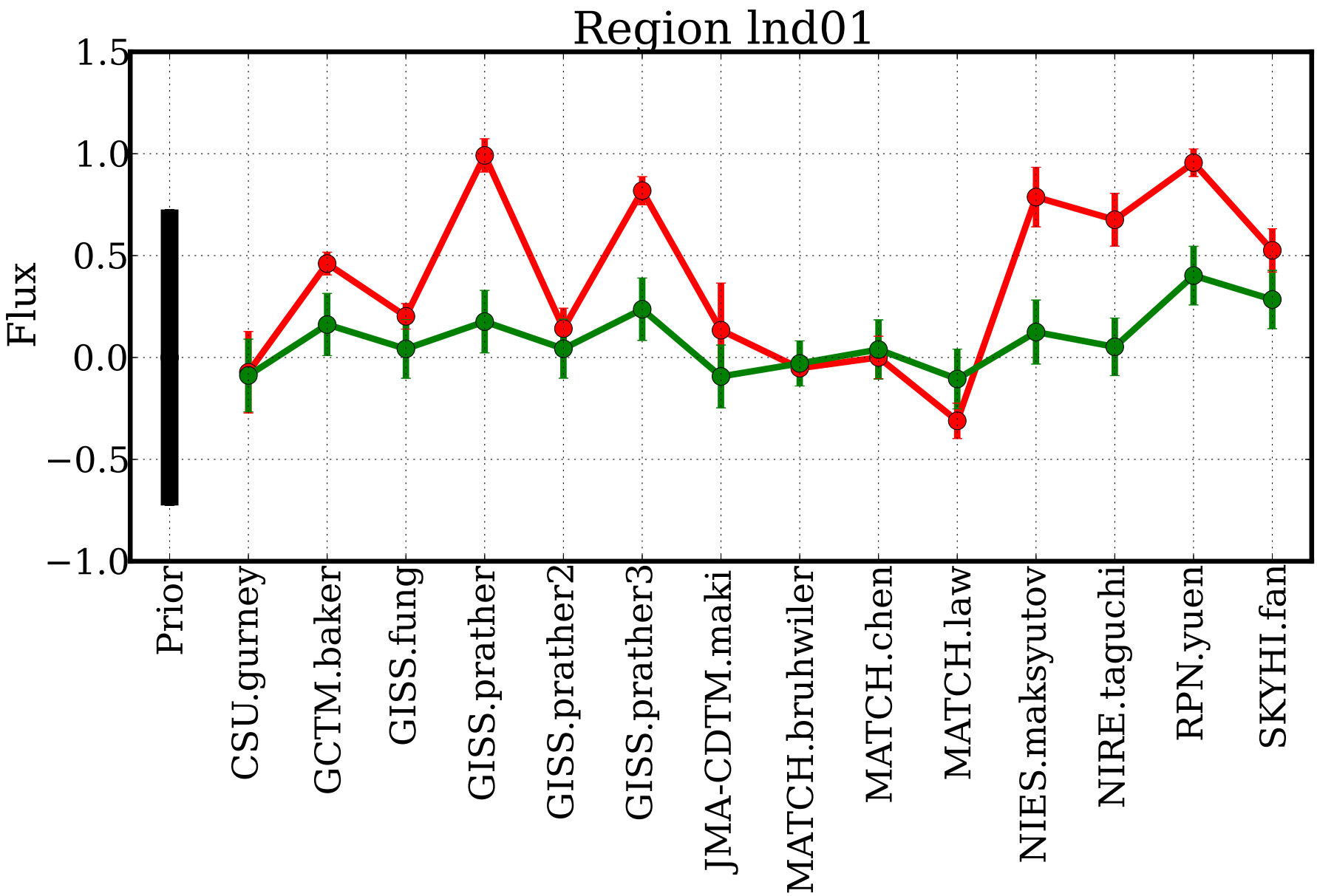
Inferred fluxes show less variability across models



