Model Error Representation via Density Estimation

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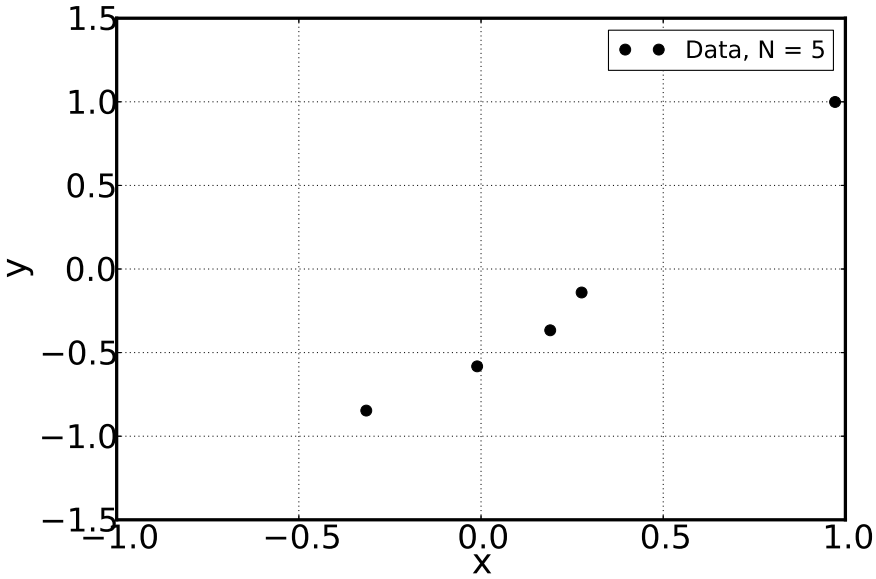
Main target

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

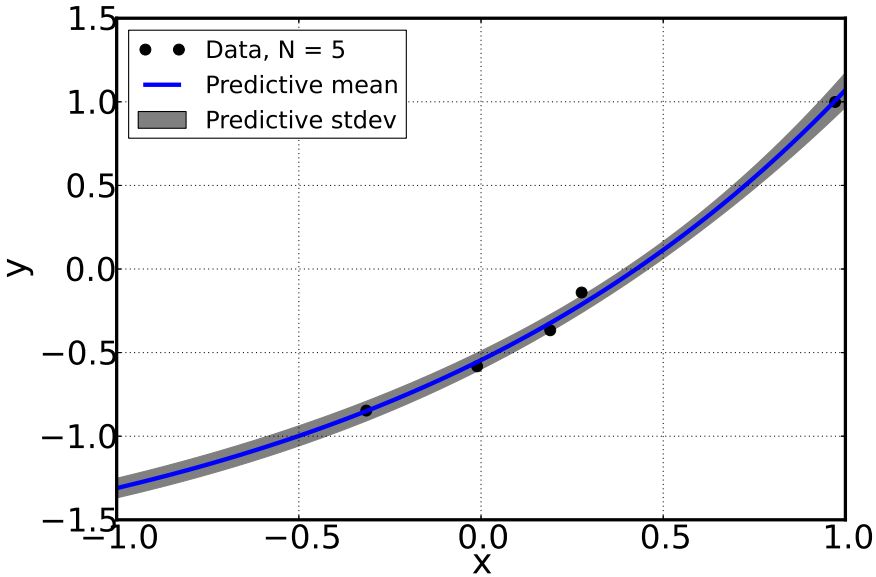
- Represent and estimate the error associated with
  - Simplifying assumptions, parameterizations
  - Mathematical formulation, theoretical framework
  - Numerical discretization
    (connection to Mesh Discretization Error Task)
- ...will be useful for
  - Model validation
  - Model comparison
  - Scientific 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

Motivation



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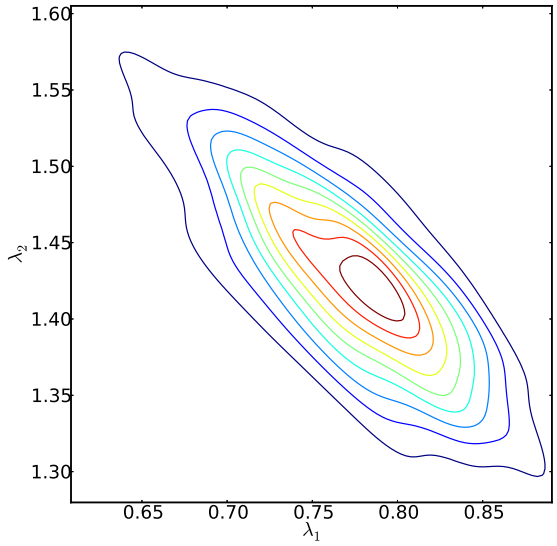
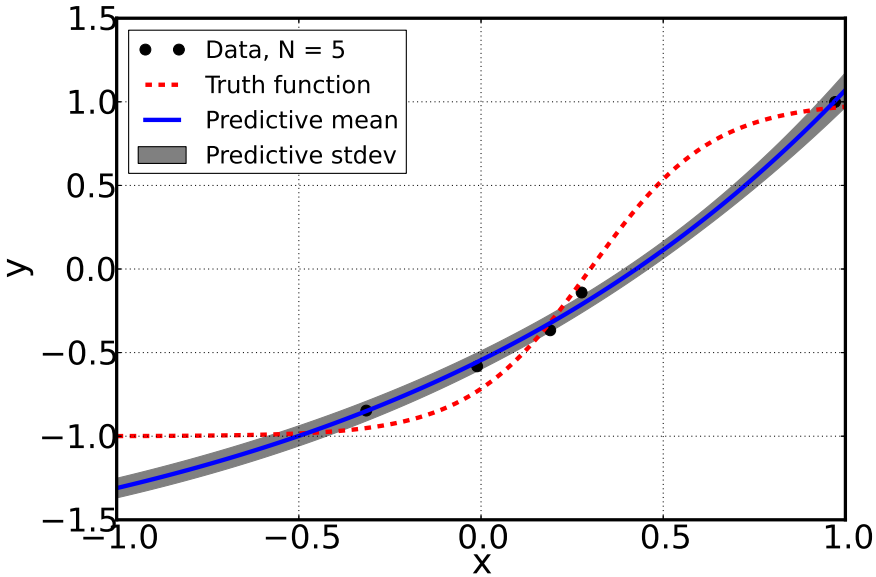


Calibrated parameters

Motivation



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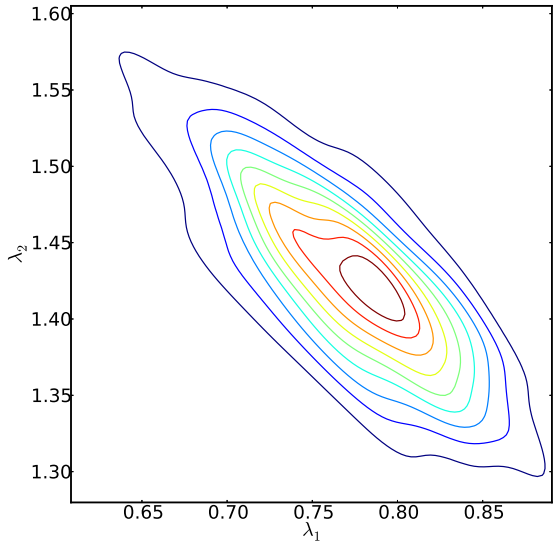

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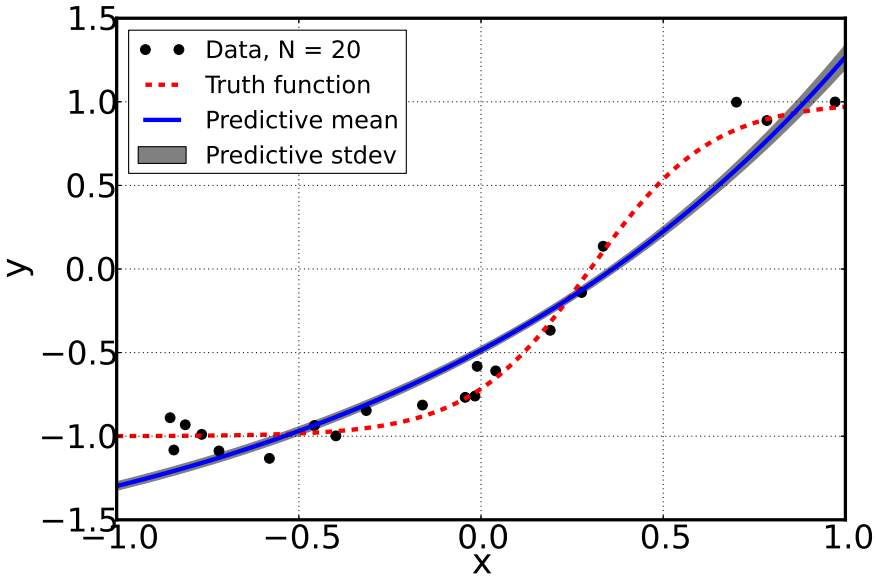

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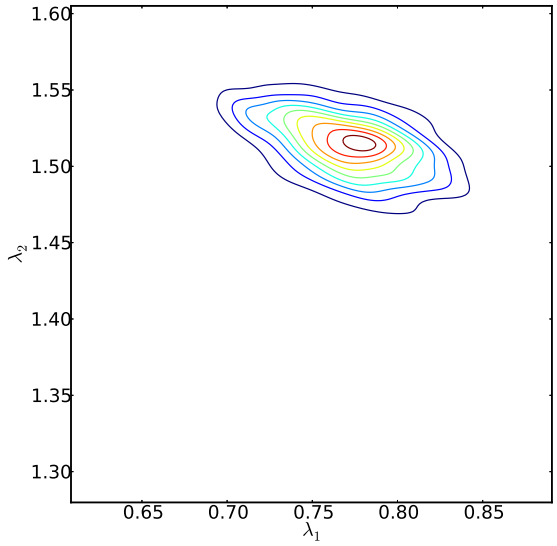

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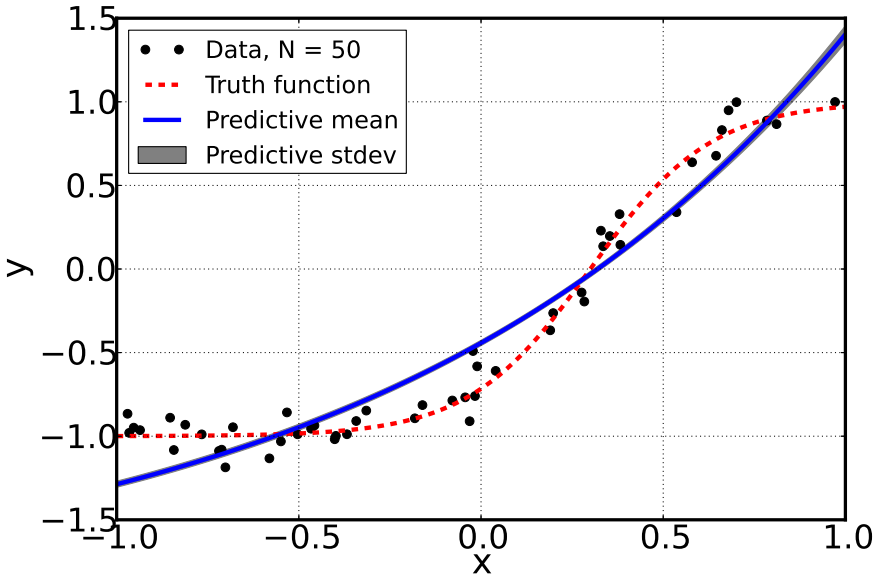
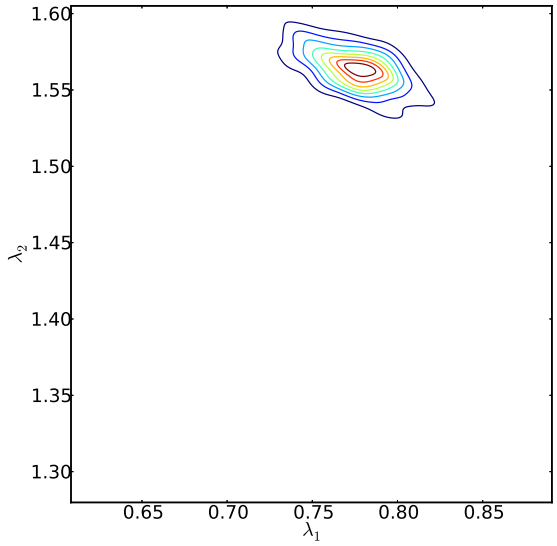


