Practical methods for characterizing solutions of stochastic equations

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- **Generalities:**
  - *Examples of stochastic problems*
  - *Discretization of probability space*

- **Surrogate models for solutions of stochastic equations (SEs)**
  - *Stochastic reduced order models (SROMs)*
  - *Surrogates for solutions of SEs*
  - *Examples:* Stochastic transport equation & Random eigenvalue problems

- **Extremes of solutions of SEs:**
  - *Matrix-valued random fields*
  - *Solution by the extreme value theory (EVT)*

GENERALITIES

- **Engineering/financial problems:**

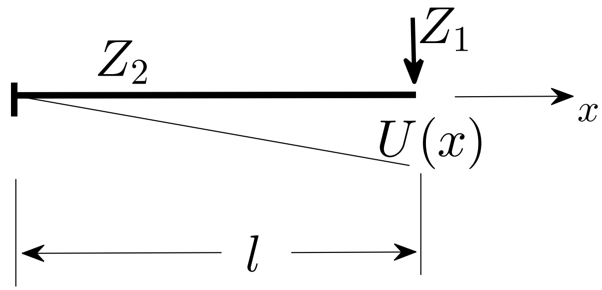
$$\boxed{\textbf{INPUT} \Longrightarrow \textbf{SYSTEM} \Longrightarrow \textbf{OUTPUT}}$$

(random) (stoch.eqs) (?)

- **Formulation of stochastic problems:**
  - *Construct* probabilistic models for input/system
  - *Calibrate* these models to the available information
    - Observable parameters (classical statistical methods)
    - Unobservable parameters (solutions of inverse problems)

- **Output characterization:**
  - *Monte Carlo simulation method:* general, computationally demanding
  - *Popular methods:* Stochastic Galerkin and collocation
  - *SROM-based method*

- **Example 1:**



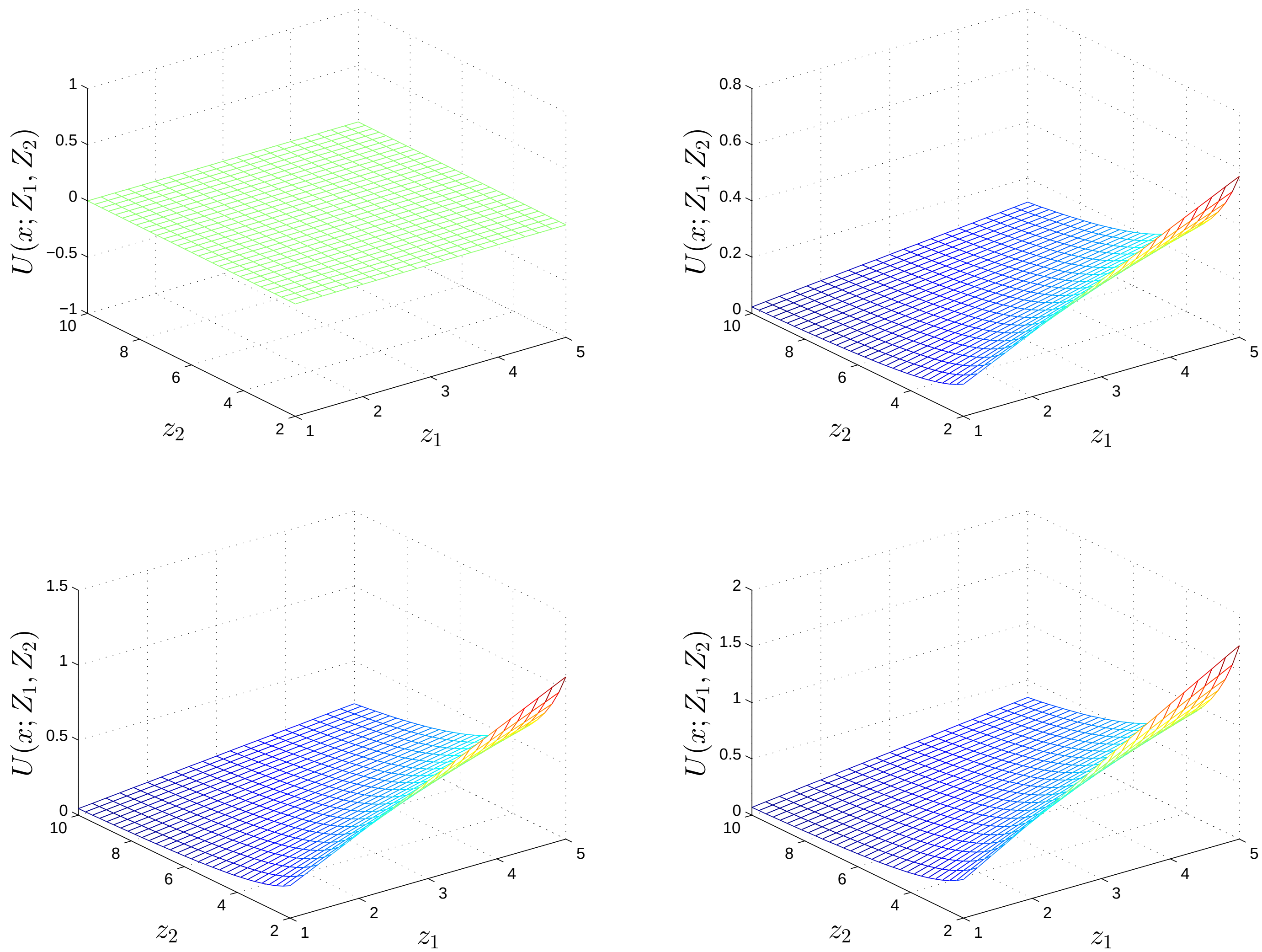
  - *Input:* $Z = (Z_1, Z_2)$ = a two-dimensional random vector