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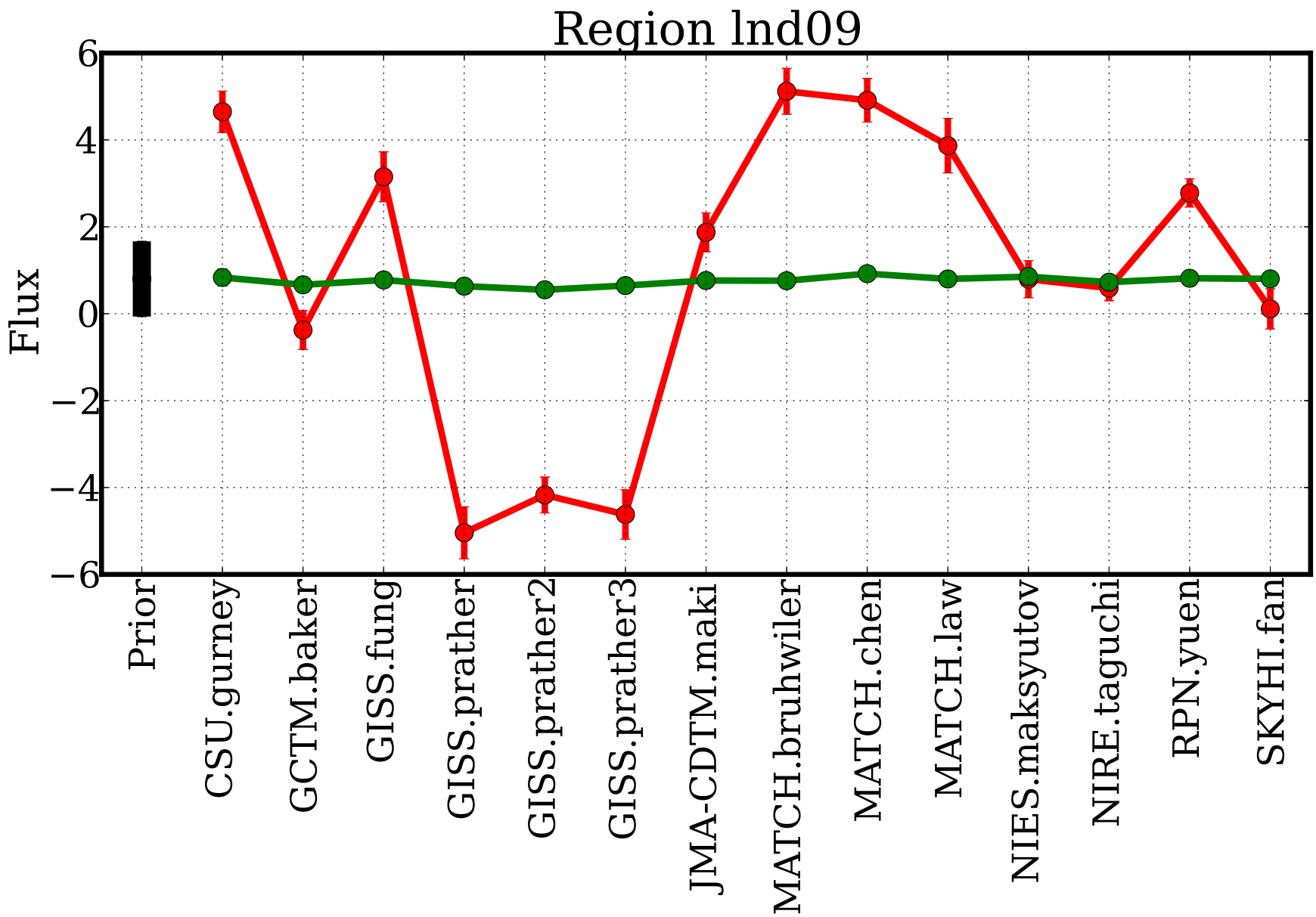

