SAND2011-2058C

Analysis of Uncertain Dynamical Network Models

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Stochastic Multiscale Methods: Bridging the Gap Between Mathematical Analysis and Scientific and Engineering Applications

BANF International Research Station, BANF, Canada
March 27 – April 1, 2011

Acknowledgement

R.G. Ghanem — Univ. Southern California, Los Angeles, CA
O.M. Knio — Johns Hopkins Univ., Baltimore, MD

This work was supported by:

- The US Department of Energy (DOE), Office of Advanced Scientific Computing Research (ASCR), Applied Mathematics program, 2009 American Recovery and Reinvesment Act.
- The DOE Office of Basic Energy Sciences (BES) Division of Chemical Sciences, Geosciences, and Biosciences.
- BS acknowledges DOE Computational Science Graduate Fellowhip support, which is provided under grant number DE-FG02-97ER25308.

Sandia National Laboratories is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94-AL85000.

Outline

Uncertainty in Network Models

- Network ODE models typically rely on empirically-based parameters/inputs
    - Uncertain parameters/inputs
    - Uncertain network structure
- Need for dynamical analysis methods that
    - Can handle uncertainty
    - Provide model reduction with quantified fidelity
        - *accounting* for uncertainty
- Uncertain ODE systems, $x(t) \in \mathbb{R}^n$

$$
\begin{aligned}
\frac{dx}{dt} &= f(x;\lambda) \\
x(0) &= x_0
\end{aligned}
$$

Deterministic Nonlinear ODE System Analysis

- Computational Singular Perturbation (CSP) analysis
- Jacobian eigenvalues provide first-order estimates of the time-scales of system dynamics: $\tau_i \sim 1/\lambda_i$
- Jacobian right/left eigenvectors provide first-order estimates of the CSP vectors/covectors that define decoupled fast/slow subspaces
- With chosen thresholds, have M “fast" modes
    - M algebraic constraints define a slow manifold
    - Fast processes constrain the system to the manifold
    - System evolves with slow processes along the manifold
- CSP *time-scale-aware* Importance indices provide means for elimination of “unimportant" network nodes and connections for a selected observable

Analysis of Uncertain ODE Systems

- Handle uncertainties using probability theory
- Every random instance of the uncertain inputs provides a “sample" ODE system
  - Uncertainties in fast subspace lead to uncertainty in manifold geometry
  - Uncertainties in slow subspace lead to uncertain slow time dynamics
- One can analyze/reduce each system realization
  - Statistics of $x(t;\lambda)$ trajectories
- This can be expensive!
- Explore alternate means

Dynamical Analysis of the Galerkin PC System

Key questions:

- How do the eigenvalues and eigenvectors of the Galerkin system relate to those of the sampled original system
- What can we learn about the sampled dynamics of the original system from analysis of the Galerkin system
  - fast/slow subspaces
  - slow manifolds
- Can CSP analysis of the Galerkin system be used for analysis and reduction of the original uncertain system

Spectral Stochastic Representations

Let (Ω, σ, ρ) be a probability space.
Let $\xi : \Omega \to \mathbb{R}^m$ be an L^2 RV.
Let $(\Xi, s, \mu) = \xi_\sharp(\Omega, \sigma, \rho)$.
Let $\{\varphi_\alpha(\xi) : \alpha = 0, 1, 2, \ldots\}$ be an orthonormal basis of $L^2(\Xi)$.
Let $X : A \times \Omega \to \mathbb{R}$ be an $L^2(\Omega)$ A-process. Its closest representative in $L^2(\Xi)$ is

$$X(a, \omega) \simeq \sum_\alpha X_\alpha(a)\, \varphi_\alpha(\xi(\omega))$$

where

$$X_\alpha(a) = \int_\Omega X(a, \omega)\, \varphi_\alpha(\xi(\omega))\, d\rho(\omega) = \langle \varphi_\alpha, X \rangle.$$

Take $m = 1$ for simplicity. $m > 1$ holds by tensor product arguments.

