Uncertainty Quantification: A Paradigm for Sufficient Modeling in Complex Systems

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s2i2 Scientific Workflows for Scattering Science
Caltech, CA January 31 2013

Outline

Motivation

Probabilistic Character of Physical Processes

is not an intrinsic property, but a consequence of loss of information about these processes.

- equilibrium processes: uncertainty about parameters from mean-field theory
- non-equilibrium processes: uncertainty about mean-field theory itself

Models of Physical Processes

are not intrinsic properties of these processes, but a consequence of our choice of Observables and Quantities of Interest (QoI).

We have a choice in **which** information to package and **how** to do that

with consequences on the way we think things depend on each others, and hence on the whole machinery of statistical inference.

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Some UQ Challenges

Purpose: $U = \hat{U}|_{h,d,p,m} + \underbrace{\epsilon_h|_{d,p,m} + \epsilon_p|_{d,m} + \epsilon_d|_m}_{\text{Limits on Predictability: Must be quantified}} + \epsilon_m$

- Quantify and manage risk
- Scientific discovery

Modeling

What is the relationship between evidence and quantities of interest ? conservation laws ? differential equations ? how much freedom do have ?

Curse of Dimensionality

How much of the complexity structure do we need to sufficiently characterize the QoI ?

Outline

Random Matrix

If a system is sufficiently complex, the state of the system is no longer important ... what is required here is a new kind of statistical mechanics, in which we renounce exact knowledge not of the state of the system but of the system itself. We picture complex nucleus as a black box in which a large number of particles are interacting according to unknown laws. The problem then is to define in a mathematically precise way an ensemble of systems in which all possible laws of interaction are equally possible" (E. Wigner, 1932; F. Dyson, 1961).

Construction of Stochastic Matrices

Most General:

Joint density function on matrix elements: too complex, requires too much information.

Known Physical Constraints:

- Invariance of measure under arbitrary rotations
- Hermitian Hamiltonians
- Accounting for additional invariances:
  - GUE (Gaussian Unitary ensemble)
  - GOE (Gaussian orthogonal ensemble)
  - GSE (Gaussian symplectic ensemble)

Applications in Mechanics:

The set of positive definite matrices constrained by experimental observations is significant.

Positive Definite Matrices

MaxEnt with following constraints:

$$\begin{cases} \int_{\mathbb{M}_n^+} A p_A dA = \bar{A} \in \mathbb{M}_n^+ \\ \int_{\mathbb{M}_n^+} p_A dA = 1 \\ E\{\|A^{-1}\|_F^\gamma\} < \infty \end{cases}$$

Then A has the Wishart distribution, characterized by its mean and dispersion coefficient

$$\delta_A = \sqrt{\frac{E\|A - \bar{A}\|_F^2}{\|\bar{A}\|_F^2}} \qquad \|A\|_F = \sqrt{\mathrm{tr}(AA^T)}$$

Bounded Matrix

Behavior of heterogeneous materials can be theoretically bound between the behavior of two equivalent homogeneous materials:

Specifically, the constitutive matrix is bounded above and below by:

$$C_l \leq C \leq C_u$$

Constrain the probabilistic model of the heterogeneous material with this information: $\mathcal{G} = \{G \in \mathbb{M}_n^+ : G_l < G < G_u\}$

$$\begin{cases} \int_{\mathcal{G}} p_{\mathcal{G}}(G) dG & = & 1 \\ \int_{\mathcal{G}} \ln\left[\det(G - G_l)\right] p_{\mathcal{G}}(G) dG & = & g_l \\ \int_{\mathcal{G}} \ln\left[\det(G - G_u)\right] p_{\mathcal{G}}(G) dG & = & g_u \end{cases}$$