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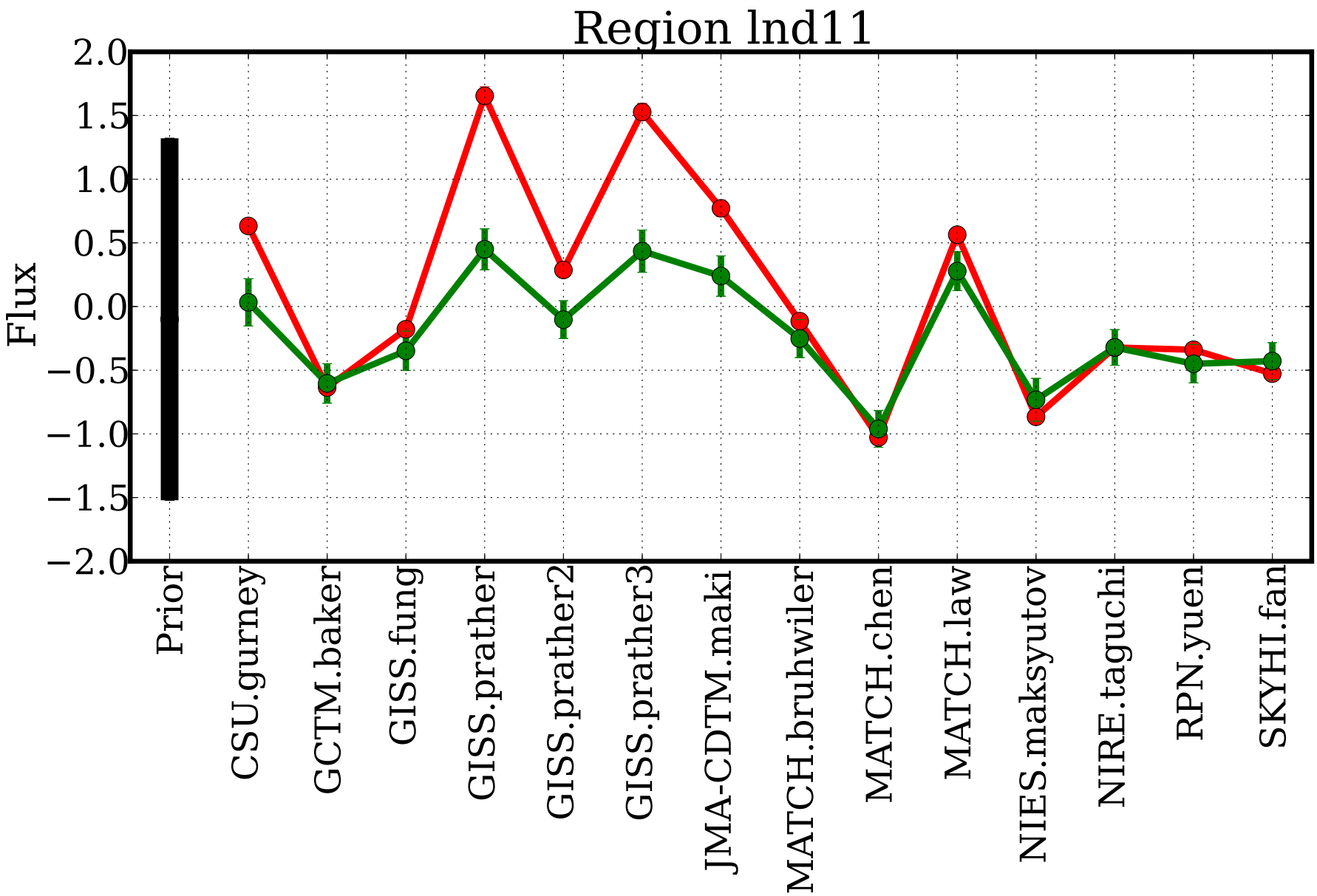