  - *System (defining equation):* $U''(x) = -Z_1\,(l - x)/Z_2, \quad 0 < x < l$
    $\Longrightarrow$ *stochastic equation (SE)*, i.e., equation with random entries

  - *Output/Solution:* $U(x) = (Z_1/Z_2)\left(l\,x^2/2 - x^3/6\right)$

  - *Note:*
    (1) Stochastic dimension of this problem is 2
    (2) $U(x)$ = *parametric random function*, i.e., deterministic function of $x \in (0, l)$ that depends on 2 RVs (stochastic dimension = 2)
    (3) Statistics of $U(x)$ can be obtained simply and efficiently by MC

(4) Solution $U(x) = U(x; Z_1, Z_2) =$ *a response surface over* (Z_1, Z_2) for each $x \in [0, l]$
($x = 0.0$, 0.5, 0.7, and 0.9: top left, top right, bottom left, and bottom right)



- **Example 2:** Suppose stiffness Z_2 varies randomly along the beam, i.e.,
  $Z_2 \mapsto$ random function $Z_2(x)$

  – *Input:* Z_1 = a random variable and $Z_2(x)$ = a random function
  Note: Stiffness $\sim$ infinite family of RVs $\{Z_2(x)\}$ indexed by $x \in (0, l)$

  – *System (defining equation):* $U''(x) = -Z_1\,(l - x)/Z_2(x), \quad 0 < x < l$
  $\Longrightarrow$ *infinite stochastic dimension*

  – *Output/Solution:* $U(x) = -Z_1 \int_0^x \left[\int_0^z \big((l - y)/Z_2(y)\big)\, dy\right] dz, \quad 0 < x < l$

  – *Statistics of $U(x)$:*

    - Generate samples Z_1 of $Z_2(x)$
    - Calculate corresponding samples of $U(x)$
    - Estimate properties of $U(x)$ from its samples

  – *Note:*

    - Samples of $U(x) \sim$ double integrals
    - Monte Carlo method is less attractive even for this very simple stochastic problem

- **General formulation:**

$$\boxed{\mathcal{L}[U(x,t)] = Y(x,t), \quad x \in D \subset \mathbb{R}^d, \quad t \in [0,\tau]} \quad \text{(with appropriate B/ICs)}$$

$\mathcal{L}$ = algebraic, differential, ... operator with random entries

$Y(x,t)$ = random input

- **Example of SPDE:** $\boxed{\nabla \cdot \big(A(x)\,\nabla U(x)\big) = B(x), \quad x \in D \subset \mathbb{R}^d}$ (+ BCs)

  $A(x), B(x)$ = random fields defined on a probability space $(\Omega, \mathcal{F}, P)$

- **Comments:**
  - If mapping $A, B \mapsto U$ is measurable $\Longrightarrow$ *U is a random field* on $(\Omega, \mathcal{F}, P)$
  - Random fields $A(x), B(x)$ = uncountable families of real-valued random variables indexed by $x \in D \Longrightarrow$ *infinite stochastic dimension*
  - We can view SPDEs as PDEs defined on (physical space)$\times$ (probability space), i.e., *the product space* $(D \times \Omega, \mathcal{B}(D) \times \mathcal{F}, \lambda \times P)$

- **Conditions that $A(x); B(x)$ must satisfy:**
  - *Mathematical conditions:* Solution existence/uniqueness (Babuška, I. M. et.al., SIAM Journal of Numerical Analysis, 2004)
  - *Physical conditions:* e.g., samples of $A(x)$ must be, e.g., realistic microstructures

- **For calculations, we need to discretize**
  - *Physical space* (FEM)
  - *Probability space* $\leftarrow$

- **Discretization of probability space:**
  - *Construct a parametric model $A_d(x, Z)$ for $A(x)$*, i.e., a deterministic function of $x \in D$ that depends on a random vector $Z = (Z_1, \ldots, Z_d)$
    $\Longrightarrow$ *finite stochastic dimension* (equal to d), e.g.,

    $$\boxed{A_d(x, Z) = \sum_{i=1}^{d} Z_i \, \varphi_i(x), \quad x \in D}$$

    ($\{\varphi_i\}$ = specified deterministic functions)
  - *KL parametric models:*
    - Can only match the first two moments of $A(x)$ (unless Gaussian)
    - Provides no information on sample properties
  - *Sample parametric models:*
    - Same functional form as KL parametric model
    - Matches target sample properties (essential if interested in output extremes)

- **Construction of sample parametric models:**
  - *Generate independent samples* $A(x,\omega)$ of $A(x)$
  - *Select a basis* $\{\psi_i(x)\}$ and set $A_d(x,Z) = \sum_{i=1}^{d} Z_i\,\psi_i(x)$
  - *Calculate corresponding samples* of $\{Z_i\}$ by minimizing the distance

$$d\big(A(x,\omega), A_d(x, Z(\omega))\big) = \sup_{x \in D} \left| A(x,\omega) - \sum_{i=1}^{d} Z_i(\omega)\,\psi_i(x) \right|,$$

  - *Store* $\{Z_i(\omega)\}$ and construct samples of $A_d(x,Z)$

- **Example:**
  - *Beta translation field:* $\boxed{A(x) = a + (b-a)\,F^{-1}_{\mathrm{Beta}(p,q)} \circ \Phi\big(G(x)\big), \quad x \in D = (0,l_1) \times (0,l_2)}$

where $a = 3$, $b = 20$, $p = 2$, $q = 6$, $l_1 = 20$, $l_2 = 10$, $\rho = 0.7$, and
$G(x)$ = homogeneous Gaussian field with $E[G(x)] = 0$ and spectral density