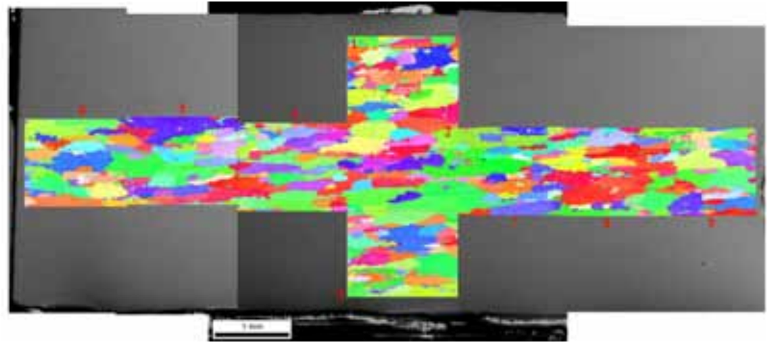
MaxEnt Distribution of Bounded Random Matrix:

$$p_G(G) = \frac{\det(G - G_l)^{a-(N+1)/2} \det(G_u - G)^{b+(N+1)/2}}{\beta_N(a, b) \det(G_u - G_l)^{(a+b)-(N+1)/2}}$$

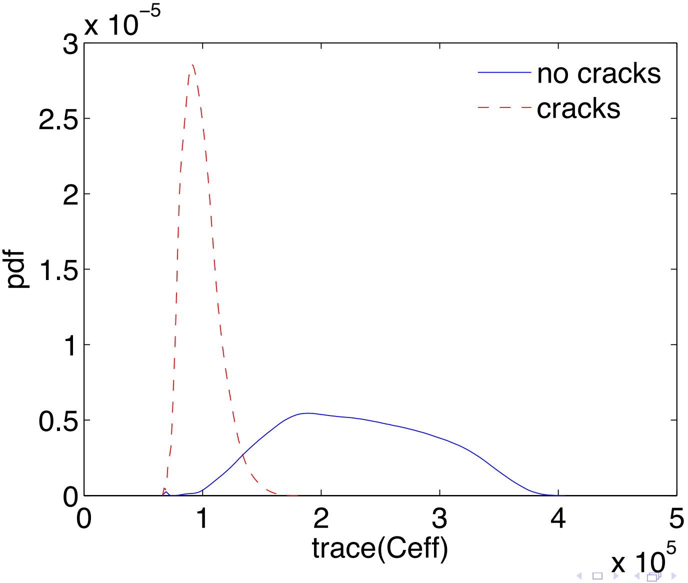
Notes:

- a, b are obtained from the MaxEnt optimization.
- efficient sampling algorithms have been developed for this distribution.

Experimental Data - with inclusions



Detection of Subscale Features

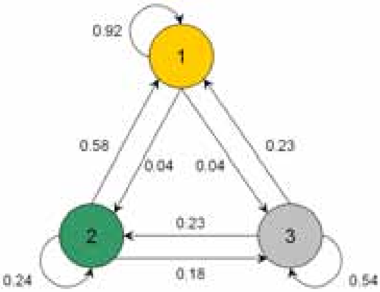


Comments

Stochastic homogenization without the asymptotics:

- Information from specific subscale (one at which instabilities initiate) is packaged into parameters for a model at a specific coarse scale (one where QoI is relevant).
- Subscale can be identified with scale at which damage must be detected.
- Coarse scale can be identified with scale at which system measurements (prognostic measurements) are made.
- Random matrices for inelastic material behavior are also completed.

Random Conservation Law or Stochastic Matrix



MaxEnt with Following Constraints:

1. $q_1(\omega) + \cdots q_n(\omega) = 1 \qquad a.s.$
2. $\mathbb{E}\ q = (\hat{q})_{ML}$
3. $\mathbb{E}(q_j - \bar{q}_j) = s^2_{q_j\,ML}$

Random Conservation Law or Stochastic Matrix

Optimization Problem

$$f_q^* = \arg\max_{f_q} \quad -\int_V f_q(q_1, \cdots, q_n) \ln f_q(q_1, \cdots, q_n) dV$$

$$\begin{aligned}
\text{s.t.} \quad \int_V f_q(q_1, \cdots, q_n) dV &= 1 \\
\int_V q_i f_q(q_1, \cdots, q_n) dV &= \bar{q}_i \qquad i = 1, \cdots, n \\
\int_V (q_i - \bar{q}_i)^2 f_q(q_1, \cdots, q_n) dV &= \sigma_{q_i}^2 \qquad i = 1, \cdots, n
\end{aligned}$$

where the domain V is characterized by

$$V = \left\{ [q_1, \cdots, q_n] \subset \mathbb{R}^n \mid \sum_{i=1}^{n} q_i = 1 \; ; \; q_i \geq 0, \; i = 1, \cdots, n \right\}$$