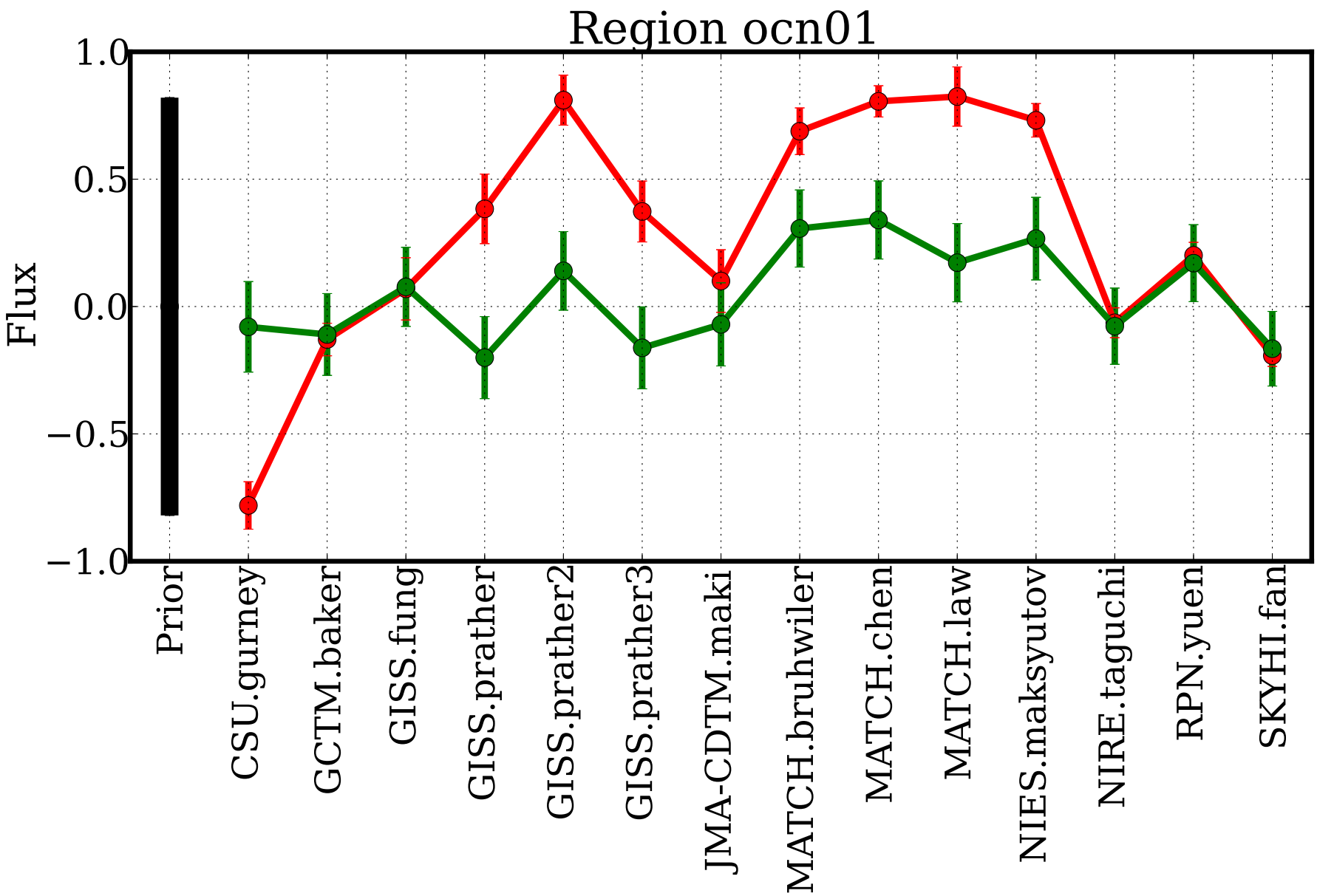
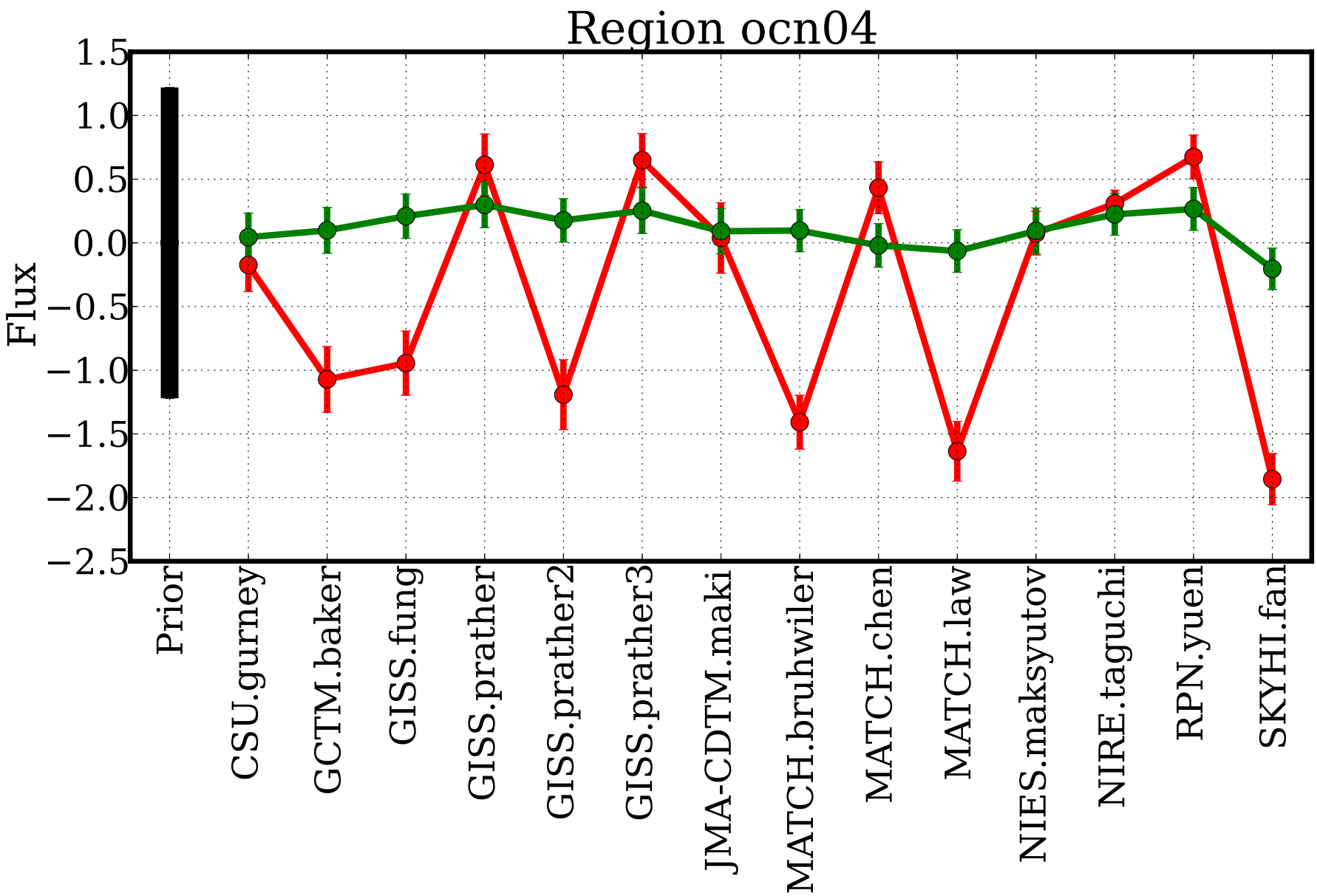