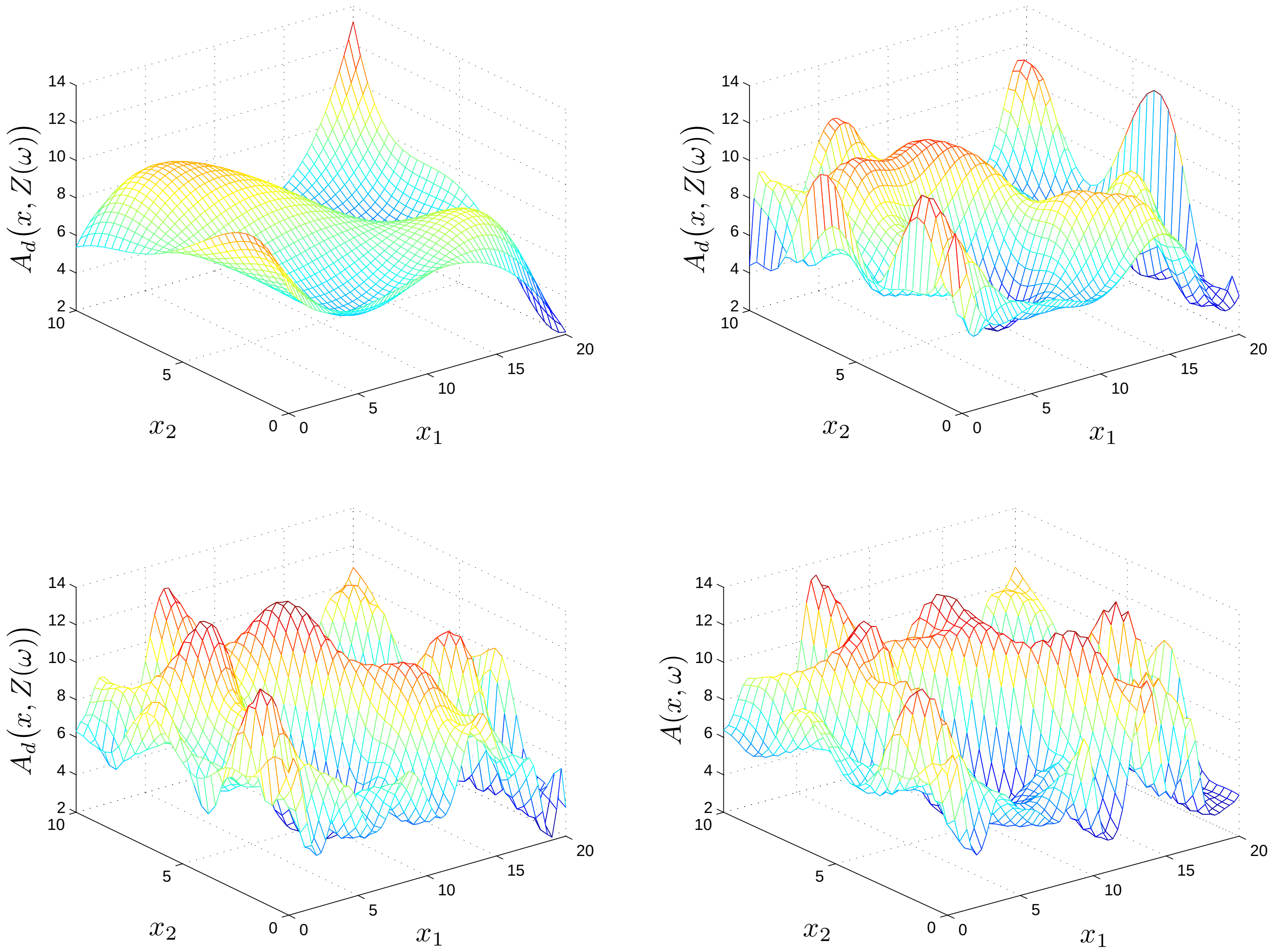
$$s(\lambda) = \frac{1}{2\,\pi\,\sqrt{1-\rho^2}} \exp\left(- \frac{\lambda_1^2 - 2\,\rho\,\lambda_1\,\lambda_2 + \lambda_2^2}{2\,(1-\rho^2)} \right), \quad \lambda \in \mathbb{R}^2, \quad |\rho| < 1.$$

  - *Parametric model for* $A(x)$*:*

$\boxed{A_d(x,Z) = \sum_{i=1}^{d} Z_i\,\psi_i(x)}$ ($\{\psi_i\}$ = product of Chebyshev polynomials in x_1 and x_2)

– *Samples of $A_d(x, Z)$ and $A(x)$:*

Samples of $A_d(x, Z)$ with $d = 25$ (left top panel), $d = 100$ (right top panel), and $d = 225$ (left bottom panel) and target sample of $A(x)$



SURROGATE MODELS

- **Objective:** *Construct surrogate models* $\tilde{U}_L(x, Z)$ for solutions $U(x, Z)$ of SPDEs, i.e., accurate + efficient approximations of $U(x, Z)$

- **Ingredients of $\tilde{U}_L(x, Z)$:**
  - *Stochastic reduce order models (SROMs)* $\tilde{Z}$ with samples $\{\tilde{z}_k\}$ for Z
  - *Deterministic solutions* of SPDEs for $\{Z = \tilde{z}_k\}$ and gradients of these solutions