Galerkin Reformulation

Consider an ODE

$$\dot{x} = f(\xi, x) \qquad x(\xi, 0) = x_0(\xi)$$

with $x(t, \omega) \in \mathbb{R}^n$. Represent x as

$$x(\xi, t) = \sum_{\alpha} x_\alpha(t)\, \varphi_\alpha(\xi)$$

where

$$x_\alpha(t) = \langle \varphi_\alpha(\xi),\, x(\xi, t) \rangle$$

and so these coefficients have dynamics

$$\begin{aligned} \dot{x}_\alpha &= \left\langle \varphi_\alpha(\xi),\, \frac{d}{dt} x(\xi, t) \right\rangle \\ &= \langle \varphi_\alpha(\xi),\, f(\xi, x) \rangle \\ \dot{x}_\alpha &= g(x_*) \end{aligned}$$

Jacobian of Sampled System

The dynamical system can be locally characterized by the eigenstructrure of the Jacobian matrix. The enteries of the Jacobian matrix J of the sampled system is given by

$$J_{ij}(\xi, t) = \frac{\partial f^i}{\partial x^j}(\xi, x(\xi, t))$$

At each value of time, $J(\xi, t)$ is a random matrix.

Jacobian Matrix of Reformulated System

The Jacobian matrix of the coefficient system can be thought of as a block matrix with blocks

$$\begin{aligned}\mathcal{J}_{\alpha\beta}(t) &= D_{x_\beta} \int_\Xi f(\xi, x(\xi,t))\, \varphi_\alpha(\xi)\, d\mu(\xi) \\ &= \int_\Xi \varphi_\alpha(\xi)\, J(\xi,t)\, \varphi_\beta(\xi)\, d\mu(\xi) \\ &= \langle \varphi_\alpha, J\varphi_\beta \rangle\end{aligned}$$

Truncate the representation so that $\alpha, \beta = 0, \ldots, P$.
$\mathcal{J}$ is then a $n(P+1) \times n(P+1)$ matrix.

Essential Numerical Range of J

The numerical range of a matrix M is

$$W(M) = \{v^* M v : v \in \mathcal{C}^m, v^* v = \|v\|^2 = 1\}.$$

Note that

$$\text{spect}(M) \subset W(M).$$

The essential numerical range of $J(\xi)$ is

$$\tilde{W}(J) = \bigcup_{\text{a.e. } \xi} W(J(\xi)).$$

n-dimensional system – Key Results

1. The spectrum of $\mathcal{J}^P$ is contained in the convex hull of the essential range of the random matrix J.

$$\text{spect}(\mathcal{J}^P) \subset \text{conv}(\widetilde{W}(J))$$

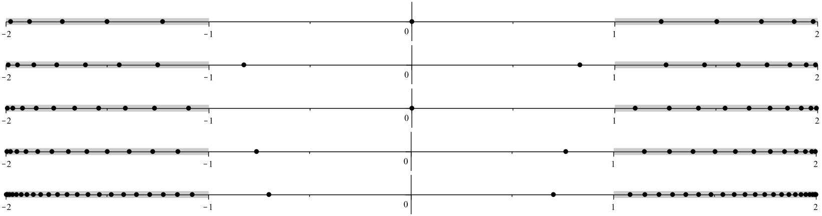
2. For any orthonormal basis $\{\phi_\alpha\}_{\alpha=0}^{\infty}$:

   As $P \to \infty$, the eigenvalues of $\mathcal{J}^P(t)$ converge weakly, *i.e.* in the sense of measures, toward $\bigcup_{\omega\in\Omega} \text{spect}(J(\omega))$.

Sonday *et al.*, *SISC*, in press
Berry *et al.*, in review

- Interpolating Galerkin system eigenvalues approximates random eigenvalues
- Eigenpolynomials and Eigenvalues can be used to construct the PCE for the random eigenvalue.

1D Example



$$\dot{x}(\xi, t) = a(\xi)x(\xi, t); \quad \xi(\omega) \sim U[-1, 1];$$

$$J = a(\xi) \equiv \begin{cases} \xi + 1 & \text{for} \quad \xi \geq 0, \\ \xi - 1 & \text{for} \quad \xi < 0. \end{cases}$$

$$\widetilde{W}(J) = [-2, -1] \cup [1, 2]; \qquad \text{conv}(\widetilde{W}(J)) = [-2, 2].$$