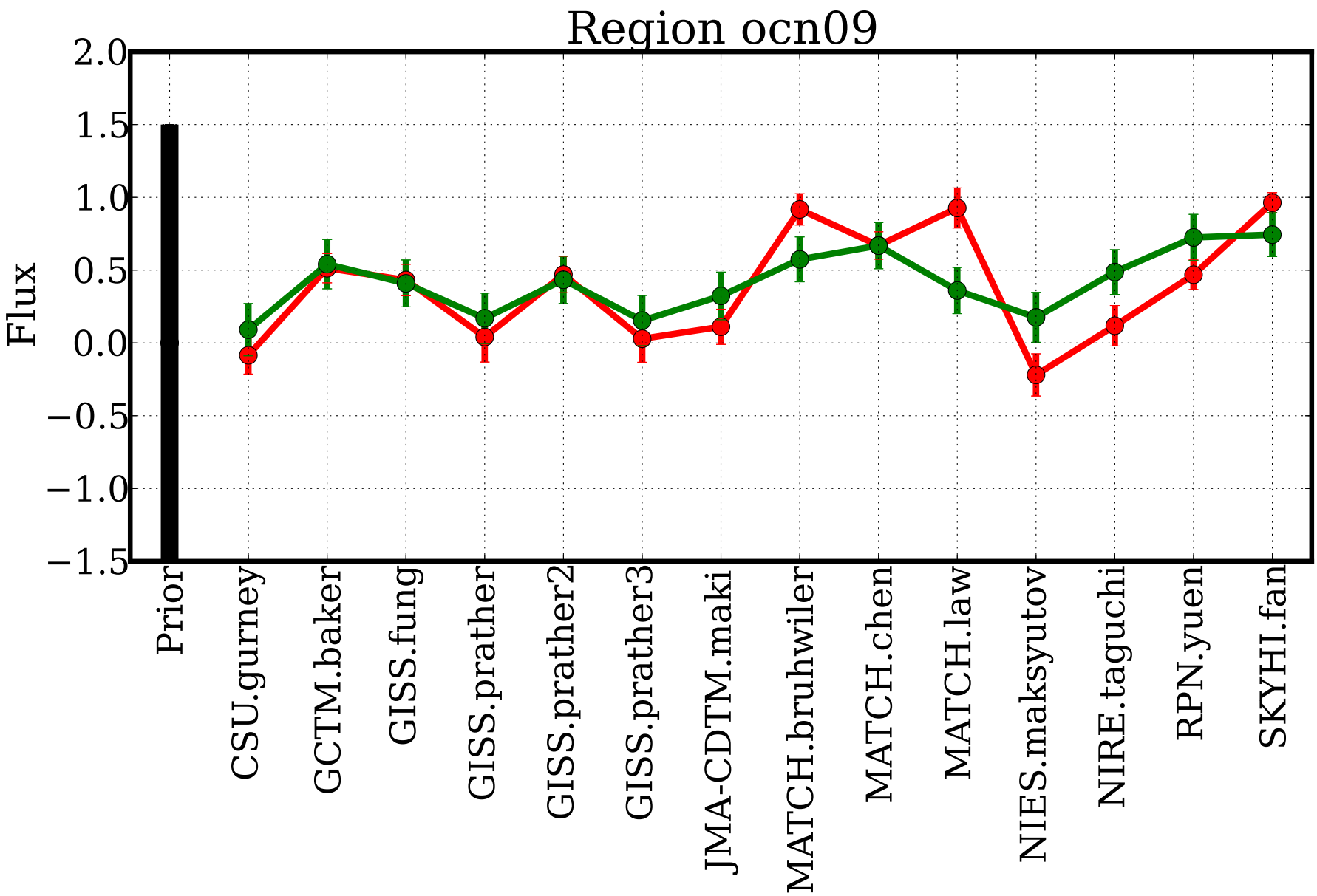
Inferred fluxes show less variability across models