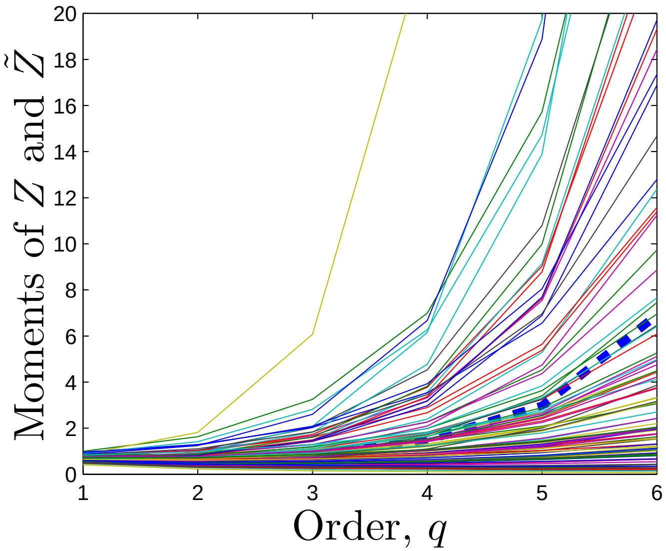
- **SROM $\tilde{Z}$ for Z:** a random vector defined on the probability space of Z such that
  - Dimension$(\tilde{Z})$ = Dimension(Z);
  - $\tilde{Z}$ has a finite number of samples $\{\tilde{z}_k\}$, $k = 1, \ldots, m$; and
  - PL$(\tilde{Z}) \sim$ PL(Z)

- **Algorithm for constructing $\tilde{Z}$:**
  - *Select m samples of Z at random* and partition the range $\Gamma = Z(\Omega)$ of Z in Voronoi cells $\{\Gamma_k\}$ centered on $\{\tilde{z}_k\}$, where $\Gamma_k = \{z \in \Gamma : \ \|z - \tilde{z}_k\| \leq \|z - \tilde{z}_l\|, l \neq k\}$
  - *Calculate the discrepancy* between PL$(\tilde{Z})$ and PL(Z) (Note: $\{\tilde{z}_k\}$ and $\{P(Z \in \Gamma_k)\}$ define the law of $\tilde{Z}$)
  - *Repeat previous steps to select the optimal pair* $\{\tilde{z}_k, \Gamma_k\}$, i.e., the pair that minimizes the discrepancy between PL$(\tilde{Z})$ and PL(Z)

- **Example of SROM:** $Z \sim \text{Gamma}(2,3)$:
  - *Discrepancy between* $\text{PL}(\tilde{Z})$ *and* $\text{PL}(Z)$ can be measured by, e.g.,

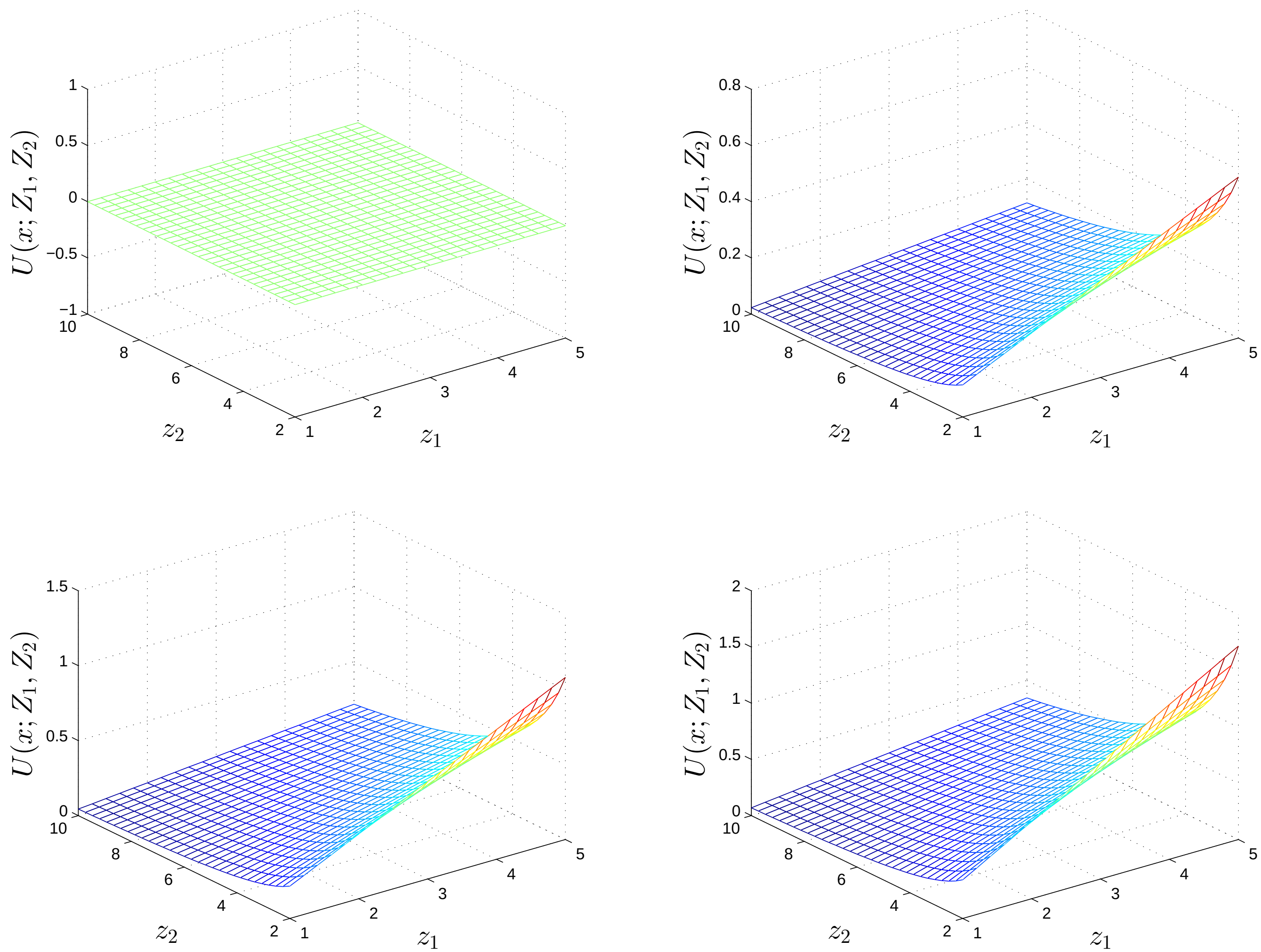
$$\sum_{r=1}^{\bar{r}} \left(E[Z^r] - E[\tilde{Z}^r]\right)^2 + \int \left(F(\alpha) - \tilde{F}(\alpha)\right)^2 d\alpha$$