Model-data fit



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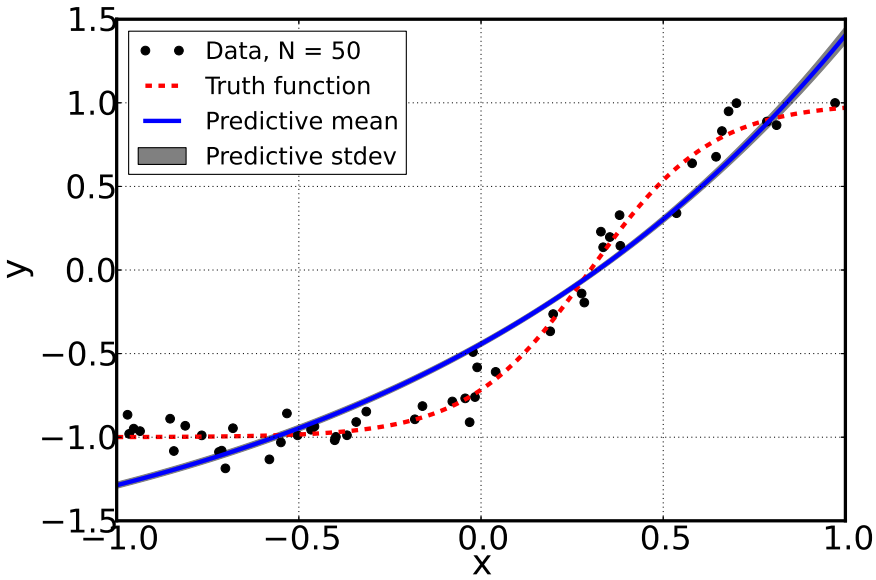
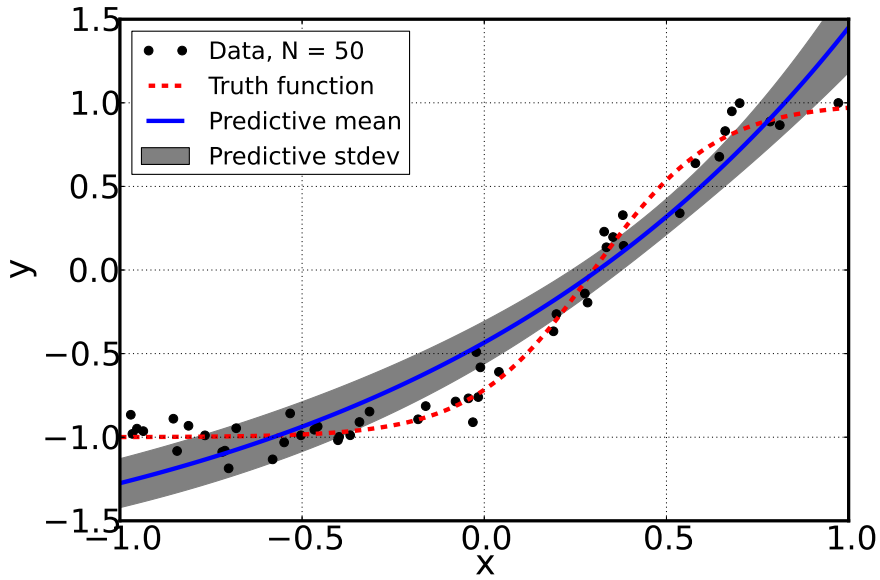


Model-data fit



What we want

- If the model is structurally deficient, more data does not help!
- We target model-vs-truth discrepancy

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

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

Statistical modeling of errors in calibrating $f(x;\lambda)$

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

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

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

State-of-the-art: 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 $\quad y_{mod}(x) = f(x;\lambda) + \delta(x)$
- Potential violation of physical constraints
  - *e.g.* incompressible flow: $\nabla \bullet v = 0$
- 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 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

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

- 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

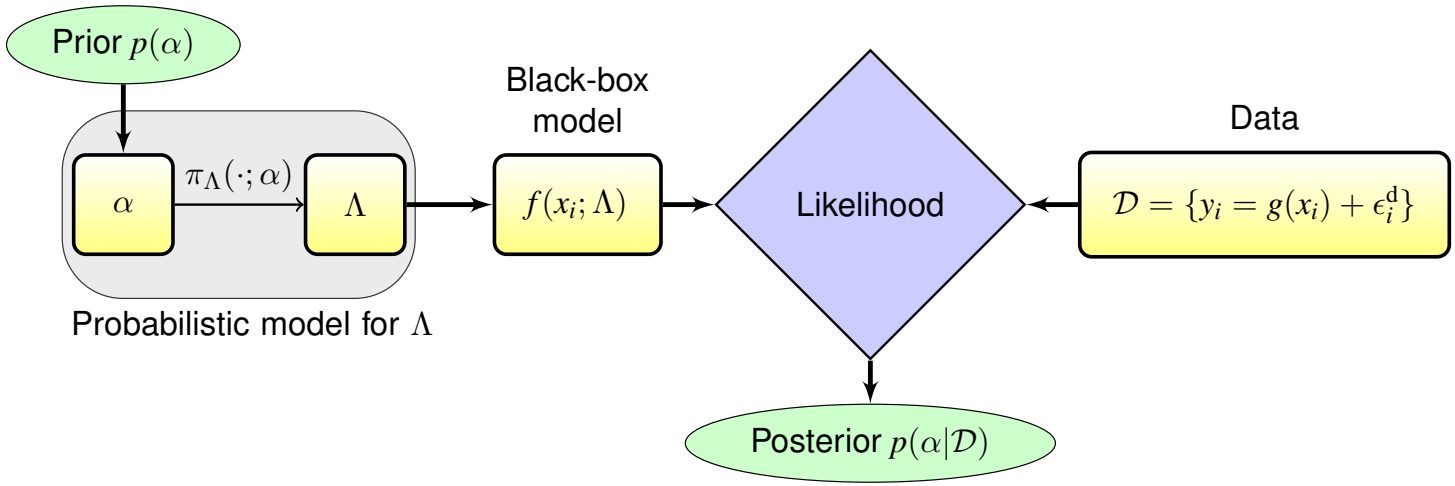
Model error embedding: Bayesian formulation

- In the simplest setting, cast λ as a random variable Λ

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

- Calibration turns into density estimation for the PDF of Λ
- Polynomial Chaos parameterization for $\Lambda = \sum_{k=0}^{K} \alpha_k \Psi_k(\xi)$
- Back to parameter estimation, now for $\alpha = (\alpha_0, \ldots, \alpha_K)$

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



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.

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 noise $\epsilon_i^{\mathrm{d}} = \sigma_{\mathcal{D}} \xi_{d+i}$; Full PC germ $\hat{\xi} = (\underbrace{\xi_1, \ldots, \xi_d}_{\text{Model error}}, \underbrace{\xi_{d+1}, \ldots, \xi_{d+N}}_{\text{Data noise}})$
- Infer $\hat{\alpha} = (\alpha, \sigma_{\mathcal{D}})$
- Data generation model; to aid likelihood $p(\mathcal{D}|\hat{\alpha})$ construction

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

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 $\Sigma(\hat{\alpha})$

Likelihood options

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- Full Likelihood: $L(\hat{\alpha}) = p(\mathcal{D}|\hat{\alpha}) = p(y_1,\ldots,y_N|\hat{\alpha}) = \pi_{\boldsymbol{h}}(\boldsymbol{y})$
  - 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

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

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

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

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 $\Sigma(\hat{\alpha})$

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

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

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:

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

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*:

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

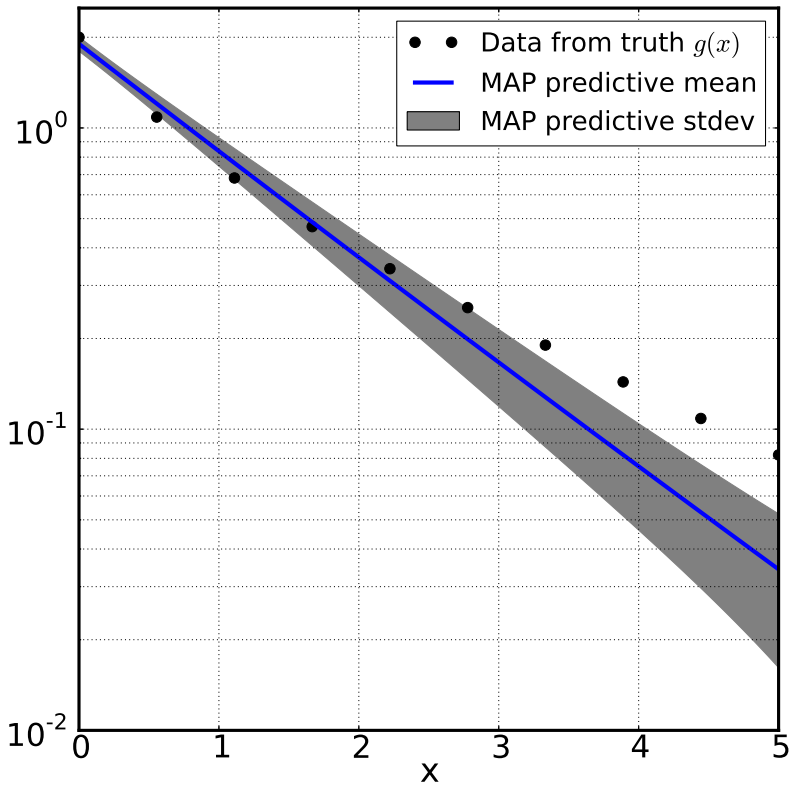
Posterior predictive variance:

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

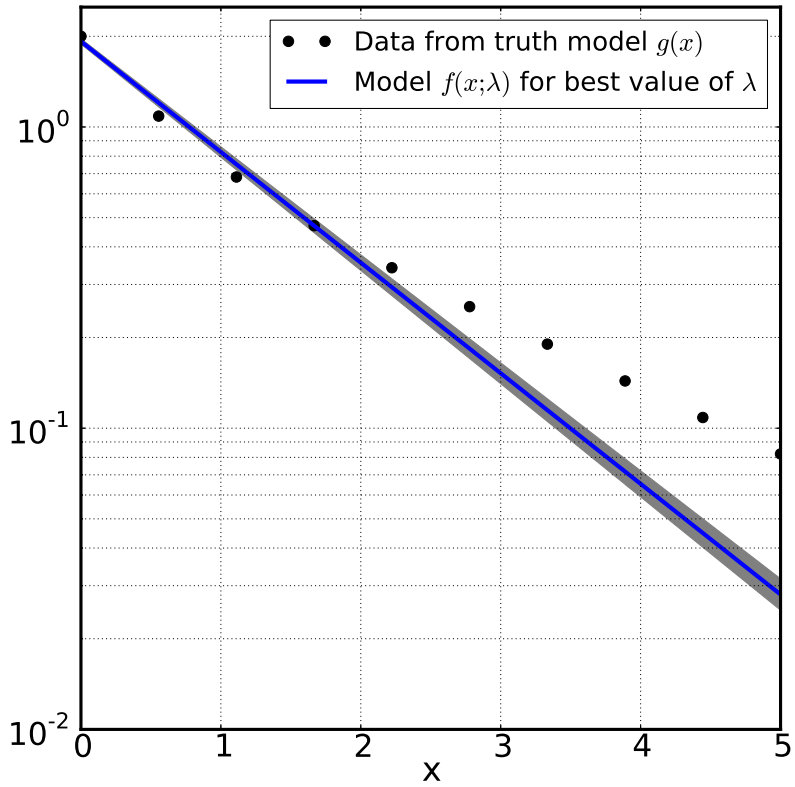
Predictions account for model error

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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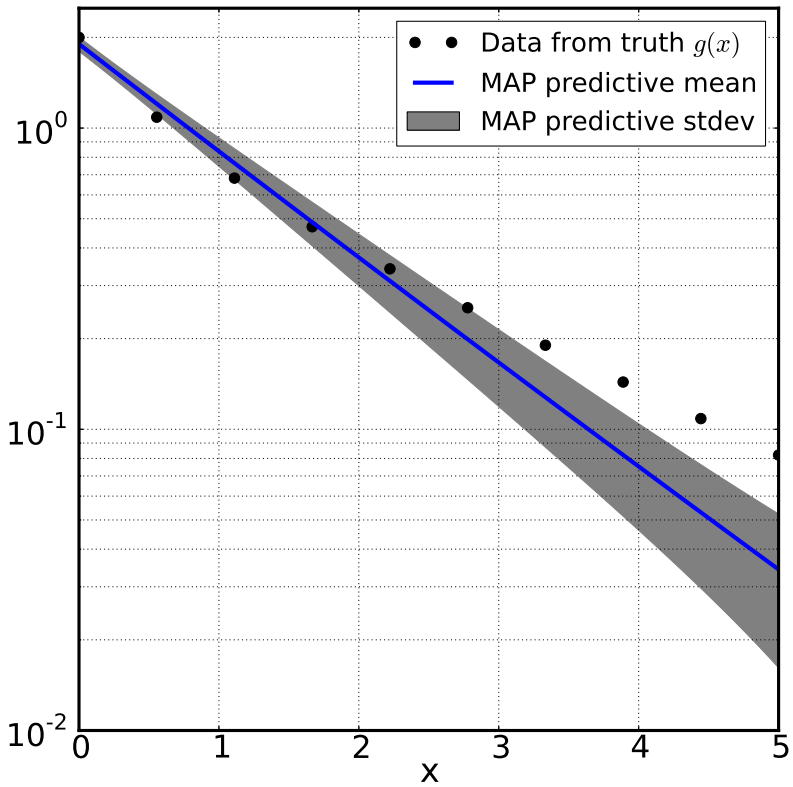
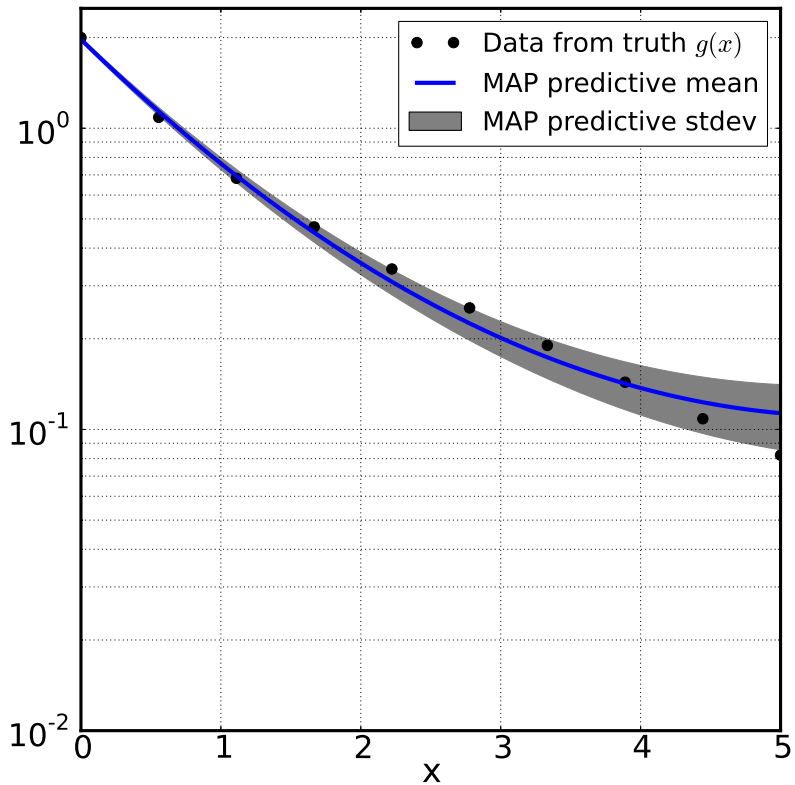
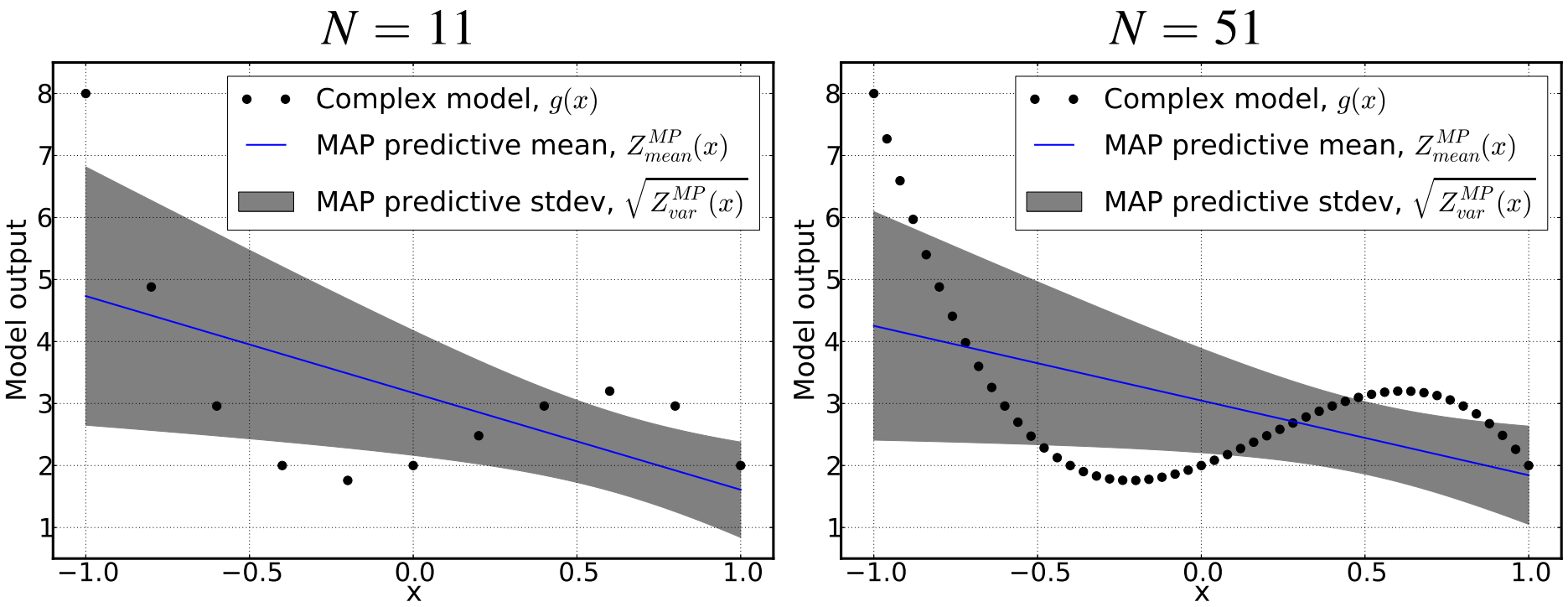


Quadratic-exponential $f_2(x, \lambda) = e^{\lambda_1 + \lambda_2 x + \lambda_3 x^2}$

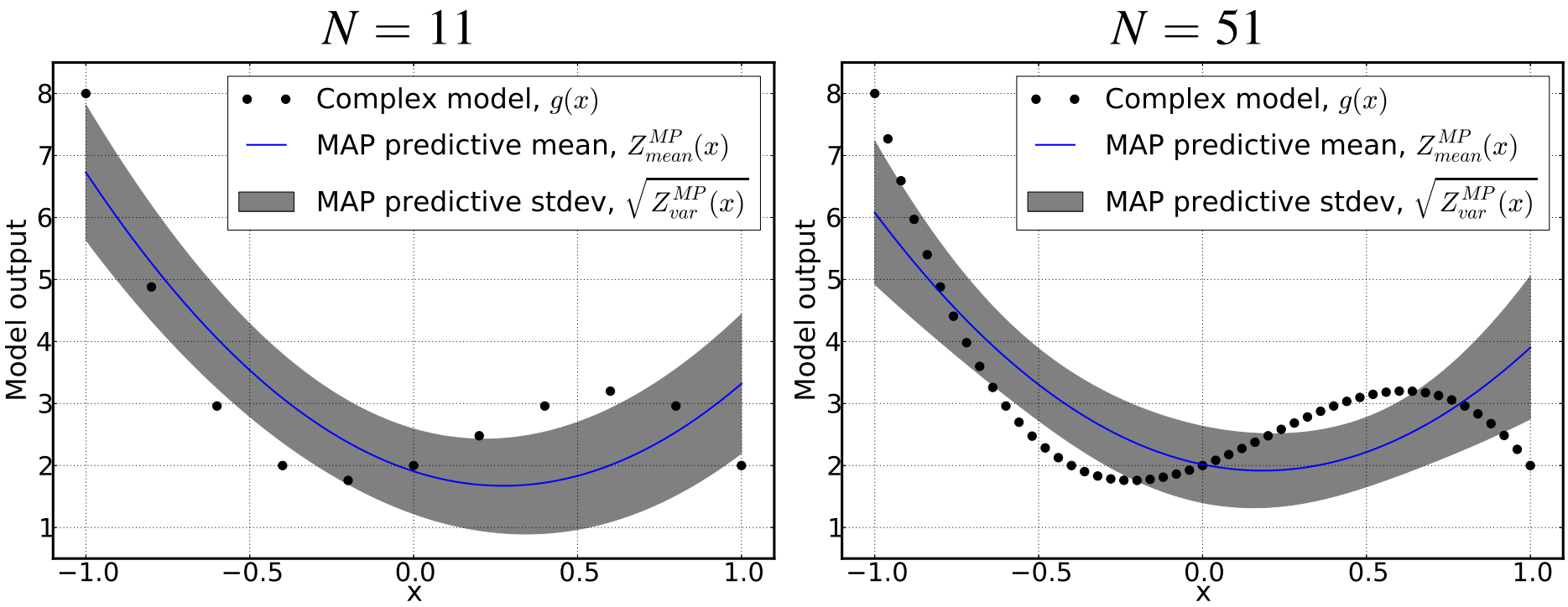


Test problem – Cubic data fit by a line – ABC



- 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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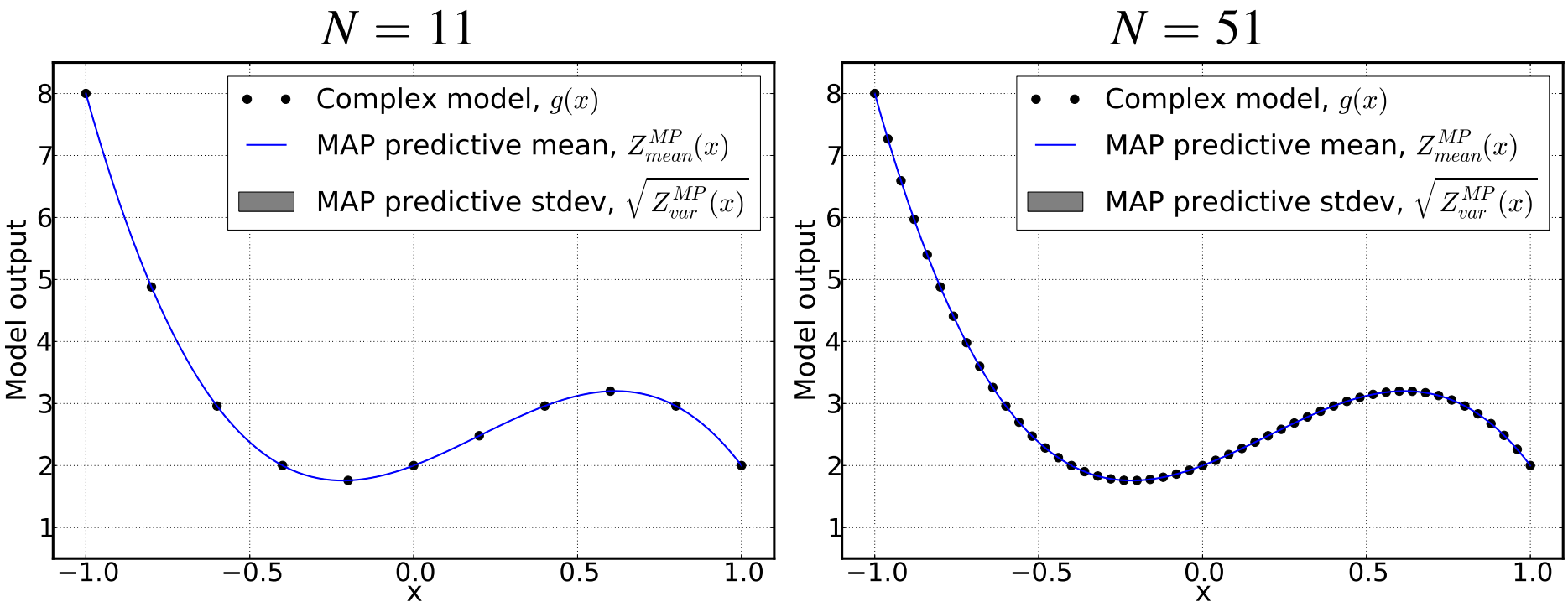
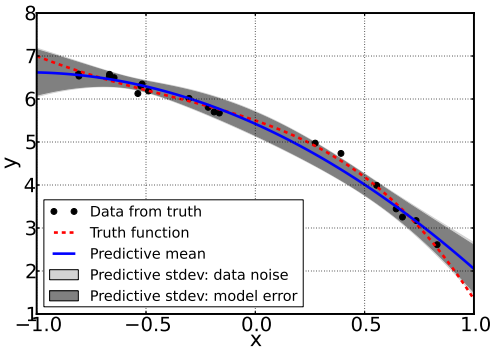


- MAP predictive mean centered on data
- MAP predictive standard deviation captures range of discrepancy
- Increasing number of data points has a small effect on both predictive mean and stdev.

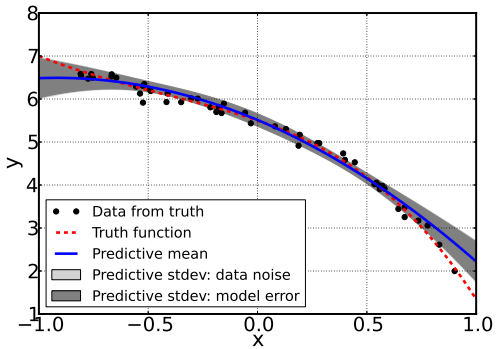
More data leads to 'leftover' model error

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 $\sigma = 0.1$.