Inferred fluxes show less variability across models



Inferred fluxes show less variability across models



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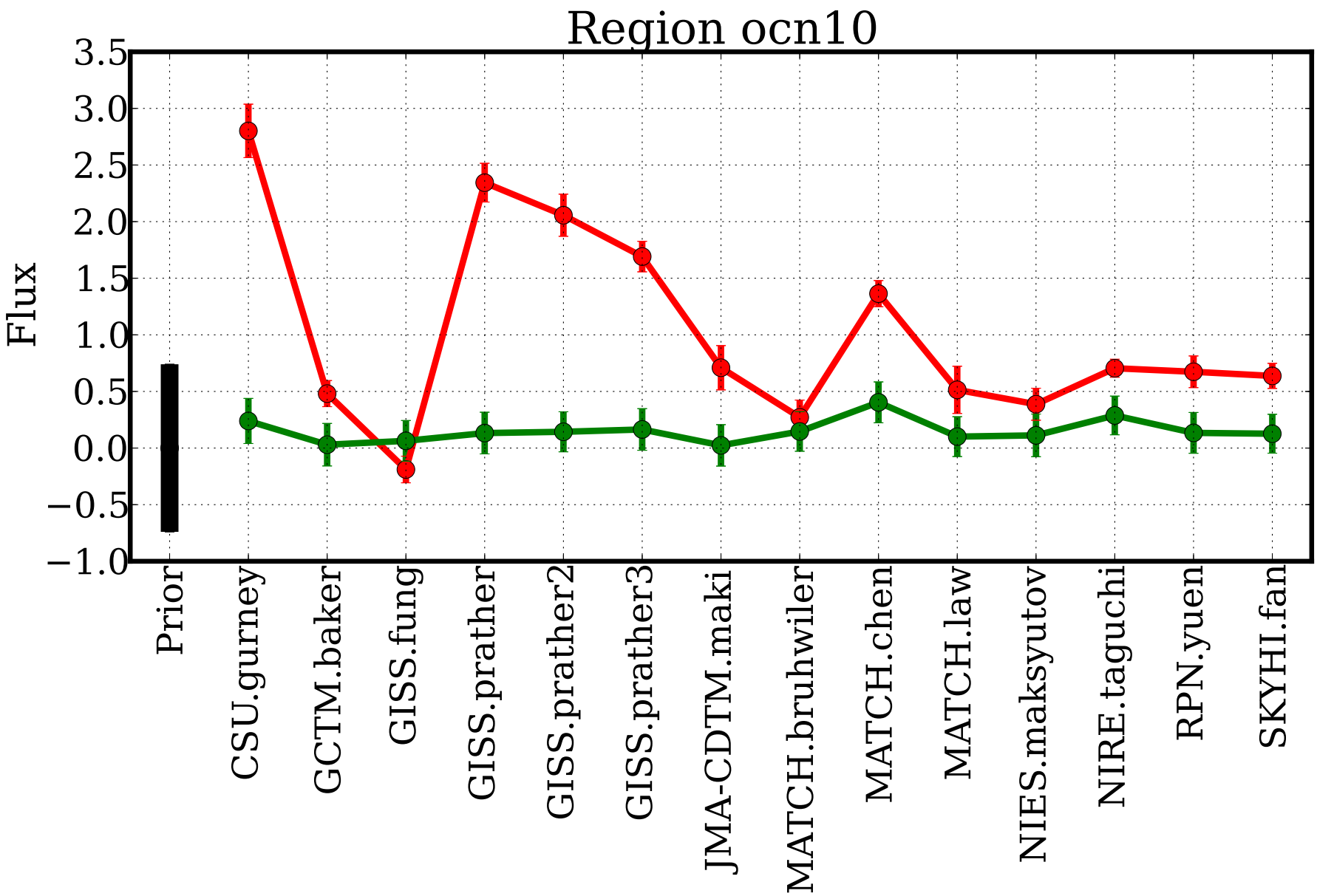
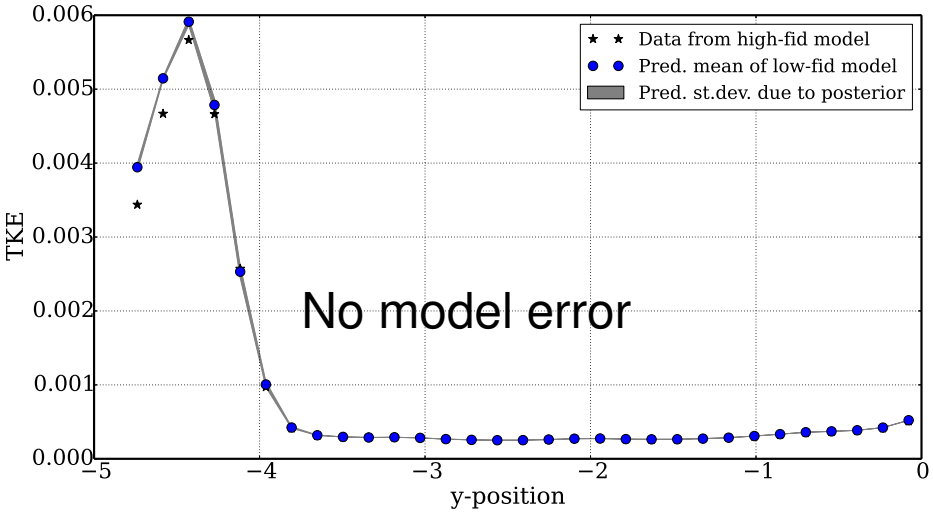