  - *First 6 moments of Z* by an SROM $\tilde{Z}$ with $m = 20$ (dash heavy line) and by MC corresponding to 100 sets of 20 samples (thin solid lines)



- **Note:**
  - SROM moments $\simeq$ exact moments
  - MC moments exhibit significant sample-to-sample variation and can be inaccurate

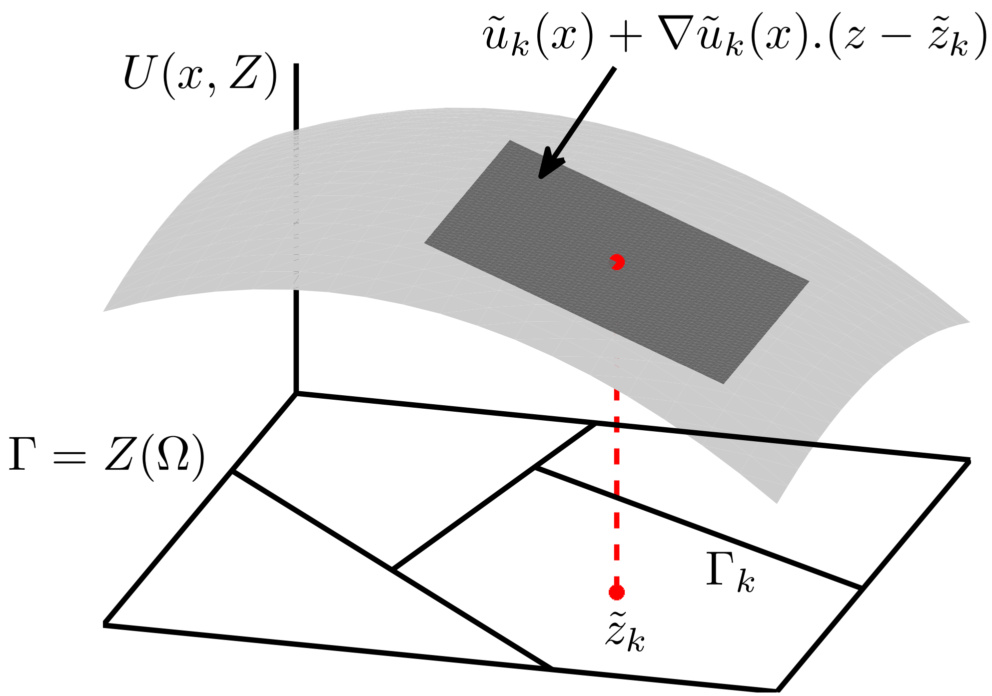
- **Surrogate model** for the *mapping* $x \mapsto U(x, Z)$ defined by the first example of SE
  Recall the response surfaces for the displacement $U(x; Z_1, Z_2)$ of a stochastic beam ($x = 0.0$, 0.5, 0.7, and 0.9: top left, top right, bottom left, and bottom right)



• **Surrogate model** for a *mapping* $x \mapsto U(x,Z)$ defined by an arbitrary SE:

$$\boxed{\tilde{U}_L(x,Z) = \sum_{k=1}^{m} 1\big(Z \in \Gamma_k\big) \left[\tilde{u}_k(x) + \nabla \tilde{u}_k(x) \cdot (Z - \tilde{z}_k)\right]}$$

$$\tilde{u}_k(x) = U(x, \tilde{z}_k)$$
$$\nabla \tilde{u}_k(x) = \big(\partial U(x,Z)/\partial z_1, \dots, \partial U(x,Z)/\partial z_d\big) \text{ for } Z = \tilde{z}_k$$



• **Note:** *Samples of* $\tilde{U}_L(x,Z)$ result from samples of Z by elementary calculations

Example 1: Stochastic transport equation

- **Problem definition:** $\boxed{\nabla \cdot (A(x)\, \nabla U(x)) = 0}$

  $x \in D \subset \mathbb{R}^2$, $D = (0, l_1) \times (0, l_2)$

  $U(0, x_2) = 0$, $U(l_1, x_2) = 1$, $\partial U(x_1, 0)/\partial x_2 = \partial U(x_1, l_2)/\partial x_2 = 0$

  – *Beta conductivity field:* $\boxed{A(x) = \alpha + (\beta - \alpha)\, F^{-1}_{\mathrm{Beta}(p,q)} \circ \Phi\big(G(x)\big)}$

  $G(x) =$ homogeneous Gaussian field with mean 0, variance 1, and spectral density given in a previous slide

  – *Parametric model:* $\boxed{A(x) \simeq A_d(x, Z) = \sum_{i=1}^{d} Z_i\, \psi_i(x), \quad x \in D}$