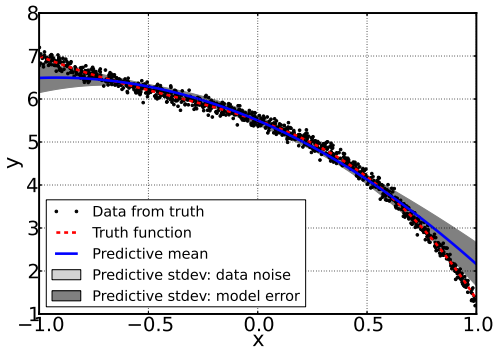
$N = 20$



$N = 50$

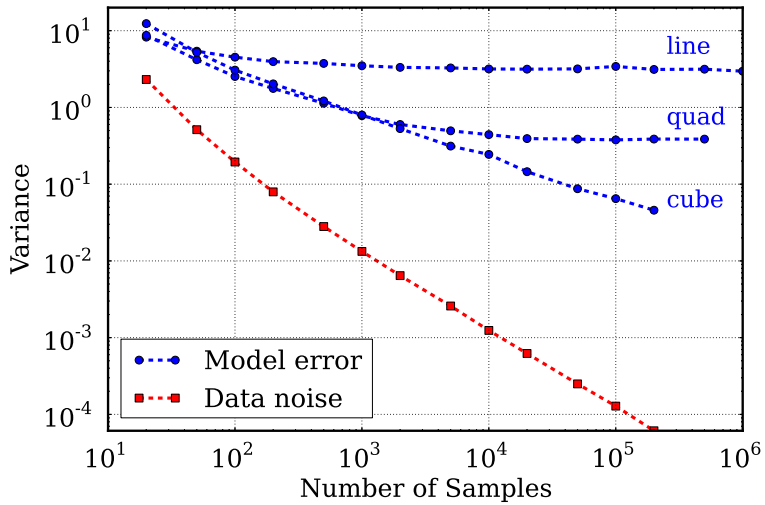


$N = 1000$



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



ScramjetUQ plan

- FY16
  [M5.1: Demo ME estimation and propagation for P1]
  - Identify a set of low fidelity models [Oct-Jan]
  - Embed ME in a few parameters at a time [Jan-Mar]
  - Calibrate with estimation of model error terms [Apr-Jun]
  - Propagate ME for observable and other QoIs [Jul-Sep]

- FY17-18
  - Automate and explore calibration over range of conditions of high-fidelity model
  - Attribute predictive model error to different parameters
  - Scale up to P2
  - Include experimental data

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, including LIS

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

  $\Rightarrow$ More informative priors/regularization

Current status: low-fi versus high-fi calibration

- Task: Low fidelity model calibration with respect to data from high-fidelity model
- Data: the nominal run from forward UQ study (quadrature point at the origin)
- QoI: 1D profiles/slices of temperature and/or pressure; potentially parameterized if common shapes emerge
- Simplified (low-fi) model to be calibrated: constant (in time and space) assumptions for Smagorinsky constant C_R and turbulent Prandtl number Pr_t.

$$f(x;\lambda) \approx g(x), \text{ where } \lambda = (C_R, Pr_t)$$

As a first step, pre-build a surrogate for $f(x;\lambda)$. That means a set of (~ 20) runs at predefined values of $\lambda = (C_R, Pr_t)$.

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- Simplified (low-fi) model to be calibrated: constant (in time and space) assumptions for Smagorinsky constant C_R and turbulent Prandtl number Pr_t.

$$f(x;\lambda) \approx g(x), \text{ where } \lambda = (C_R, Pr_t)$$

As a first step, pre-build a surrogate for $f(x;\lambda)$. That means a set of (~ 20) runs at predefined values of $\lambda = (C_R, Pr_t)$.

Main demo: Run $f(x;\lambda)$ on-the-fly, during calibration. Hands-on P1.

Code status

`UQTk`: lightweight UQ library, mostly C++ with Python interface (www.sandia.gov/uqtoolkit)

- `pce` : PC utilities, both intrusive and non-intrusive
- `quad` : Quadrature generation, including sparse
- `mcmc` : MCMC sampling, single-site and adaptive

- `infer` : Inference with density estimation; multivariate P.C. R.V., includes

```
infer_model(*Func, likelihoodType, ...)
```

- `model_inf` : Command line MCMC sampler, employs a few standard forward functions, e.g. a polynomial surrogate.

Ideally, a black-box C/C++ function `Func(...)` needs to be implemented using LES code-base to replicate $f(x;\lambda)$.

Connections to other tasks

- Major dependence on LES code/availability

  Conceptual connections: support and take advantage of

- GSA/Forward UQ:
  - pick the nominal run as a high-fidelity data
  - model error attribution similar in flavor to Sobol/GSA

- Multifidelity:
  - stochastic representation of model discrepancy from surrogate
  - compare with embedded model error representation

- Mesh discretization error:
  - low-fi (coarse mesh) versus high-fi (dense mesh)
  - represent error induced by resolution coarsening

Summary

What we have done

- The methodology is tested and fine tuned
- Identified ‘model simplification’ axis for the first set of demos
- Code base is ready to be unleashed
- Xun up to speed (and more!) with the method

What will we do next

- Carefully select conditions and output quantities of interest for calibration
- Build surrogates for static constant treatment cases for demo
- Get hands on a working case and implement model error calibration directly
- Keep talking to MDE, Multifi and Forward UQ.

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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 $\sigma_i^2(\alpha) = \mathrm{V}_\xi[f(x_i, \lambda(\xi,\alpha))]$:

    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:

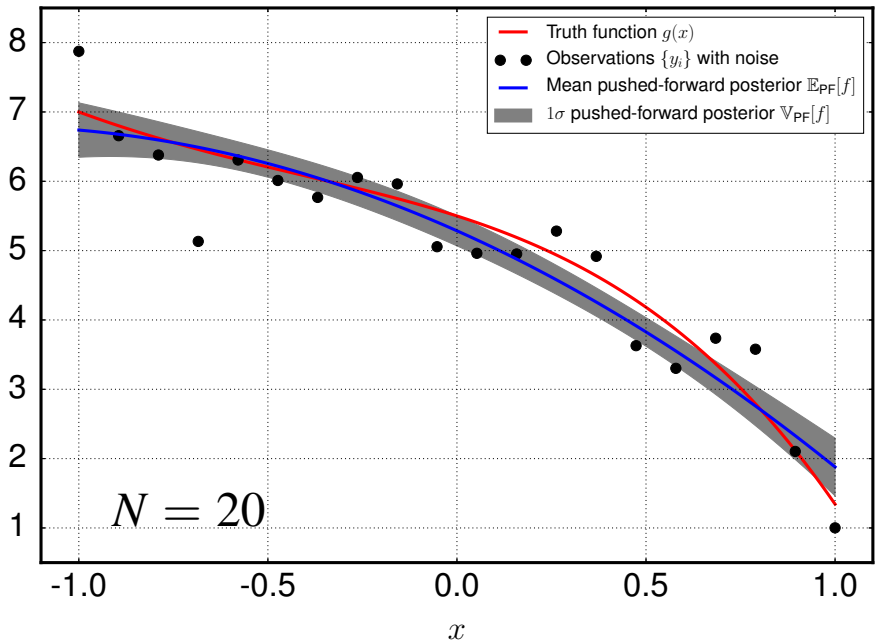
$$L_{\mathrm{ABC}}(\alpha) = \frac{1}{\epsilon} K\left(\frac{\rho(\mathcal{S})}{\epsilon}\right)$$

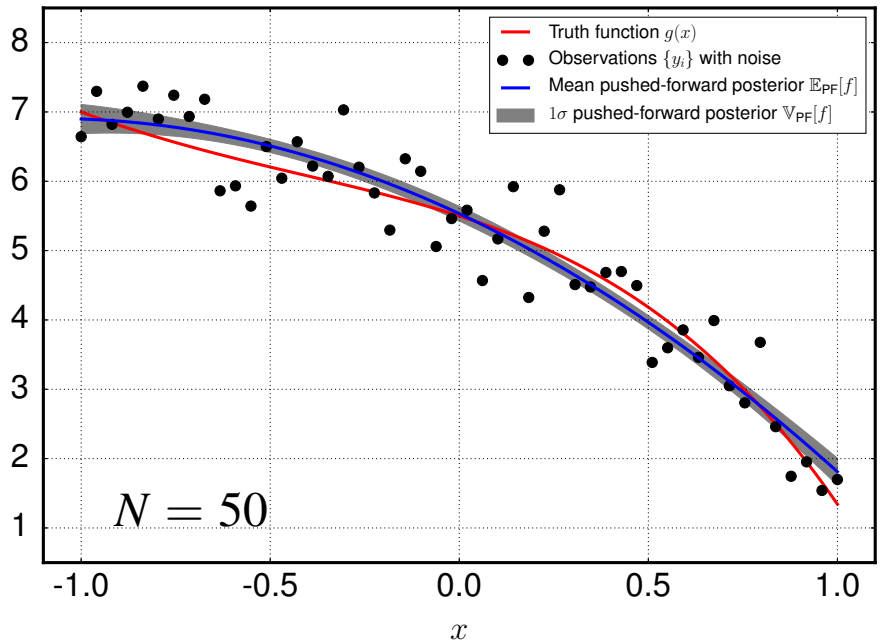
where ϵ controls the severity of the consistency control

Propose the Gaussian kernel density:

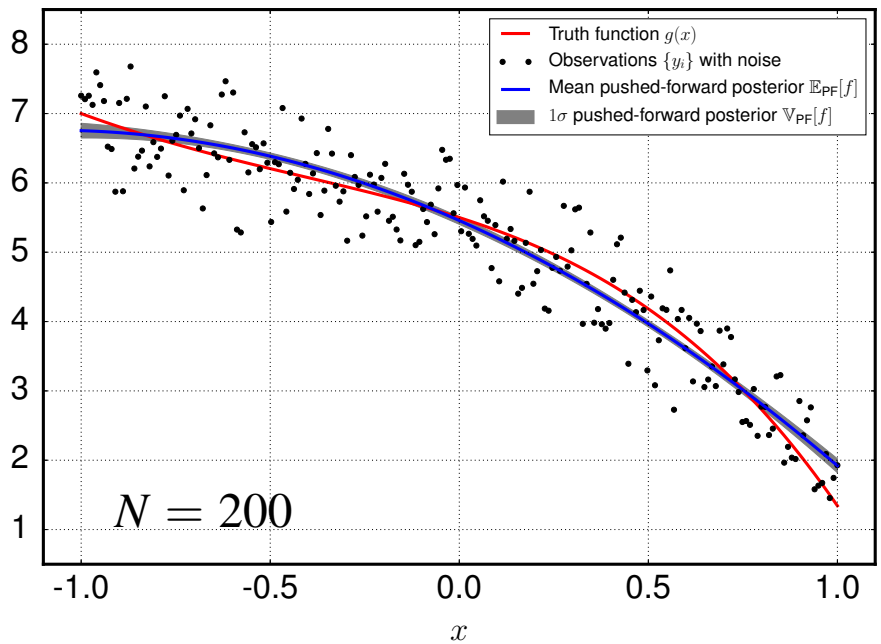
$$L_{\epsilon}(\alpha) = \frac{1}{\epsilon\sqrt{2\pi}} \prod_{i=1}^{N} \exp\left(-\frac{(\mu_i(\alpha) - y_{\mathrm{d},i})^2 + (\sigma_i(\alpha) - \gamma|\mu_i(\alpha) - y_{\mathrm{d},i}|)^2}{2\epsilon^2}\right)$$