Preliminary results – embed model err in C_R

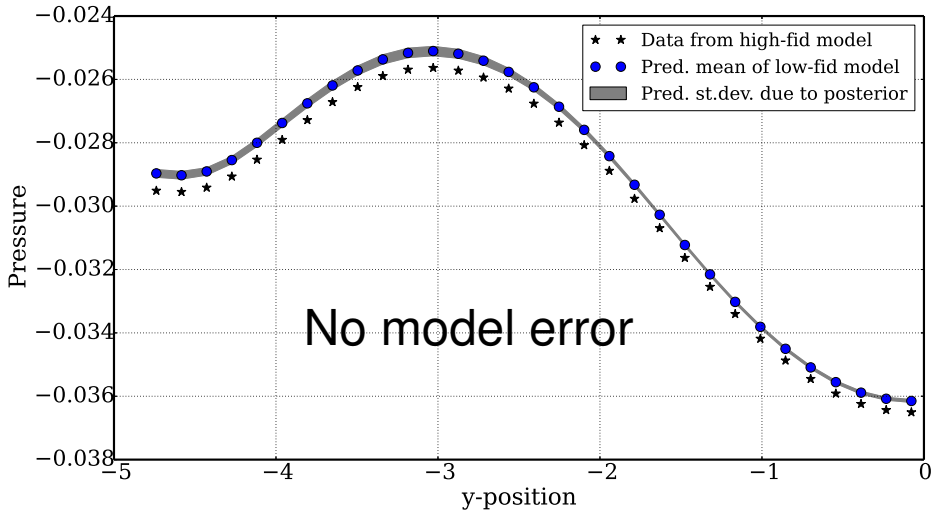
Calibrate with TKE data, predict both TKE and Pressure

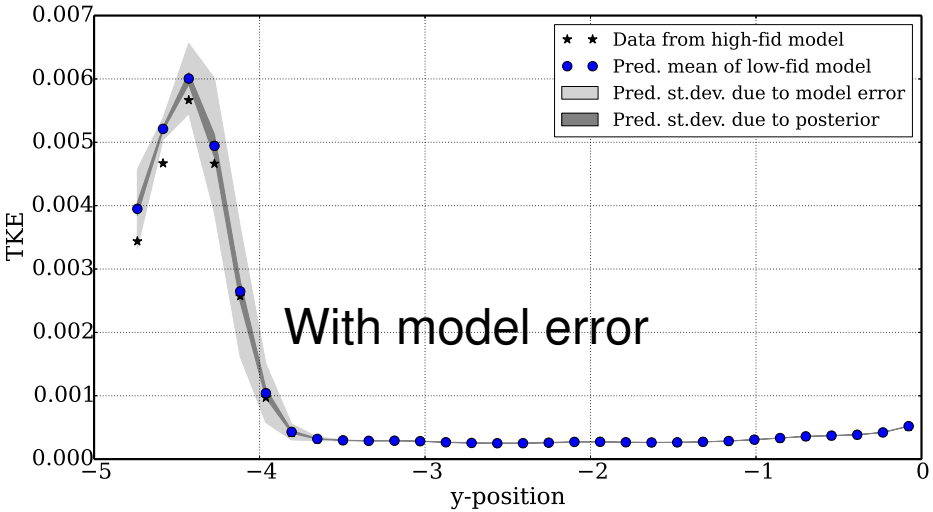
Pushed forward posterior

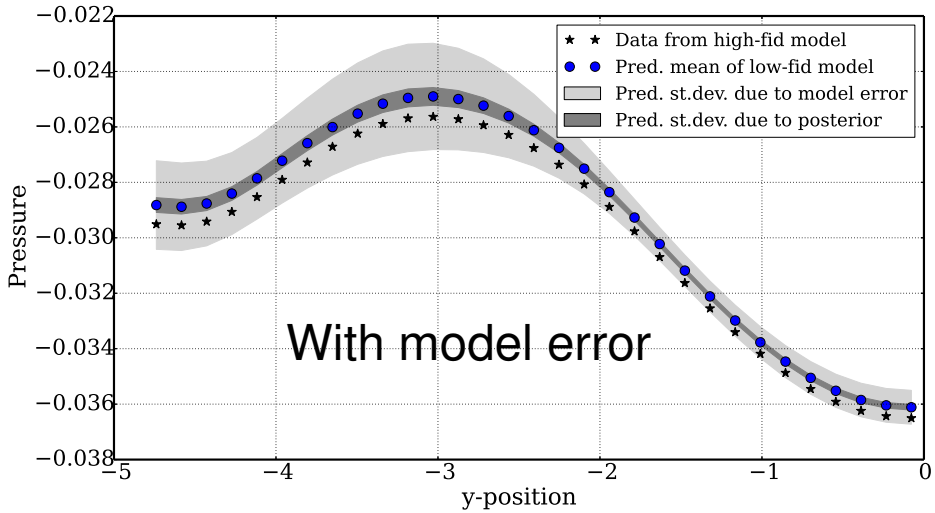
TKE



Pressure







Summary and Future

Thank You

- Represent, quantify and propagate physical model errors
- Parameter estimation $\Rightarrow$ density estimation
- Bayesian machinery to find parameters of the PDFs
- Approximate/empirical likelihoods impose constraints of interest
- Differentiates from data noise; allows model-to-model calibration
- Implemented in UQTk
- Applied in chemistry, climate modeling, LES computations
- K. Sargsyan, H. Najm, and R. Ghanem. "On the Statistical Calibration of Physical Models". *International Journal for Chemical Kinetics*, 47(4): 246-276, 2015.