LU PC: eigenvalues of $\mathcal{J}^P$ shown for $P = 10, 15, 20, 25, 45$

Eigenvectors

Let $\lambda_{i\alpha}$, $v_{i\alpha}$ be an eigenvalue/vector pair of $\mathcal{J}^P$:

$$\mathcal{J}\, v_{i\alpha} = \lambda_{i\alpha} v_{i\alpha}.$$

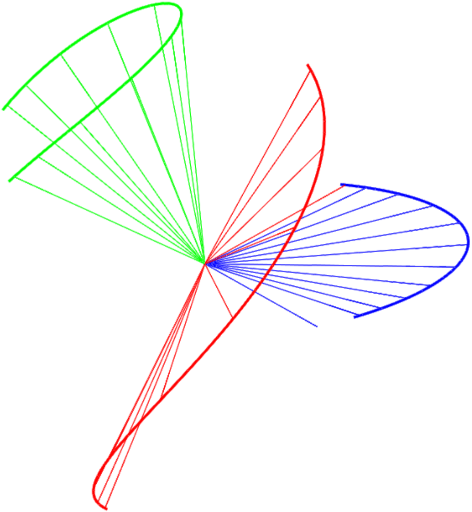
Alternatively,

$$\langle \varphi_\beta(\xi),\, (J(\xi) - \lambda_{i\alpha})\, \mathfrak{v}_{i\alpha}(\xi) \rangle = 0 \qquad \text{for } \beta = 0 \ldots P$$

where $\mathfrak{v}_{i\alpha}(\xi)$ in an n-vector with components

$$\mathfrak{v}^k_{i\alpha}(\xi) = \sum_{\gamma=0}^{P} v^{k\gamma}_{i\alpha}\, \varphi_\gamma(\xi).$$

Stochastic Vectors composed of Galerkin eigenvectors approximate the stochastic eigenvectors well



CO Oxidation Example

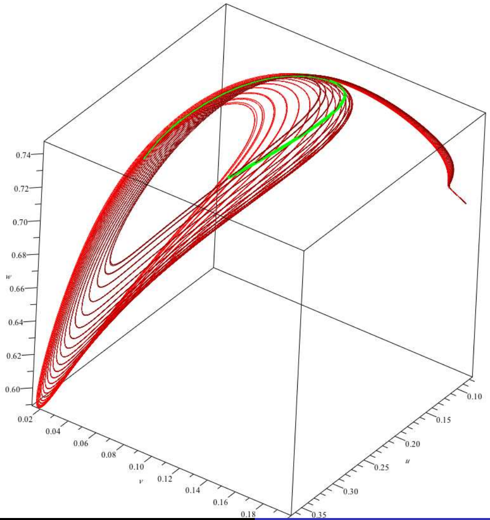
The oxidation of CO on a surface can be modeled as (Makeev et al., JCP, 2002)

$$\dot{u} = az - cu - 4duv \qquad \dot{v} = 2bz^2 - 4duv$$
$$\dot{w} = ez - fw \qquad z = 1 - u - v - w$$
$$a = 1.6, b = 20.75 + .45\xi, c = 0.04, \quad d = 1.0, e = 0.36, f = 0.016$$