Quadratic-fit – Classical Bayesian likelihood

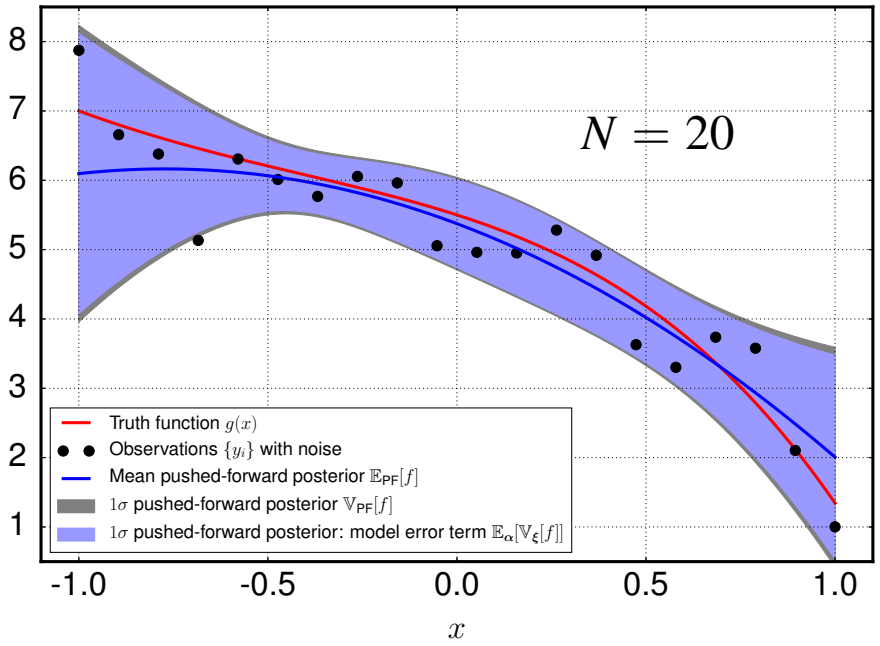


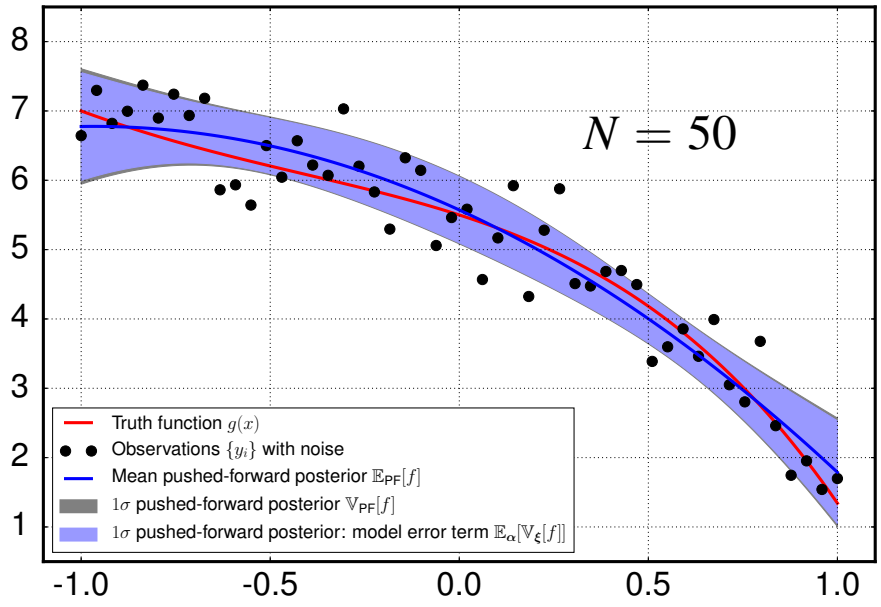


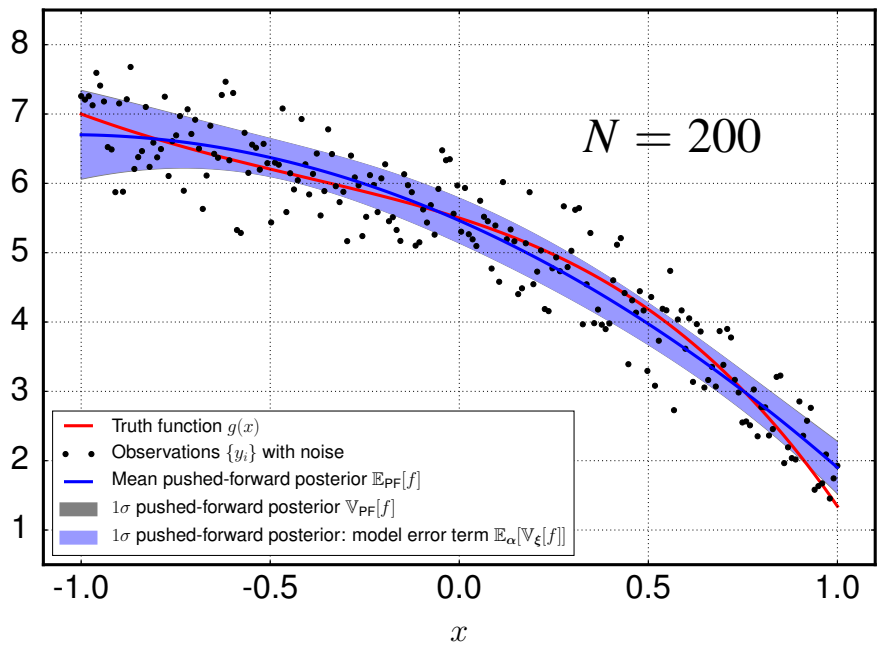
- With additional data, predictive uncertainty around the wrong model is indefinitely reducible
- Predictive uncertainty not indicative of discrepancy from truth



Quadratic-fit – ModErr – MargGauss

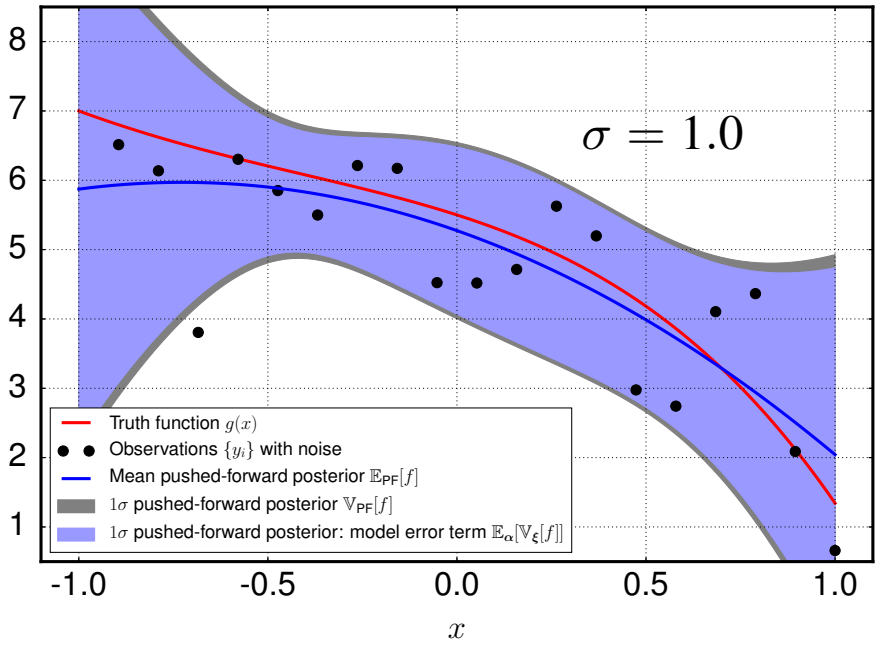


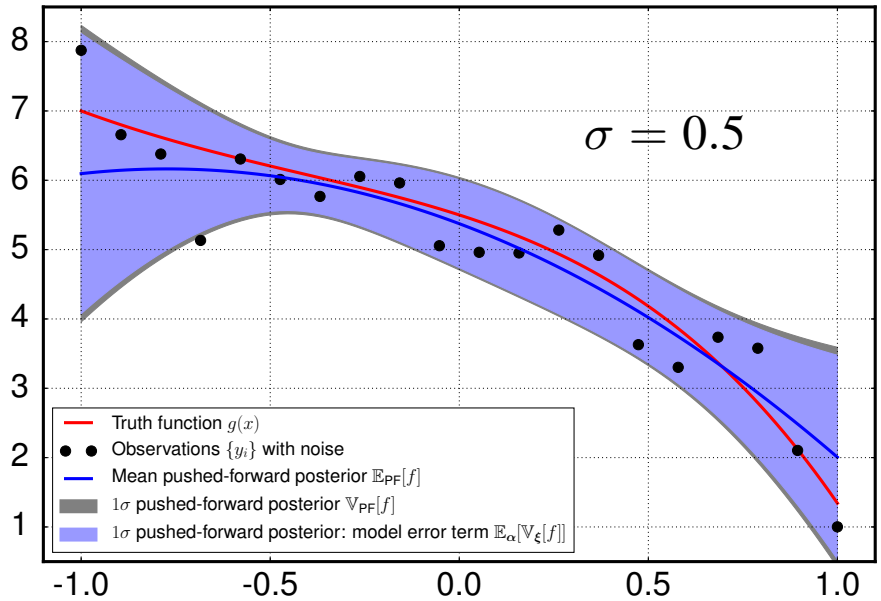


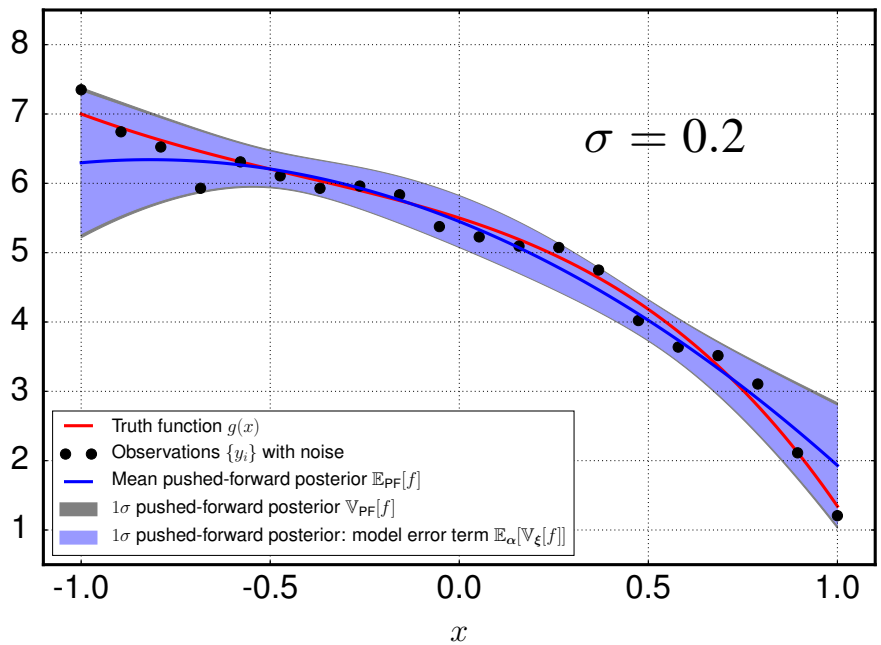


- With additional data, predictive uncertainty due to data noise is reducible
- Predictive uncertainty due to model error is not reducible

Quadratic-fit – ModErr – MargGauss

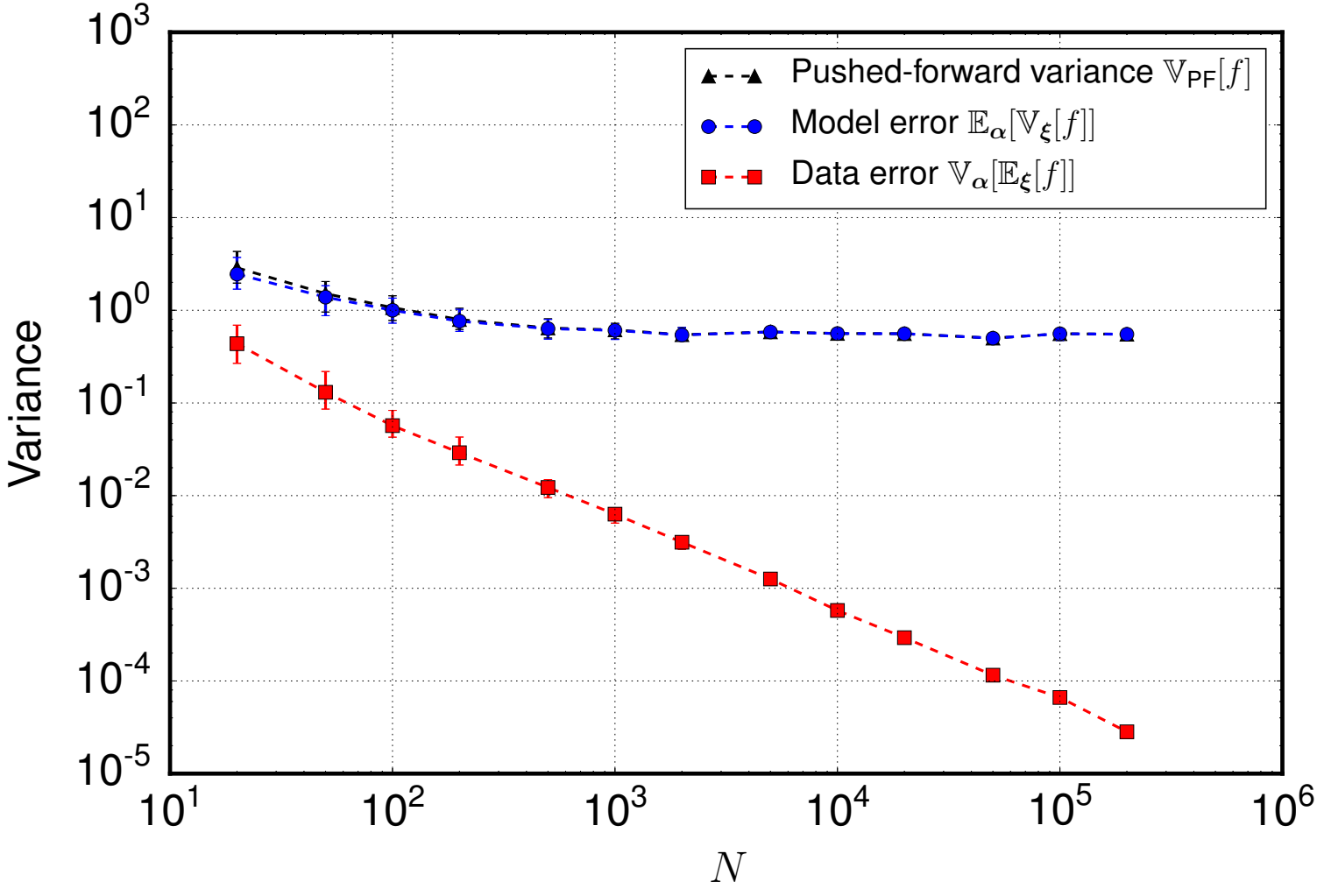






- Predictive uncertainty composed of both model-error and data-noise components
- The data-noise component is reducible with lower-noise in the data