Random Conservation Law or Stochastic Matrix

Solution

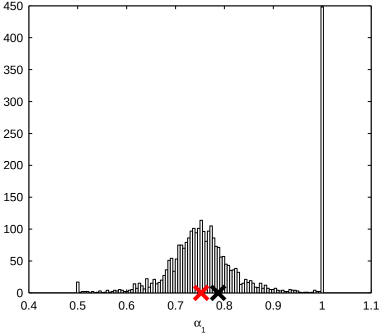
With only mean constraint:

$$f_q^*(q) = e^{(\mu-1)} \exp\left((\boldsymbol{\lambda}, q)\right) \mathbb{1}_V(q)$$

With mean and variance constraints:

$$f_q^*(q) = e^{(\mu-1)} \exp\left((\boldsymbol{\lambda}, q) + \sum_{i=1}^{n-1} \eta_i q_i^2\right) \mathbb{1}_V(q)$$

Example from Epidemiology



Uncertainty associated with optimal decisions are computed. Important for risk assessment.

Outline

A Cameron-Martin Theorem

Let $x(t)$ be a Brownian motion, and let:

- $\{\alpha_i(t)\}$ is a CONS in $L^2[0,1]$
- $\Phi_{m,p}(x) = H_m\left[\int_0^1 \alpha_p(t)dx(t)\right] \quad m = 1, 2, \cdots \;\; p = 0, 1, \cdots$
- $\Psi_{m_1 \cdots m_p}(x) = \Phi_{m_1,1}(x) \cdots \Phi_{m_p,p}(x)$

Then

$$\lim_{N \to \infty} \int_C^w \left| F[x] - \sum_{m_1,\cdots,m_N}^{N} A_{m_1,\cdots,m_N} \Psi_{m_1 \cdots m_N}(x) \right|^2 d_w x = 0$$

The polynomial chaos decomposition of any square-integrable functional of the Brownian motion converges in mean-square as N goes to infinity.

For a finite-dimensional representation, the coefficients are functions of the missing dimensions. That is, the coefficients are themselves random variables dependent on the dimensions excluded from the representation.

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Polynomial Chaos

$$\alpha(x,\theta) = \sum_{i=0}^{\infty} \alpha_i(x)\ \Psi_i(\boldsymbol{\xi}(\theta))$$

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Note

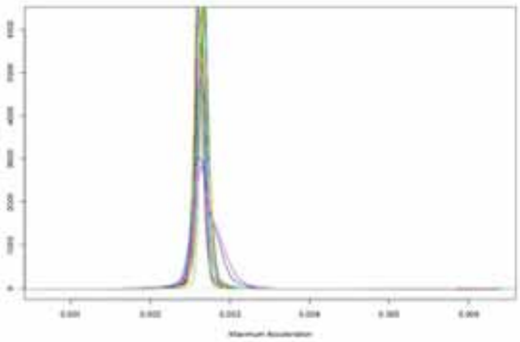
- Must estimate α_i constrained by information:
  - experimental constraints (known only through distributions):
    -$\boldsymbol{\xi}$ captures endogenous sources of uncertainty.
  - physics constraints (deterministic maps):
    -α depends on $\boldsymbol{\xi}$ through a conservation law that must be honored.
- Dimension of $\boldsymbol{\xi}$ reflects complexity of the process α.
- Probability measure of $\boldsymbol{\xi}$ determines the geometry in which analysis and approximation are carried out.

Uncertainty on Uncertainty

$$\alpha(x,\theta) = \sum_{i=0}^{\infty} \alpha_i(x)\Psi_i(\xi(\theta))$$

Coefficients are uncertain

$$\alpha_i = \sum_j \alpha_{ij}\Psi_j(\eta_i)$$



$$\alpha(x,\theta) = f(x, \underbrace{\xi_1, \cdots, \xi_n}_{\text{Aleatoric Uncertainty}}, \underbrace{\xi_{n+1}, \cdots, \xi_m}_{\text{Model/Data Uncertainty}})$$

$$= \sum_i \alpha_i(x) \Psi_i(\boldsymbol{\xi})$$

Characterization of Chaos Expansions of Model Output

Given a model:

$$\mathcal{M}_{\boldsymbol{\xi}} u = 0$$

We want:

$$u(\boldsymbol{\xi}) = \sum_i (u, \psi_i)_{L^2(\Omega)} \psi_i(\boldsymbol{\xi})$$