  ($\{\psi_i(x)\}$ = Chebyshev polynomials)

  $\Longrightarrow U(x) \simeq U(x, Z)$ is a parametric random field with stochastic dimension d

  – *Surrogate model:* $\boxed{U_L(x, Z) = \sum_{k=1}^{m} 1(Z \in \Gamma_k)\, \big[\tilde{u}_k(x) + \nabla \tilde{u}_k(x) \cdot (Z - \tilde{z}_k)\big]}$

  (piecewise linear approximation of $U(x, Z)$)

  – *Numerical results for:* $l_1 = 20$, $l_2 = 10$, $a = 3$, $b = 20$, $p = 2$, $q = 6$, $\rho = 0.7$, and stochastic dimension $d = 200$

- **Implementation of surrogate models:**

  – *SPDE with* $Z = \tilde{z}_k \Longrightarrow \tilde{u}_k(x)$, $k = 1, \ldots, m$

  – *Gradient equations:* $\partial(\mathrm{SPDE})/\partial \mathrm{Z_r}$, $r = 1, \ldots, d$

$$\nabla \cdot (A_d(x, Z)\, \nabla V_r(x, Z)) = -\nabla \cdot \left(\frac{A_d(x, Z)}{\partial Z_r} \nabla U(x, Z) \right) \quad \text{for } Z = \tilde{z}_k,$$

  where $V_r(x, Z) = \partial U(x, Z)/\partial Z_r$

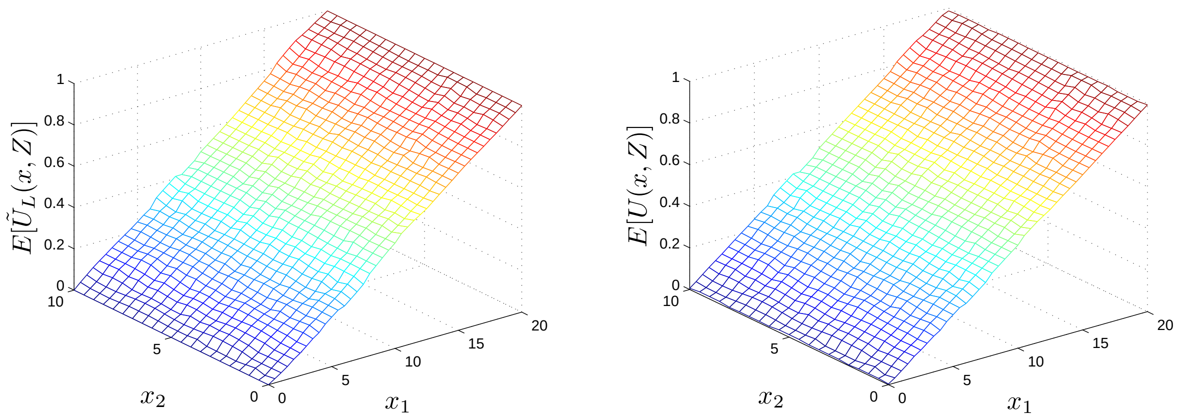
- **Calls of deterministic solver:**
  $(m + 1)\, d = 4020$ *calls for* $d = 200$ *and* $m = 20$
  $\Longrightarrow$ Impractical for large stochastic dimensions

- **Alternative surrogate model $U_L^*(x, Z)$:**

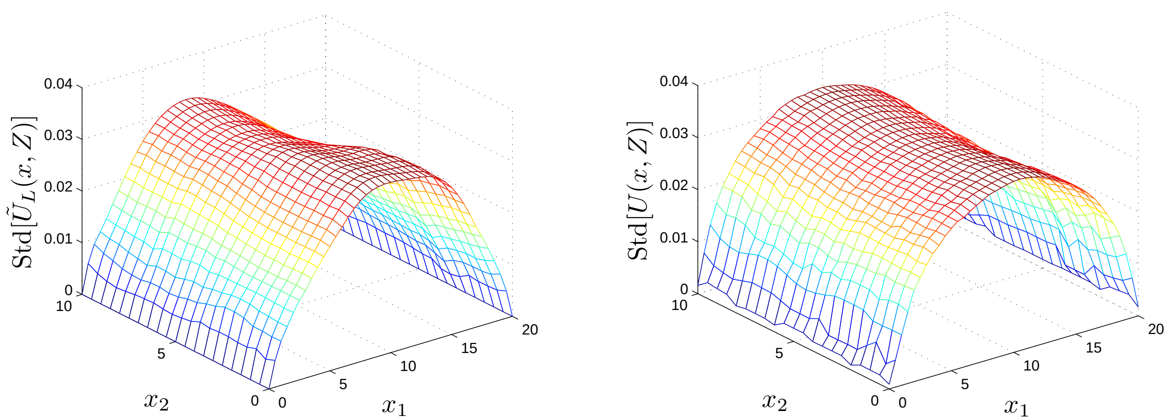
  – *Main idea:* Approximate Z by its projection on the subspace spanned by the dominant eigenvectors of its covariance matrix

  – *Calls of deterministic solvers:*
  $(m + 1)\, d^* = 120$ for $d^* = 5$ and $m = 20$, where $d^* = \#\{\text{retained eigenvectors}\}$

- **Solution statistics:**
  - *Note:* Statistics of $U_L^*(x, Z) \simeq$ Statistics of $U_L(x, Z)$, e.g.,
  - *Estimates of* $E[U(x, Z)]$ by $\tilde{U}_L(x, Z); \tilde{U}_L^*(x, Z)$ (left panel) and MC (right panel)