Quadratic-fit – ModErr – MargGauss

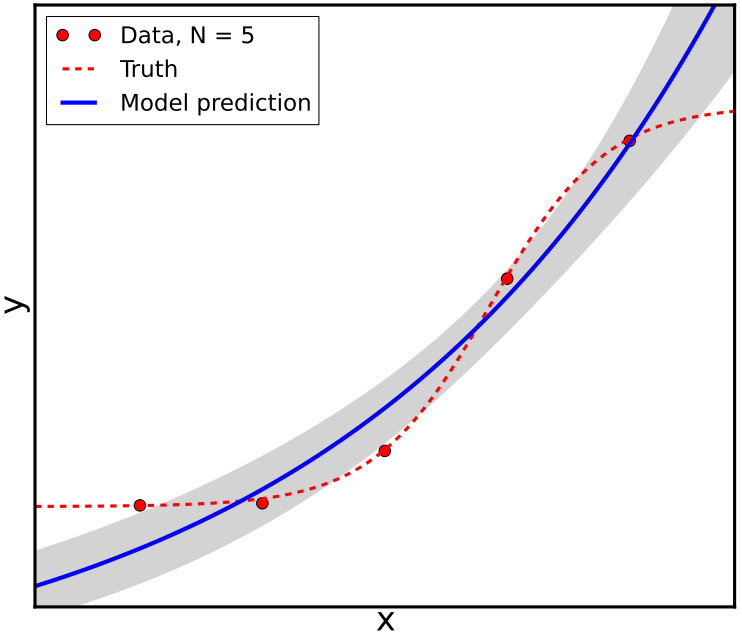


Calibrating a quadratic $f(x)$ w.r.t. $g(x) = 6 + x^2 + 0.5(x+1)^{3.5}$

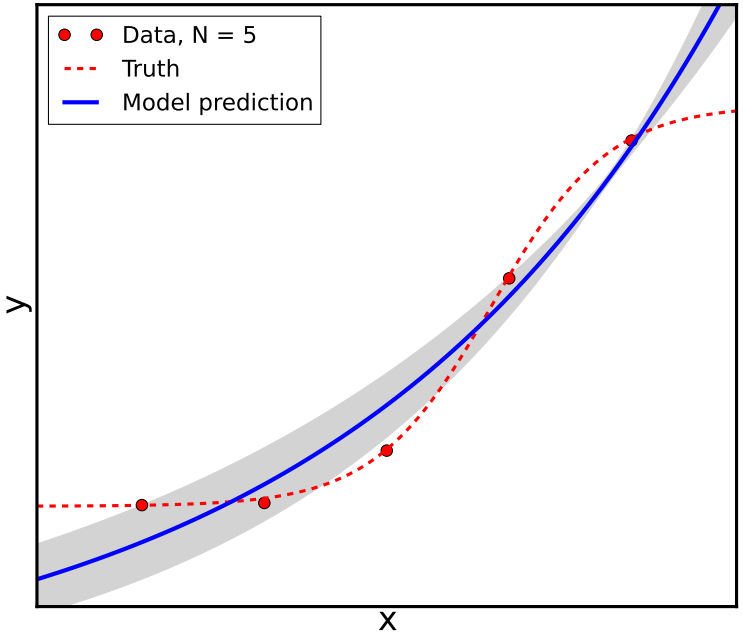
Predictions account for model error: example 1

Calibrating an exponential model $f(x; \lambda_1, \lambda_2) = \lambda_2 e^{\lambda_1 x} - 2$
with data from a hyperbolic tangent model $g(x) = \tanh(3(x - 0.3))$

Additive Gaussian error



Embedded model error



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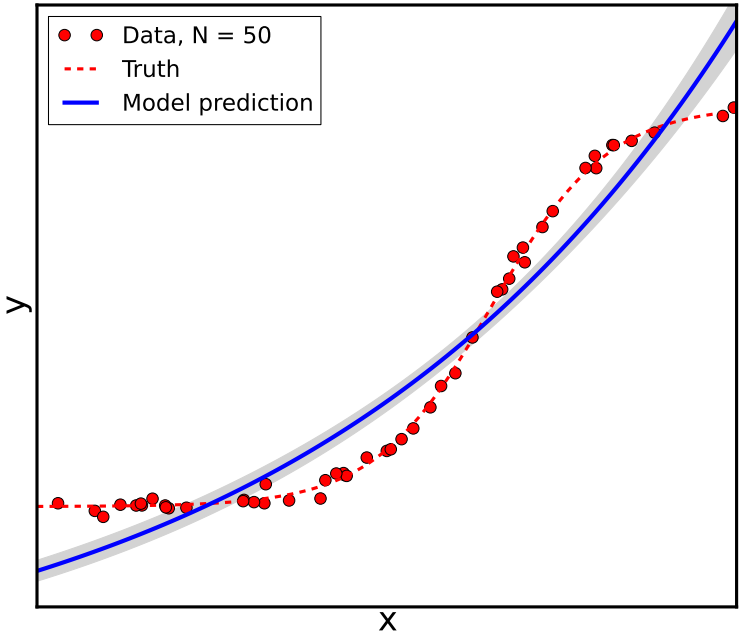

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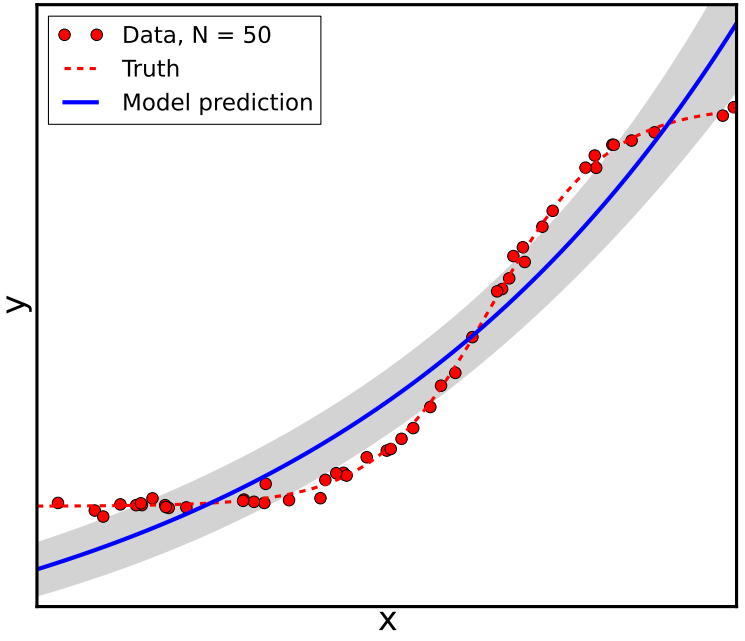


Model Error formulation – noisy data

$$y = f(x, \lambda) + \epsilon$$

Let $\epsilon \sim N(0, \sigma^2)$. With N *i.i.d.* data points we have

$$y_i = f(x_i, \lambda) + \epsilon_i, \quad i = 1, \ldots, N$$

For Hermite-Gaussian PC:

$$\begin{aligned}
\lambda &= \sum_{k=0}^{P} \alpha_k \Psi_k(\xi_1, \cdots, \xi_d), \qquad \alpha \equiv (\alpha_0, \cdots, \alpha_P) \\
f(x, \lambda) &= \sum_{k=0}^{P} f_k(x, \alpha) \Psi_k(\xi_1, \cdots, \xi_d) \\
y_i &= h(x_i, \alpha, \sigma, \xi) = \sum_{k=0}^{P} f_k(x_i, \alpha) \Psi_k(\xi_1, \cdots, \xi_d) + \sigma \xi_{d+i}
\end{aligned}$$

Augmented PC germ $\xi = (\xi_1, \cdots, \xi_d, \xi_{d+1}, \cdots, \xi_{d+N})$

Chemistry problem – ABC

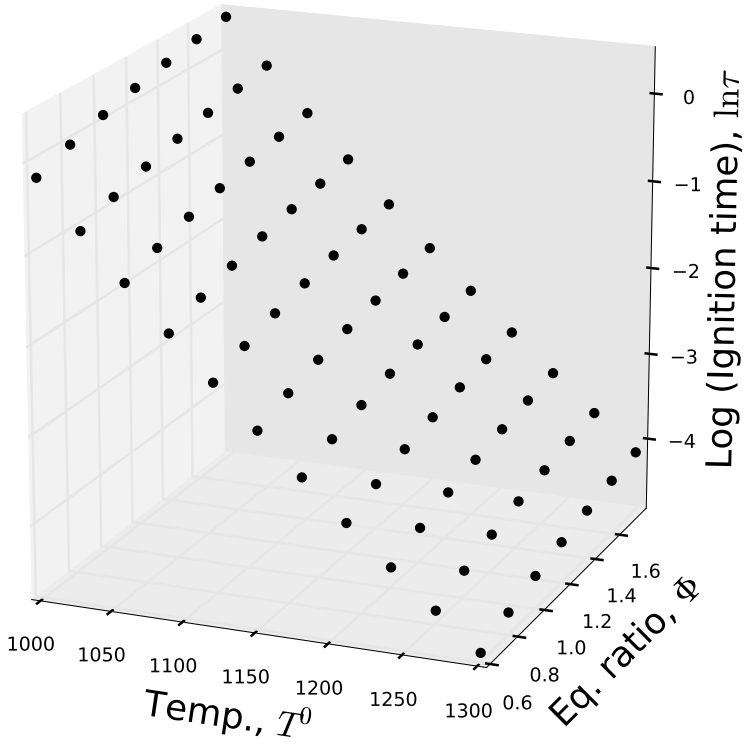
- Homogeneous ignition, methane-air mixture
- Single-step global reaction model calibrated against a detailed chemical kinetic model

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

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

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

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

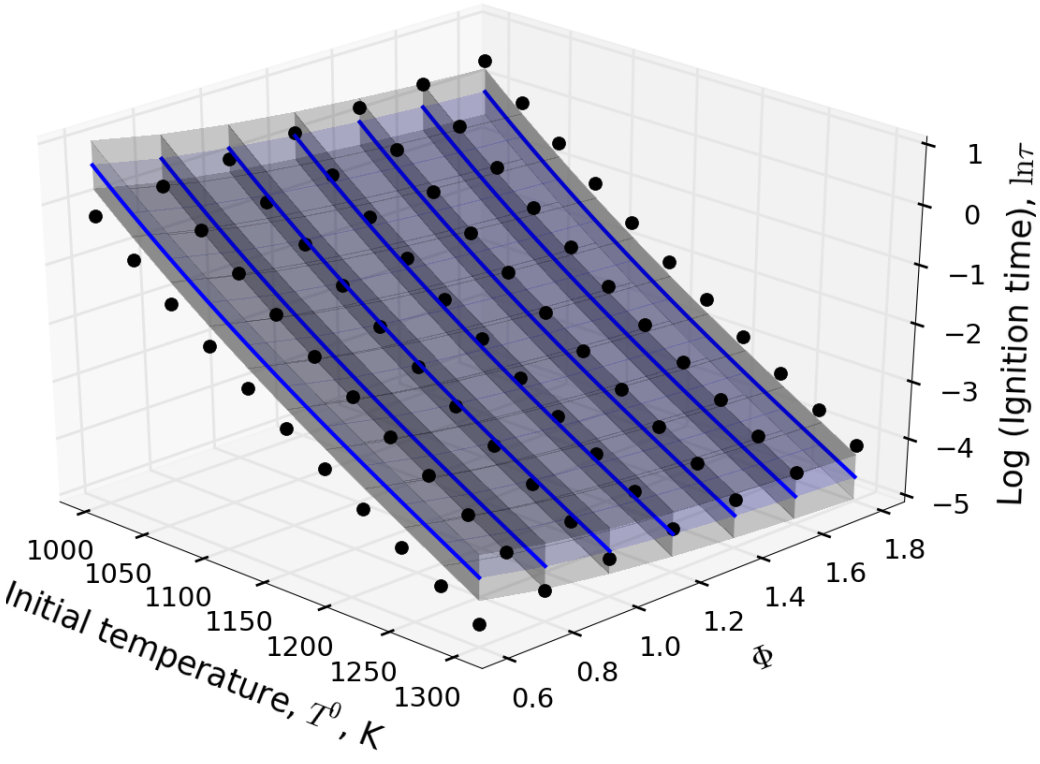


Quality of Uncertain Calibrated Model Predictions

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, HNN, 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

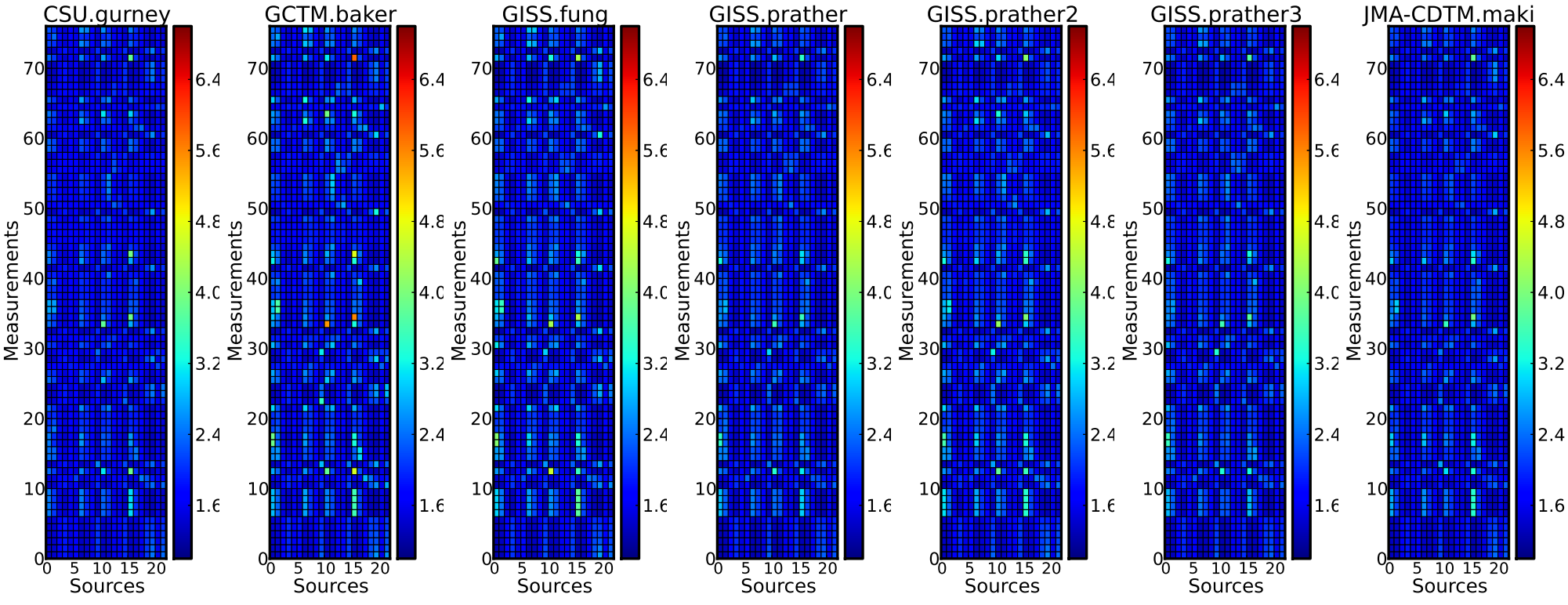
[Gurney *et al.*, Tellus B, 2003]