- Optimal design for maximum information
- Bayesian problem still hard
- Hierarchical Bayesian formulation
- More intrusive embedding; problem specific

Additional Material

Likelihood construction – variants

- Full Likelihood

$$L(\alpha) = p(D|\alpha) = p(y_{\text{data},1}, \ldots, y_{\text{data},N}|\alpha)$$

- Marginalized Likelihood

$$L(\alpha) = p(D|\alpha) = \prod_{i=1}^{N} p(y_{\text{data},i}|\alpha)$$

- Approximate Bayesian Computation (ABC)
  – seek to satisfy the constraints:
  - $p(y|D)$ is "centered" on the data
  - The width of the distribution $p(y|D)$ is "consistent" with the spread of the data around the nominal model prediction

Full Likelihood

$$L(\alpha) = p(D|\alpha) = \pi_f(y_{\text{data},1}, \ldots, y_{\text{data},N}|\alpha)$$

where:
$\pi_f(\cdot, \alpha)$: N-variate density of the random variable $(f_1, \ldots, f_N)$
with $f_i = f(x_i, \lambda(\alpha))$

Problem: $\pi_f(\cdot)$ is degenerate in general when $N > M$

Consider a case with $M = 1$, $\lambda \sim N(\mu, \sigma^2)$, and $f = \lambda x$
Let $N = 2$, hence $(f_1, f_2) = (\lambda x_1, \lambda x_2)$ for any λ sample
With $f_1/x_1 = f_2/x_2 = \lambda$, (f_1, f_2) are dependent and
$\pi_f(\cdot|\mu, \sigma)$ is non-zero only along the line $f_2 = (x_2/x_1)f_1$

hence $\pi_f(y_{\text{data},1}, y_{\text{data},2}|\mu, \sigma)$ is non-zero only along the line
$y_{\text{data},2}/x_2 = y_{\text{data},1}/x_1$

Marginalized Likelihood

$$L(\alpha) = p(D|\alpha) = \prod_{i=1}^{N} \pi_{f_i}(y_{\text{data},i}|\alpha)$$

where $\pi_{f_i}(\cdot, \alpha)$ is the univariate density of the RV $f_i = f(x_i, \lambda(\alpha))$

Problem: the likelihood has multiple singularities corresponding to α values leading to vanishing marginal variances at each x_i

Gaussian example: Let $f_i \sim \mathrm{N}(\mu_i(\alpha), \sigma_i(\alpha)^2)$, then

$$L(\alpha) = \frac{1}{(2\pi)^{N/2}} \prod_{i=1}^{N} \frac{1}{\sigma_i(\alpha)} \exp\left(\frac{(\mu_i(\alpha) - y_{\text{data},i})^2}{2\sigma_i(\alpha)^2} \right)$$

Multiple singularities, $\sigma_i(\alpha) = 0$, $i = 1, \ldots, N$

Posterior maximization always finds one of these singularities, fitting one point perfectly, while misfitting the rest ($\Rightarrow$ priors)

Approximate Bayesian Computation (ABC)

Employ a kernel density as a pseudo-likelihood to enforce select constraints:

- Uncertain prediction $p(y|D)$ is centered on the data
  - With $\mu_i(\alpha) = \mathrm{E}_\xi[f(x_i, \lambda(\xi;\alpha))]$: minimize $\|\mu_i(\alpha) - y_{\mathrm{data},i}\|_2^2$
- The width of the distribution $p(y|D)$ is consistent with the spread of the data around the nominal model prediction
  - With $\sigma_i(\alpha)^2 = \mathrm{V}_\xi[f(x_i, \lambda(\xi,\alpha))]$:
    minimize $\|(\sigma_i(\alpha) - \gamma|\mu_i(\alpha) - y_{\mathrm{data},i}|)\|_2^2$
  - γ is a factor that specifies the desired match between σ_i and the discrepancy $|\mu_i(\alpha) - y_{\mathrm{data},i}|$, on average

ABC Likelihood

With $\rho(\mathcal{S})$ being a metric of the statistic $\mathcal{S}$, use the kernel function as an ABC likelihood:

$$L_{\mathrm{ABC}}(\alpha) = \frac{1}{\epsilon} K\left(\frac{\rho(\mathcal{S})}{\epsilon}\right)$$

where ϵ controls the severity of the consistency control

Propose the Gaussian kernel density:

$$L_{\epsilon}(\alpha) = \frac{1}{\epsilon\sqrt{2\pi}} \prod_{i=1}^{N} \exp\left(-\frac{(\mu_i(\alpha) - y_{\mathrm{d},i})^2 + (\sigma_i(\alpha) - \gamma|\mu_i(\alpha) - y_{\mathrm{d},i}|)^2}{2\epsilon^2}\right)$$