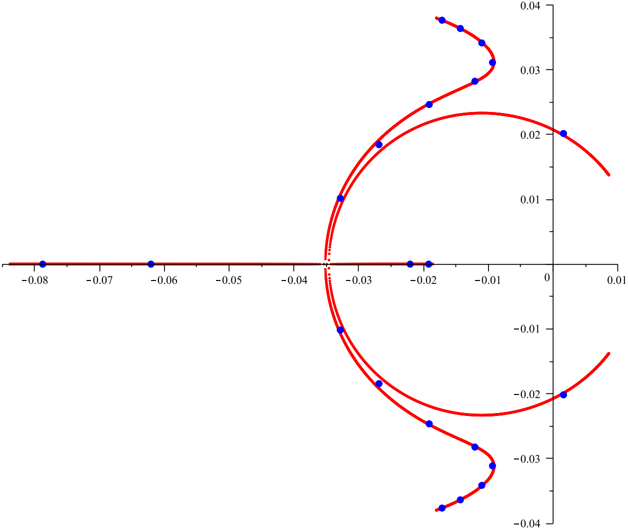
$$u(0) = 0.1, v(0) = 0.2, w(0) = 0.7$$

exhibits Hopf bifurcations for $b \in [20.3, 21.2]$

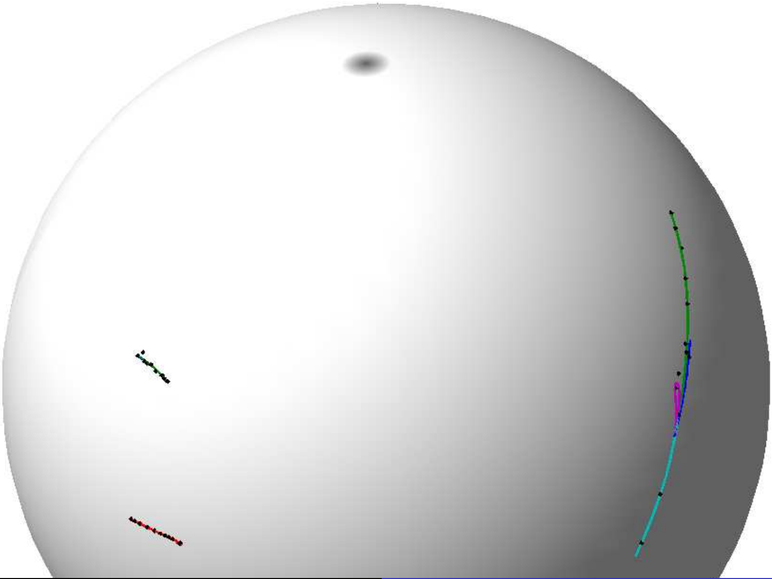
CO Oxidation: Analyzing the stochastic Jacobian at $t = 300$.



CO Oxidation: PC order 10. Slow eigenvalues.



CO Oxidation: PC order 10. Eigenvectors.



Data Free Inference (DFI)

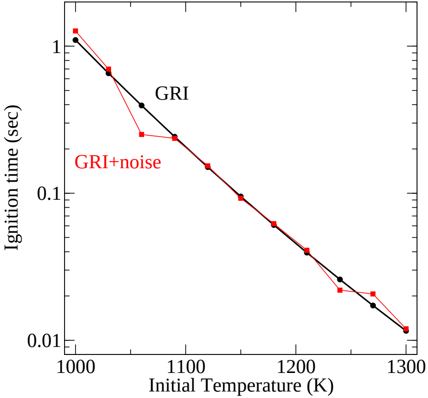
- Input uncertainties are not well characterized in many practical network models
- May have nominal parameter values and bounds
  - No information on correlations
  - No joint PDF on parameters
- Joint PDF structure can have a drastic effect on resulting uncertainties in predictions
- When original raw data is available, Bayesian inference provides the requisite posterior
- When original data is **not** available, what can be done?
  - DFI: discover a consensus joint PDF on the parameters consistent with given information

    (Berry *et al.*, JCP, in review)
  - Demonstrate on a chemical ignition problem (ODE)

Generate ignition "data" using a detailed model+noise

- Ignition using a detailed chemical model for methane-air chemistry
- Ignition time versus Initial Temperature
- Multiplicative noise error model
- 11 data points:

$$
\begin{aligned}
d_i &= t_{\mathrm{ig},i}^{\mathrm{GRI}}(1+\sigma\epsilon_i) \\
\epsilon &\sim N(0,1)
\end{aligned}
$$



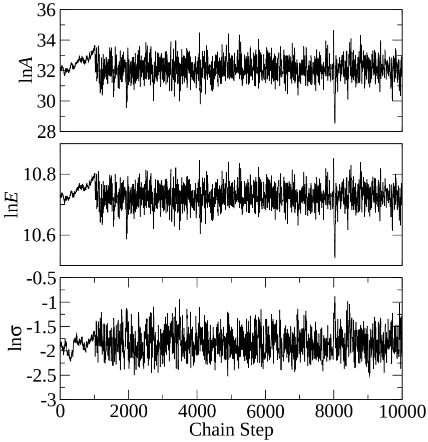
Fitting with a simple chemical model

- Fit a global single-step irreversible chemical model

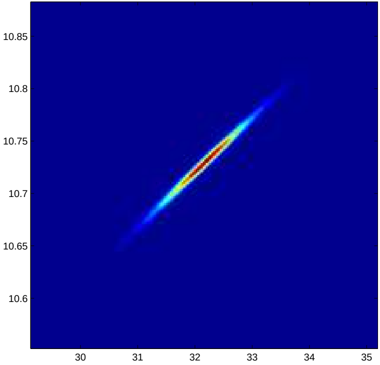
$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