- 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 $\boldsymbol{s}$: $\mathbf{d} = \mathbf{R}(\mu_{\mathbf{s}} + \mathbf{C}_{\mathbf{s}}\xi)$

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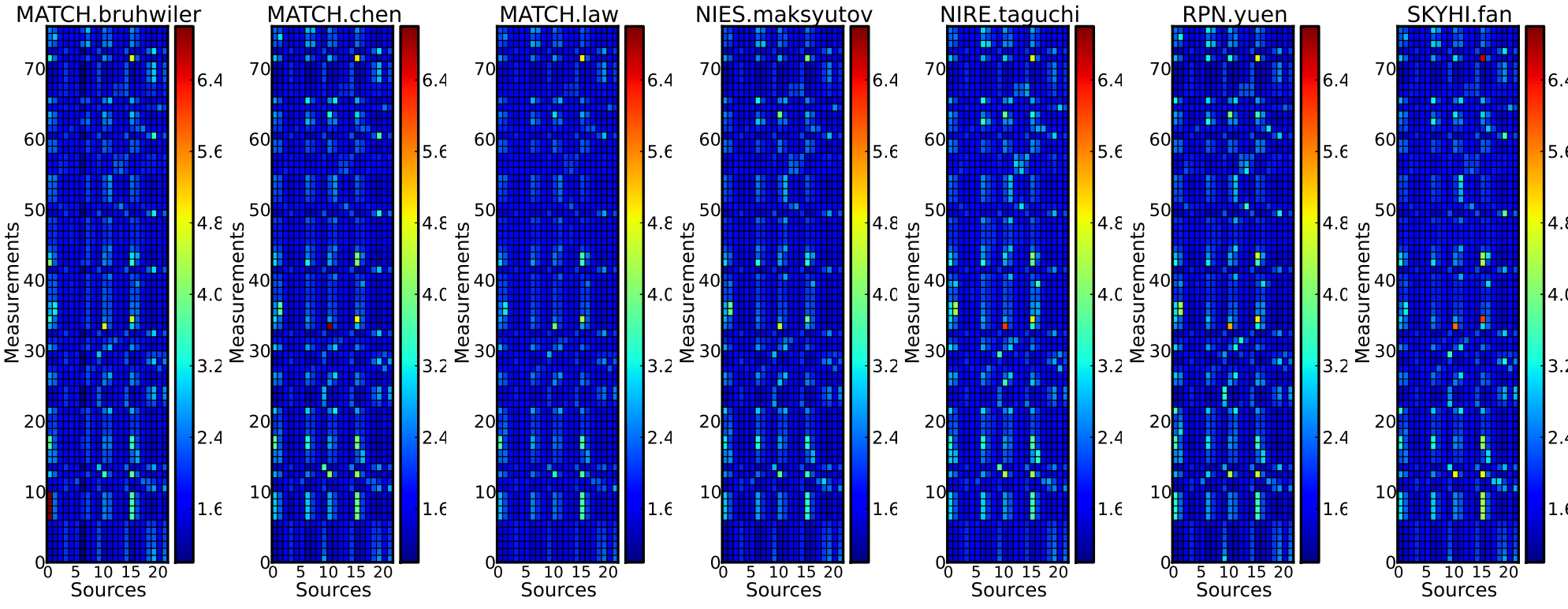

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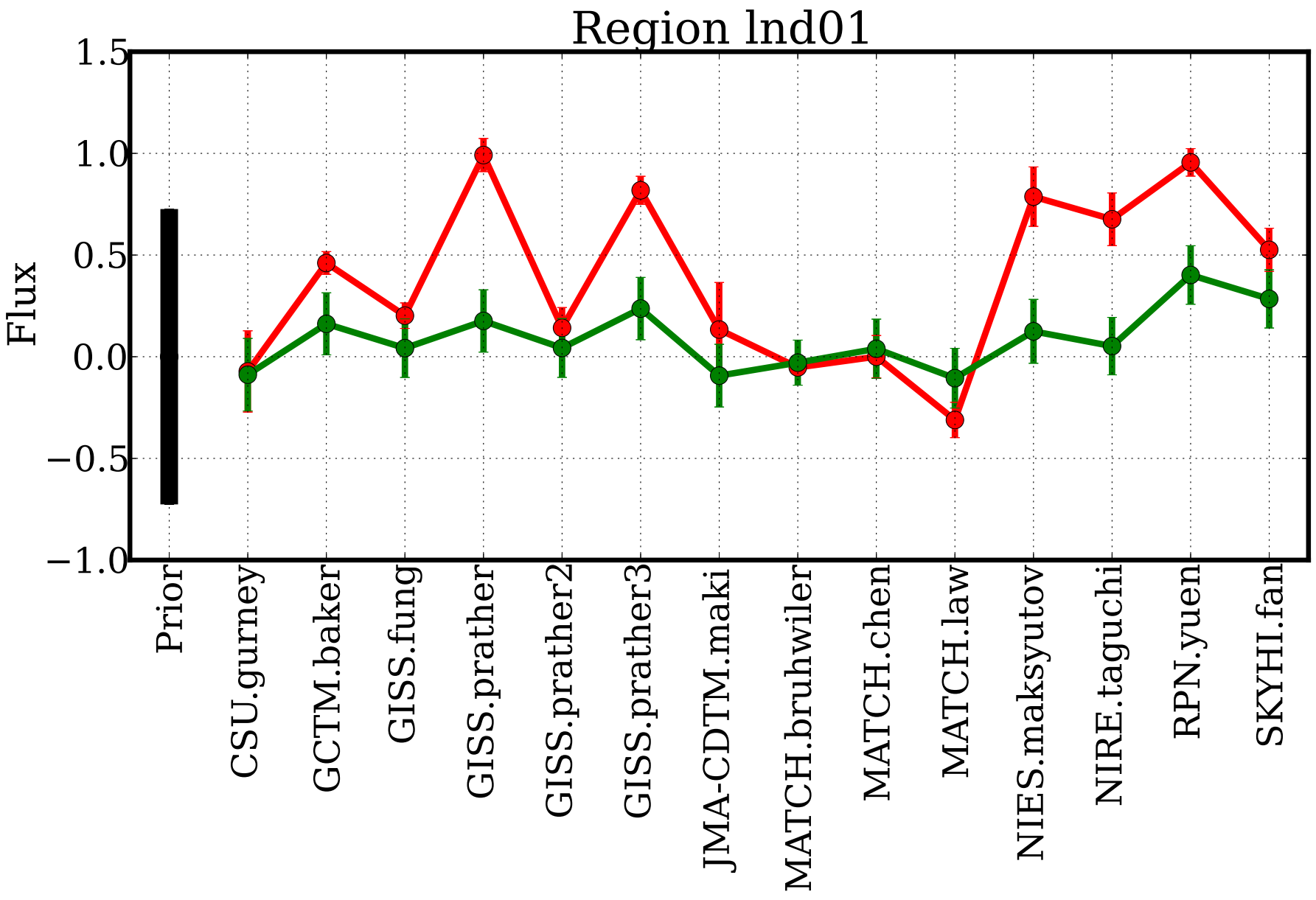
Inferred fluxes show less variability across models



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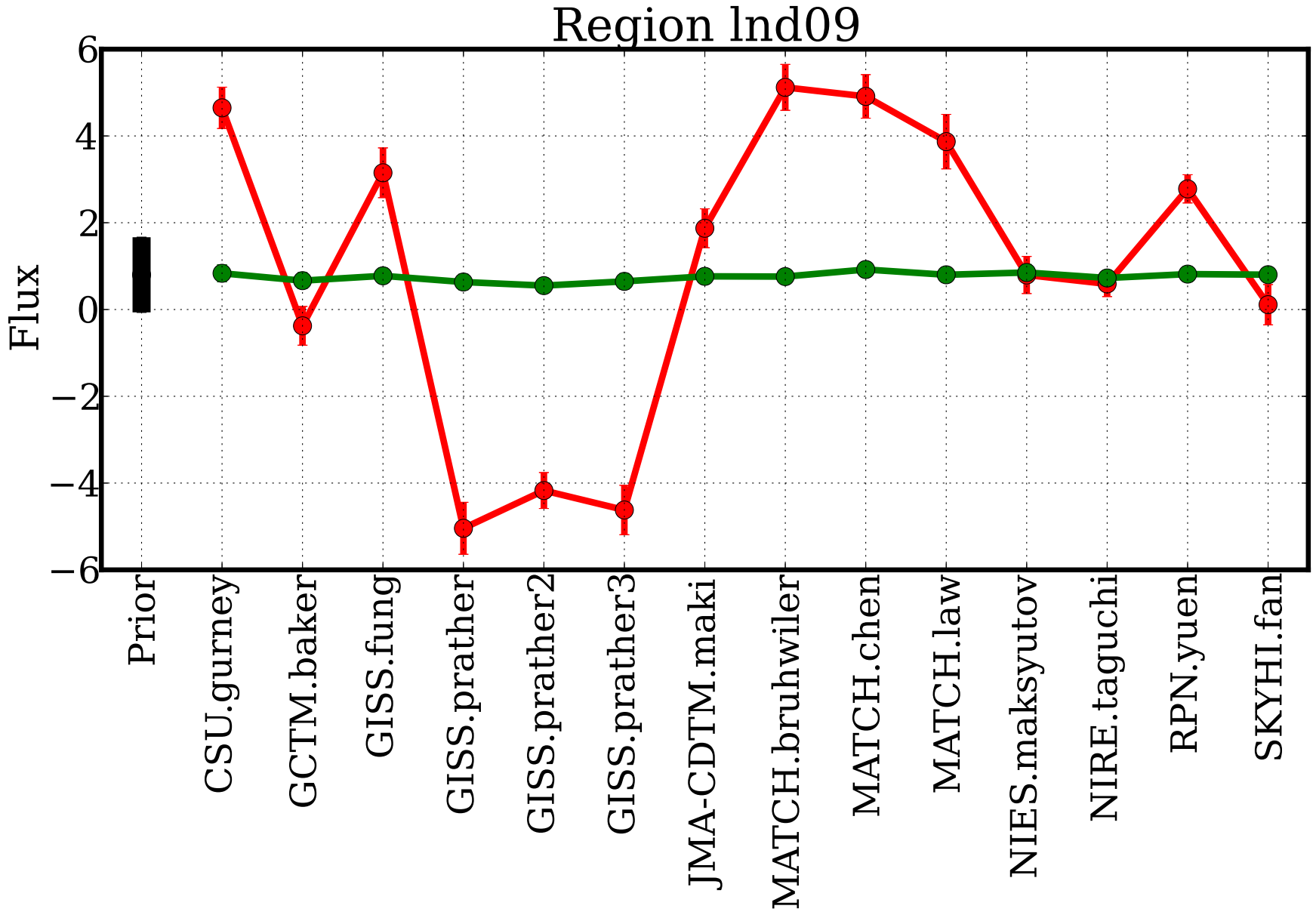