  - *Estimates of* $\mathrm{Std}[U(x, Z)]$ by $\tilde{U}_L(x, Z); \tilde{U}_L^*(x, Z)$ (left panel) and MC (right panel)



- **Estimation of unobservable parameters:**

  – *Assume the law of $A(x)$ is known up to a parameter λ*, which

    - Cannot be measured and
    - Enter the definition of a global property that can be measured, e.g., the specimen apparent conductivity $A_{\mathrm{app}}(D) = (1/l_2) \int_D A(x)\,[\partial U(x,Z)/\partial x_1]\,dx$

  – *Solution in the Bayesian framework:*

    - View λ as a random variable Λ with prior density $f'(\lambda)$
    - Construct surrogates $\tilde{U}_{L,\lambda}(x,Z)$ for $U(x,Z) \mid (\Lambda = \lambda)$, generate samples of $\tilde{U}_{L,\lambda}(x,Z)$, and calculate corresponding samples of the conditional apparent conductivity $A_{\mathrm{app}}(D) \mid (\Lambda = \lambda)$
    - Construct approximations for the density $f(\cdot \mid \lambda)$ of $A_{\mathrm{app}}(D) \mid (\Lambda = \lambda)$ by using samples of this conditional random variable
    - Construct the likelihood function $\ell(\lambda \mid \mathrm{data}) = \prod_i f(a_{\mathrm{app},i}(D) \mid \lambda)$ of λ from actual measurements $\{a_{\mathrm{app},i}(D)\}$ of $A_{\mathrm{app}}(D)$ and the densities $f(\cdot \mid \lambda)$
    - Quantify the information on λ by the posterior density $f''(\lambda) \propto f'(\lambda)\,\ell(\lambda \mid \mathrm{data})$

  – *Surrogates are efficient tools for solving this inverse problem*, i.e., finding $f''(\lambda)$

Example 2: Random eigenvalue problem

- **Problem definition:** Find eigenvalues/eigenvectors of $A = A(Z) \sim$ square matrix, where $Z = d$-dimensional random vector

  – *Surrogate model for the eigenvalues $\Lambda_i(Z)$ of $A(Z)$*

$$\tilde{\Lambda}_i(Z) = \sum_{k=1}^{m} 1(Z \in \Gamma_k) \left[\tilde{\lambda}_{i,k} + \sum_{r=1}^{d} \tilde{\lambda}_{i,k}^{(r)} (Z_r - \tilde{z}_{k,r}) \right]$$

  – *Ingredients of $\tilde{\Lambda}_i(Z)$:* $\tilde{\lambda}_{i,k} = \Lambda_i(Z)$ and $\tilde{\lambda}_{i,k}^{(r)} = \partial \Lambda_i(Z)/\partial Z_r$ for $Z = \tilde{z}_k$ (obtained by deterministic calculations)

  – *Calculation of $\tilde{\lambda}_{i,k}^{(r)}$:* Differentiate $\det(A - \Lambda\, I) = \Lambda^n + C_1\, \Lambda^{n-1} + \cdots + C_{n-1}\, \Lambda + C_n = 0$ wrt the components $\{Z_r\}$ of Z

$$n\, \Lambda^{n-1} \frac{\partial \Lambda}{\partial Z_r} + \frac{\partial C_1}{\partial Z_r} \Lambda^{n-1} + (n-1)\, C_1\, \Lambda^{n-2} \frac{\partial \Lambda}{\partial Z_r} + \cdots + \frac{\partial C_{n-1}}{\partial Z_r} \Lambda + C_{n-1} \frac{\partial \Lambda}{\partial Z_r} + \frac{\partial C_n}{\partial Z_r} = 0$$

$$\Longrightarrow \lambda_{i,k}^{(r)} = \frac{\partial \Lambda_i(Z)}{\partial Z_r}\, |_{Z=\tilde{z}_k} = -\frac{c_{1,k}^{(r)}\, \lambda_{i,k}^{n-1} + \cdots + c_{n-1,k}^{(r)}\, \lambda_{i,k} + c_{n,k}^{(r)}}{n\, \lambda_{i,k}^{n-1} + (n-1)\, c_{1,k}\, \lambda_{i,k}^{n-2} + \cdots + c_{n-1,k}},$$