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

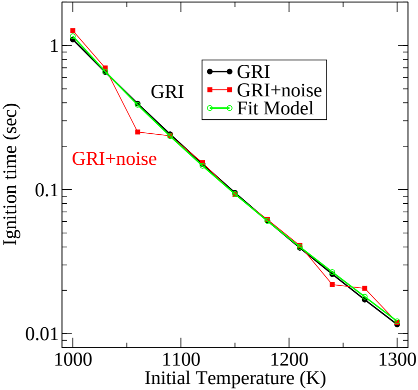
- Infer 3-D parameter vector $(\ln A, \ln E, \ln \sigma)$
- Good mixing with adaptive MCMC when start at MLE



Bayesian Inference Posterior and Nominal Prediction

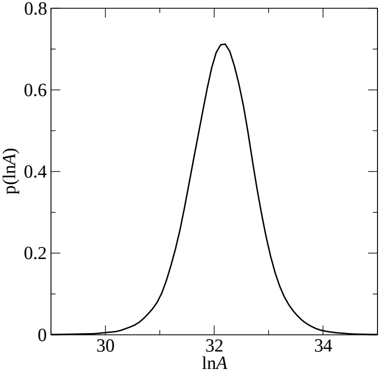


Marginal joint posterior on $(\ln A, \ln E)$ exhibits strong correlation

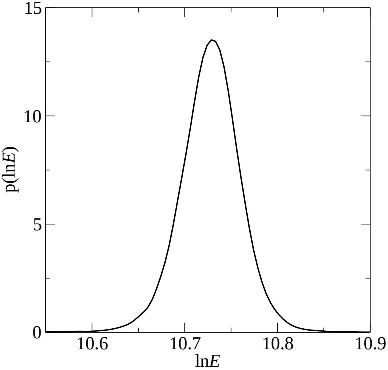


Nominal fit model is consistent with the true model

Marginal Posteriors on $\ln A$ and $\ln E$



$$\ln A = 32.15 \pm 3 \times 0.61$$



$$\ln E = 10.73 \pm 3 \times 0.032$$

Data Free Inference Challenge

Discarding initial data, reconstruct marginal $(\ln A, \ln E)$ posterior using the following information

- Form of fit model
- Range of initial temperature
- Nominal fit parameter values of $\ln A$ and $\ln E$
- Marginal 5% and 95% quantiles on $\ln A$ and $\ln E$

Further, for now, presume

- Multiplicative Gaussian errors
- $N = 8$ data points

DFI Algorithm Structure

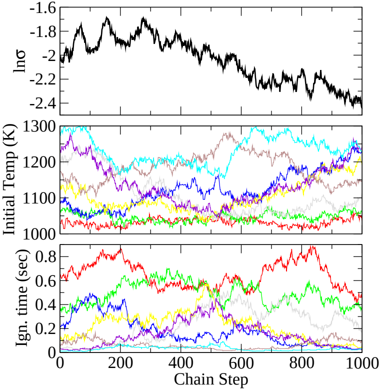
Basic idea:

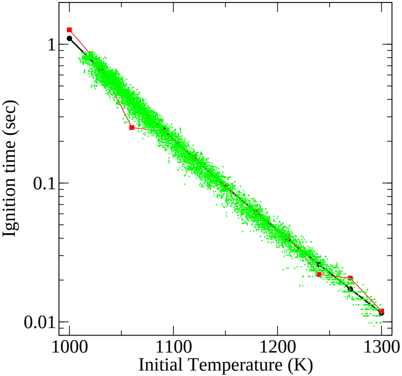
- Explore the space of hypothetical data sets
- Accept data sets that lead to posteriors that are consistent with the given information
- Evaluate pooled posterior from all acceptable posteriors

Algorithm uses two nested MCMC chains

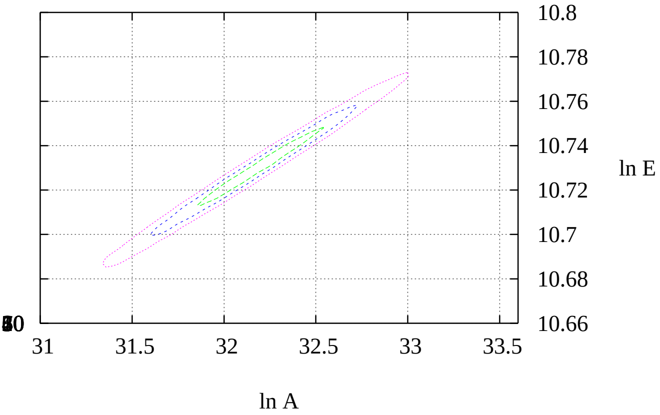
- An outer chain on the data, $(2N+1)$–dimensional
  - N data points (x_i, y_i) + σ
  - Likelihood function captures constraints on parameter nominals+bounds
- An inner chain on the model parameters
  - Likelihood based on fit-model
  - parameter vector $(\ln A, \ln E, \ln \sigma)$