If $\boldsymbol{\xi}$ are independent and have density functions:

$$u_i = \int_{\Gamma_1} \cdots \int_{\Gamma_d} u(\boldsymbol{\xi}) \psi_i(\boldsymbol{\xi}) f_1(\xi_1) \cdots f_d(\xi_d) d\xi_1 \cdots d\xi_d$$

Challenge

Curse of Dimensionality

- Dimensionality of problem is controlled by the dimension of input parameters ξ.
- We typically seek L_2 convergence in space-time-stochastic measures: solution is spatio-temporal stochastic process.

BUT:

- Often the quantities of interest are scalar random variables.

THEN:

- We discover one-dimensional representations adapted to the QoI.

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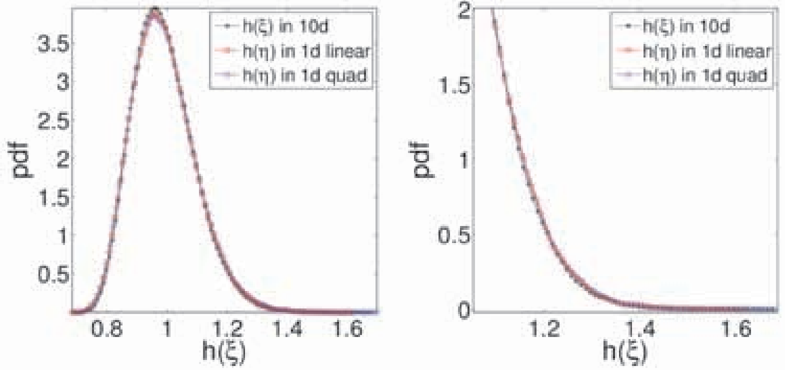
Example 1: Algebraic Model with Random Coefficients

Linear springs in series

$$h(\xi_1, \cdots, \xi_d) = \frac{d}{1+b} \quad \frac{\displaystyle\prod_{i=1}^{d}(1 + a_i\xi_i + b_i\xi_i^2)}{\displaystyle\sum_{j=1}^{d}\prod_{\substack{i=1 \\ i\neq j}}^{d}(1 + a_i\xi_i + b_i\xi_i^2)}$$

$$E\{\xi_i\xi_j\} = e^{|i-j|/l}$$



h(ξ) in 10d
h(η) in 1d linear
h(η) in 1d quad
pdf
3.5
3
2.5
2
1.5
1
0.5
0.8
1
1.2
1.4
1.6
h(ξ)
h(ξ) in 10d
h(η) in 1d linear
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1.5
1
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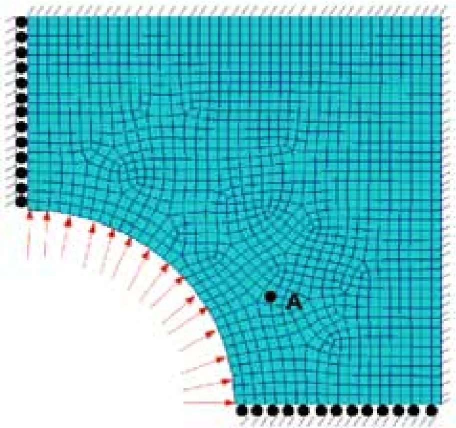
h(ξ)

Example 2: PDE with Random Coefficients

Plane Stress Problem

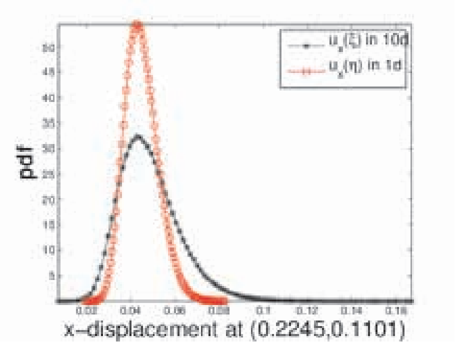


Stochastic Characterization

$C(x_1, x_2) = 0.25e^{-\frac{x_1 - x_2}{l_c}}$
$\mu = 0.25$
$\bar{E} = 1MPa$
$l_c = 0.25$
100 terms retained in KL expansion.