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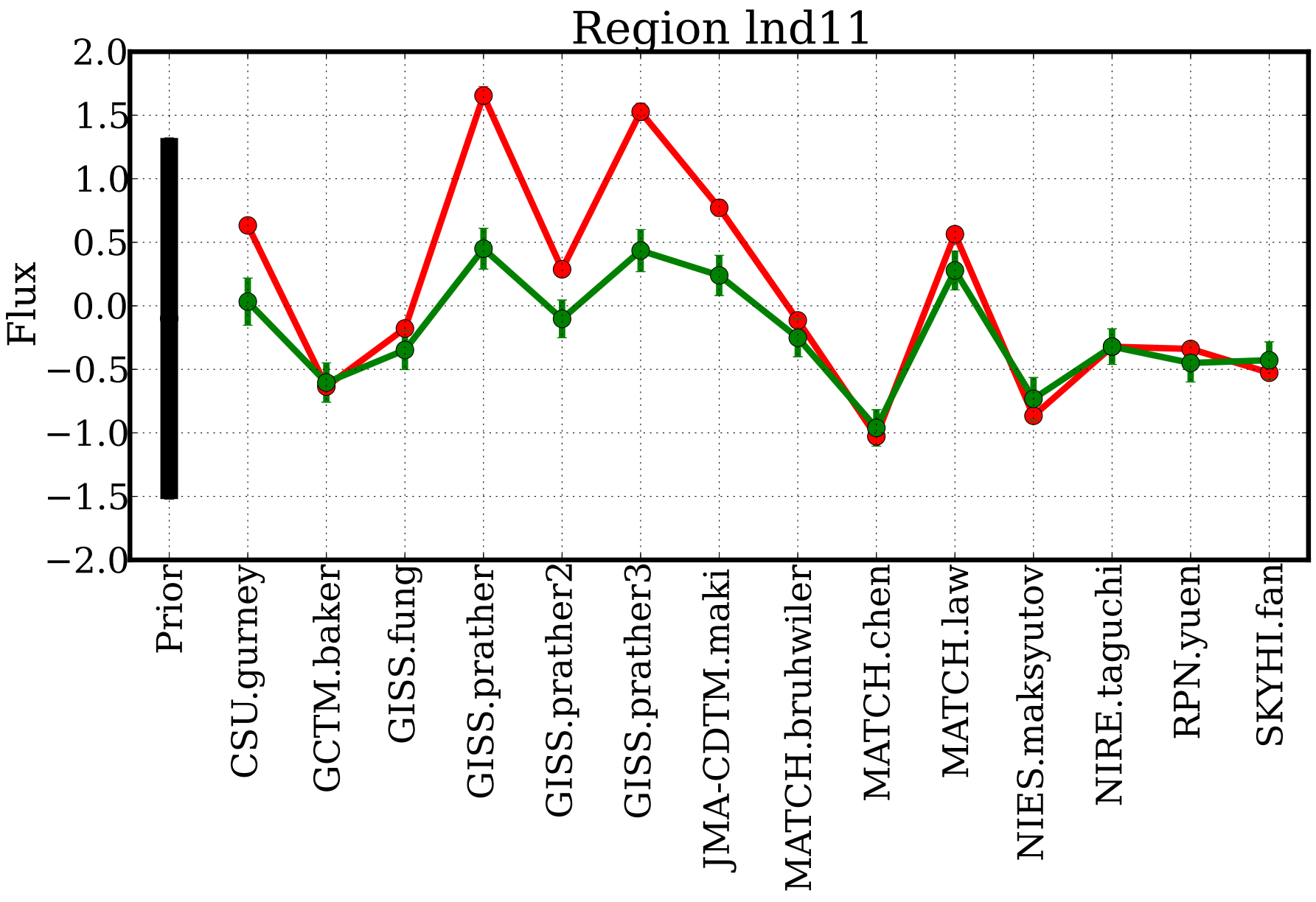

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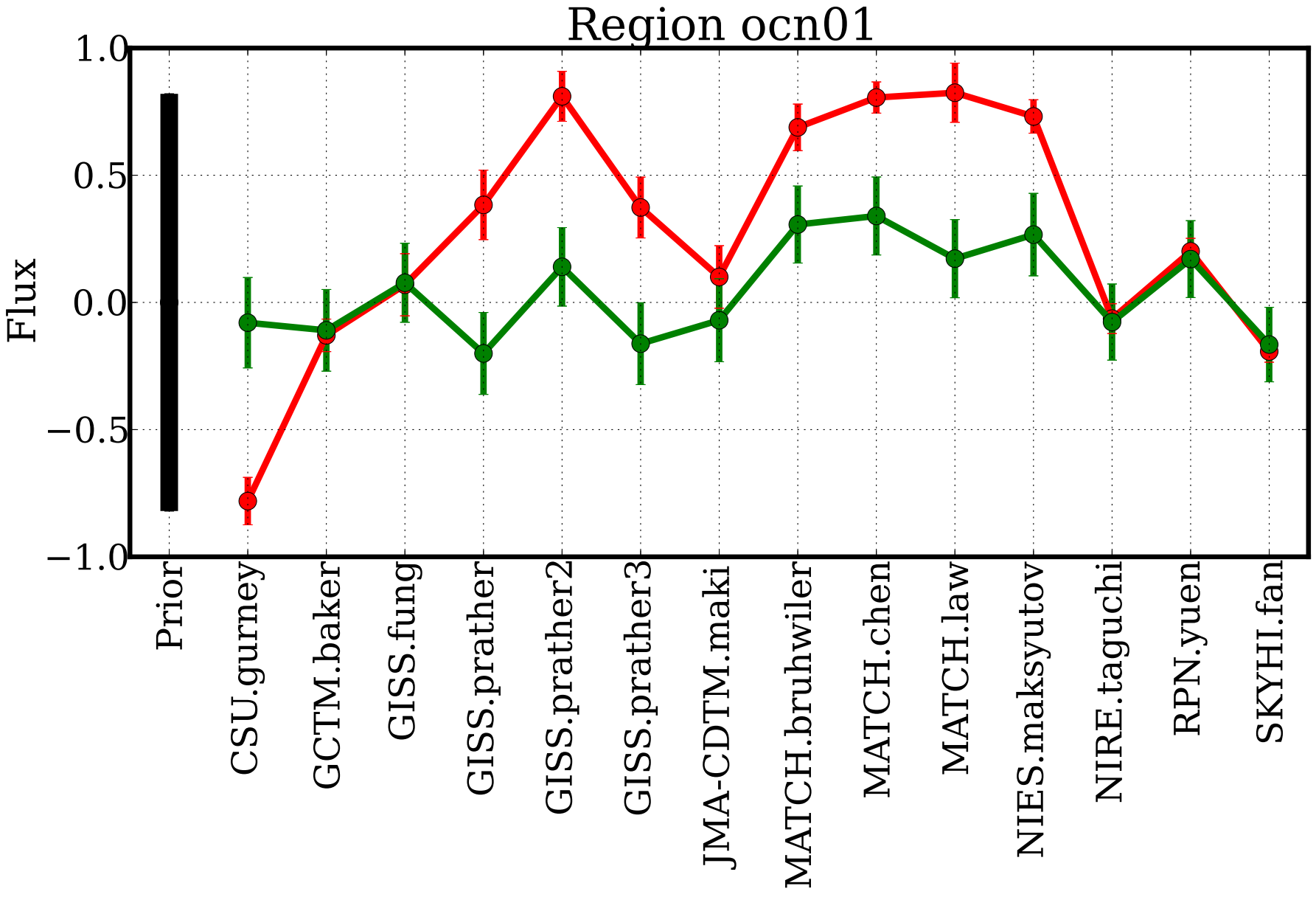

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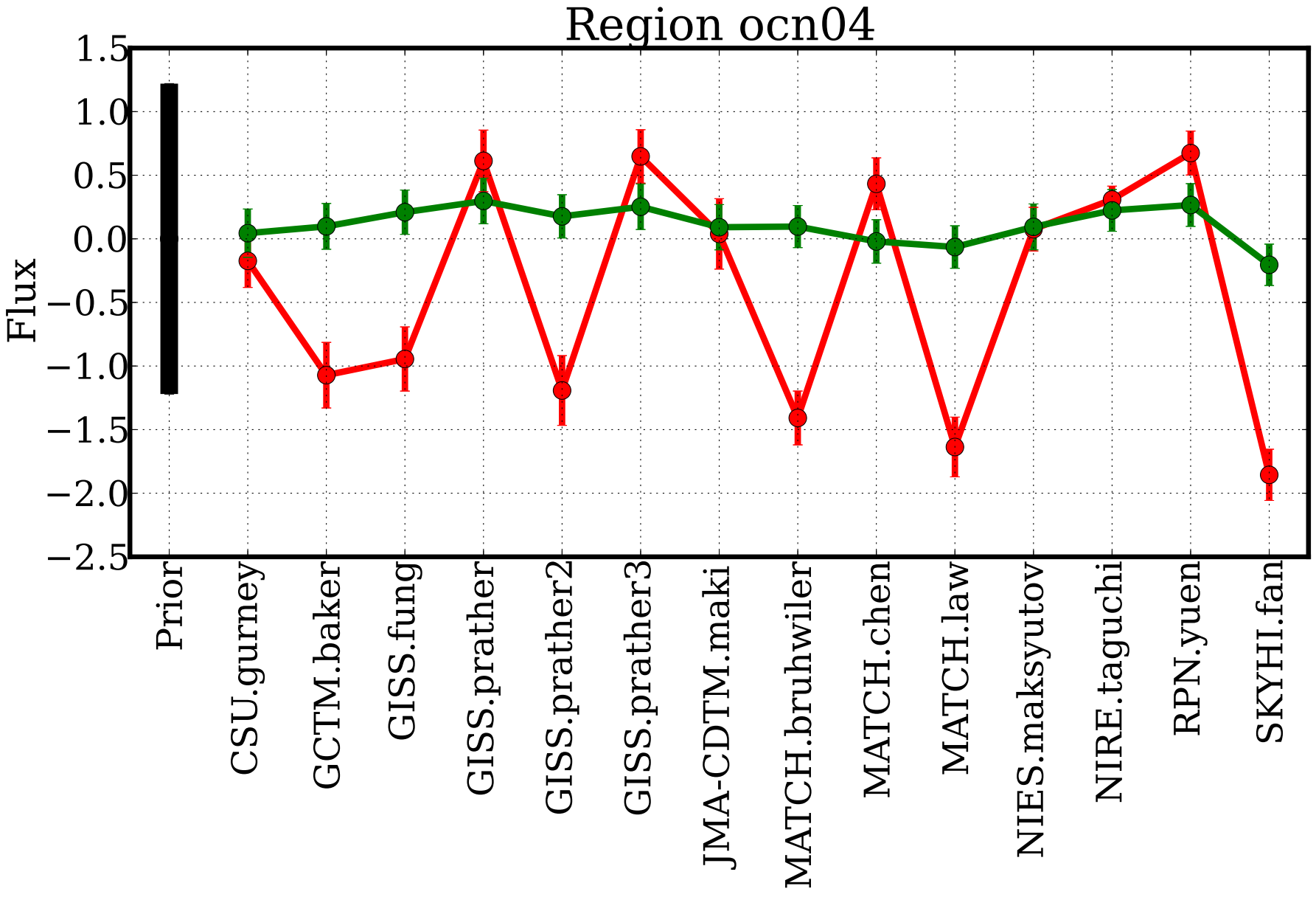

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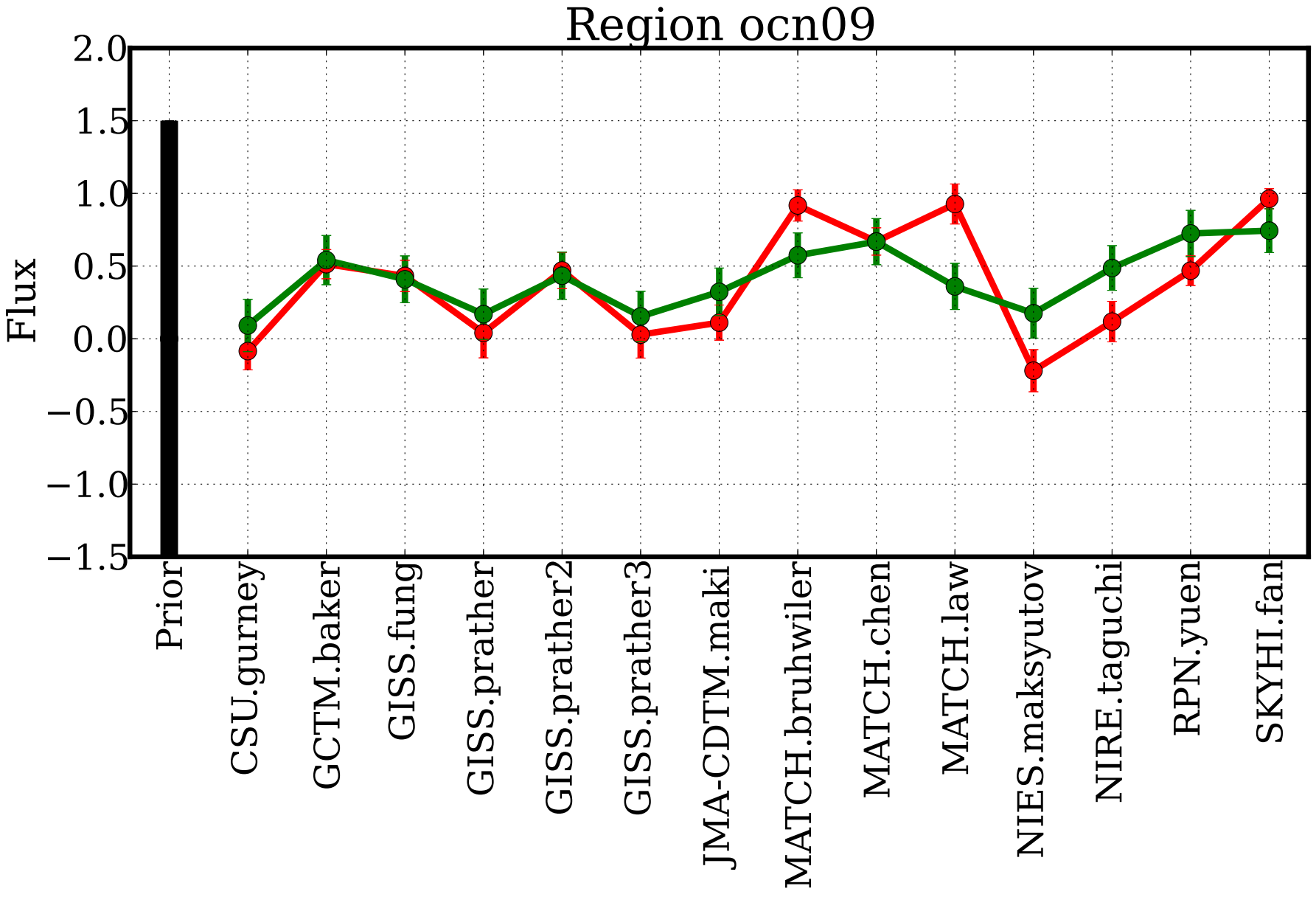

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