Short sample from outer/data chain

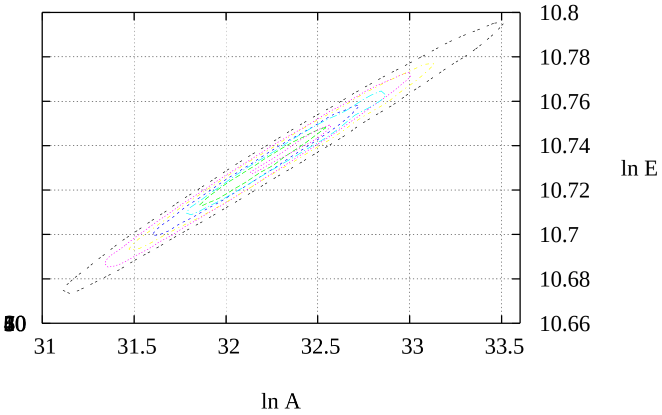




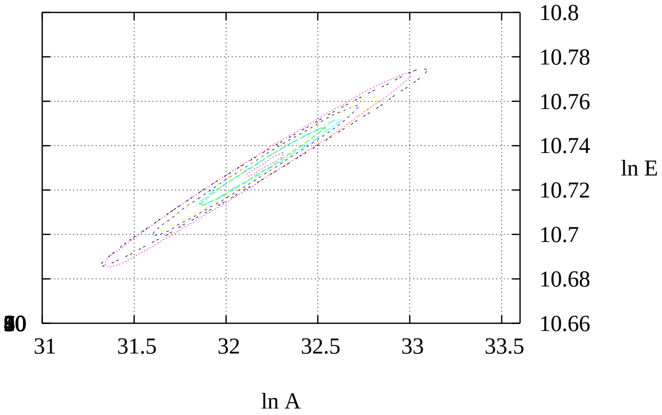
True Posterior



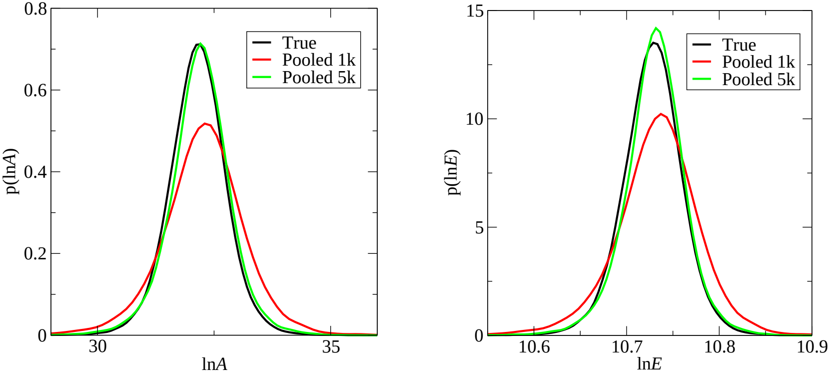
True + DFI posterior based on a 1000-long data chain



True + DFI posterior based on a 5000-long data chain



Marginal Posteriors on $\ln A$ and $\ln E$



Closure

- Analysis of uncertain network model dynamics:
    - Outlined relationship between eigen-analysis of a sampled stochastic ODE system and the Galerkin PC system.
    - Galerkin system eigenvalues/eigenvectors can be used to analyze the dynamics of the stochastic system
    - Work in progress on
        - associated stochastic model reduction strategies
        - structural uncertainty in network models
- Data Free Inference:
    - Developed a DFI procedure for estimation of self-consistent parametric posteriors in the absence of data
    - Demonstrated effective and convergent estimation of missing posterior in a chemical ignition problem
    - In progress: algorithm optimization and generalization to handle a range of different constraints