Plane Stress

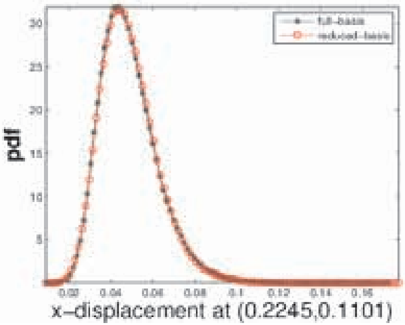
1D Approximation using Best KL component of solution

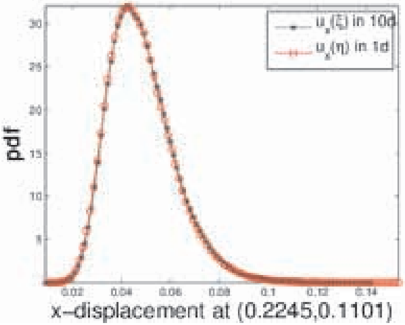


PDF of displacement at one point of the domain.

Plane Stress

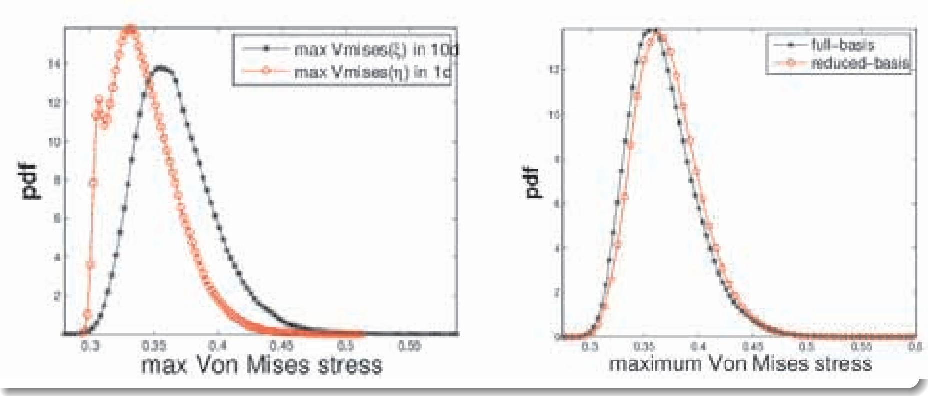
PDF of Displacement for Isometry A using linear and quadratic content





Plane Stress

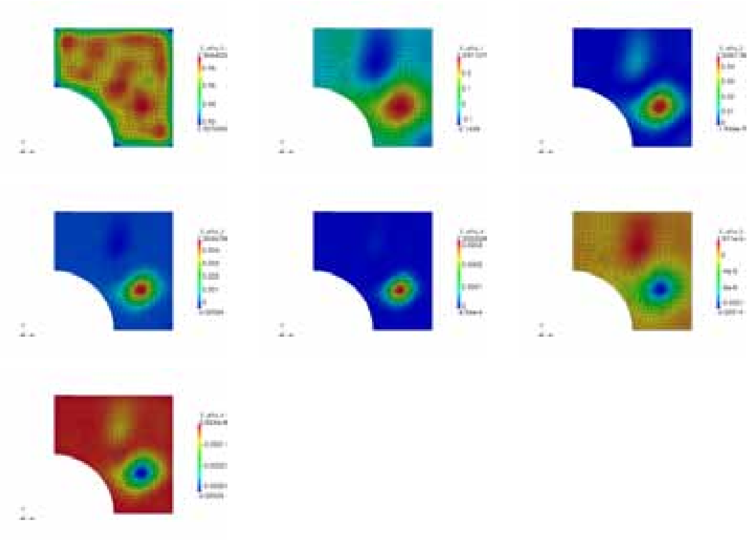
PDF for maximum von Mises Stress over the domain for Isometry A using linear and quadratic content



Observation:

If material properties in original problem are introduced in a particular reduced form ($\{k_\alpha^A\}$) then solution of original problem will be identical to the adapted solution:

Adapted Material Coordinates with Gaussian Adaptation



Outline

Concluding Remarks

Integration

UQ is paramount for the rational fusion of disparate streams of information.

Validation

UQ is paramount for assessing the credibility of model-based decisions.

Model Building

UQ can use statistical dependence to drive scientific discovery and enhance predictive models.