  where $c_{i,k}^{(r)} = \partial C_i(Z)/\partial Z_r$ at $Z = \tilde{z}_k$

- **Example:**

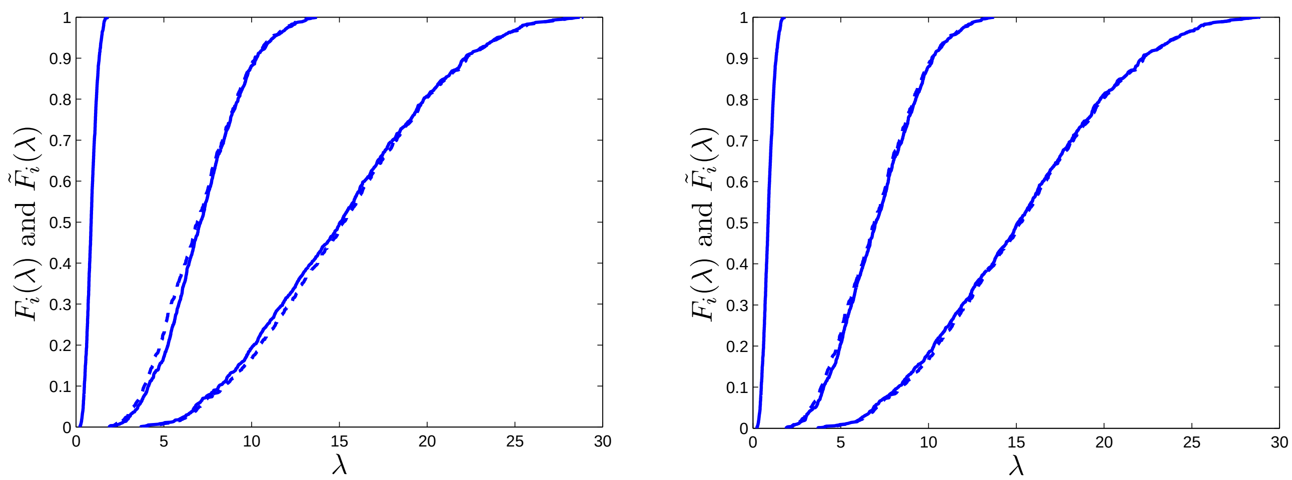
  - *Random matrix:*

$$A(Z) = \begin{bmatrix} Z_1 + Z_2 & -Z_2 & 0 \\ -Z_2 & Z_2 + Z_3 & -Z_3 \\ 0 & -Z_3 & Z_3 \end{bmatrix},$$

  with $Z_i = F^{-1} \circ \Phi(G_i)$, F = Beta cdf with range $[1, 10]$ and shape parameters $(p = 2, q = 3)$, $G_i \sim N(0, 1)$, $E[G_i\, G_j] = \rho^{|i-j|}$, $i, j = 1, 2, 3$, and $\rho = 0.7$

  - *Note:* $Z = (Z_1, Z_2, Z_3)$ = a 3-dimensional Beta vector

  - *Distributions $\{F_i(\lambda)\}$ of $\{\Lambda_i(Z)\}$* by surrogate models based on SROMs with $m = 5$ (left panel) and $m = 10$ (right panel) (Dash lines $\sim$ MC estimates based on 1000 samples)



– *Surrogate model for eigenvectors:*

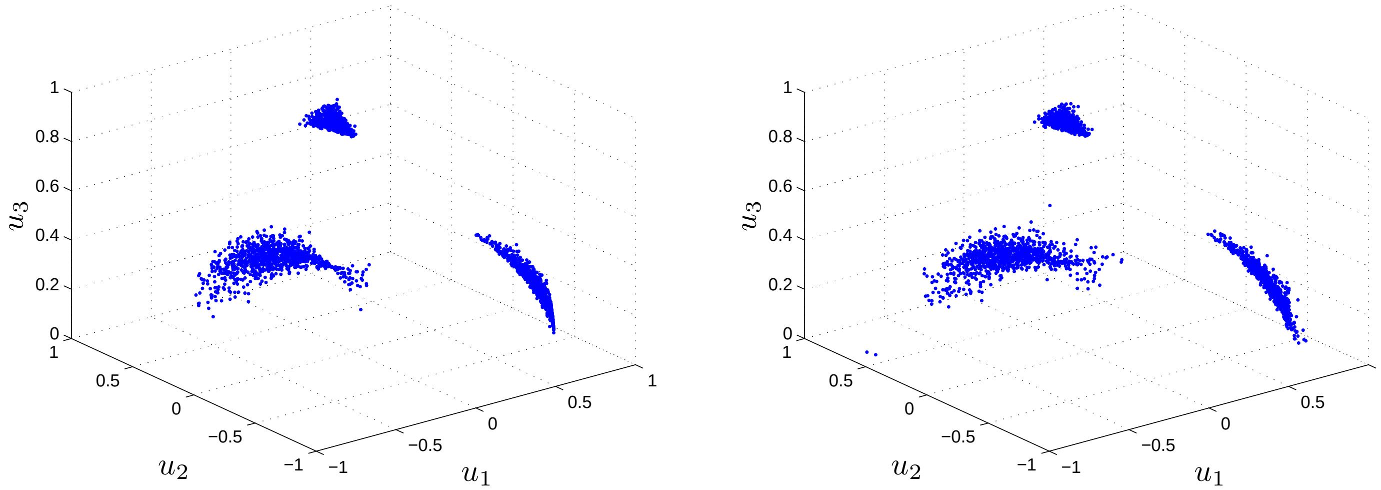
$$\tilde{U}_i(Z) = \sum_{k=1}^{m} 1\big(Z \in \Gamma_k\big) \left[\tilde{u}_{i,k} + \sum_{r=1}^{d} \tilde{u}_{i,k}^{(r)} \left(Z_r - \tilde{z}_{k,r}\right)\right],$$

– *Ingredients:* $\{\tilde{u}_{i,k} = U_i(\tilde{z}_k)\}$ = eigenvectors of $A(\tilde{z}_k)$ and $\{\tilde{u}_{i,k}^{(r)} = \partial U_i(Z)/\partial Z_r \mid_{Z=\tilde{z}_k}\}$

– *Note:* Gradients $\{\tilde{u}_{i,k}^{(r)}\}$ cannot be obtained by differentiating $A\,U_i - \Lambda_i\,U_i = 0$

– *Property:* If matrices $\tilde{a}_k = A(\tilde{z}_k)$ have distinct eigenvalues, the gradients can be calculated from $\tilde{u}_{i,k}^{(r)} = \sum_{j=1}^{n} b_{ij}^{(r)}\,\tilde{u}_{j,k}$ with $b_{ij}^{(r)} = 0$ if $i = j$ and $b_{ij}^{(r)} = \tilde{v}'_{j,k}\left(\tilde{\lambda}_{i,k}^{(r)}\,I - \tilde{a}_k^{(r)}\right)\tilde{u}_{i,k}/\big(\tilde{\lambda}_{j,k} - \tilde{\lambda}_{i,k}\big)$ if $i \neq j$, where $\tilde{v}_{j,k} = V_j(\tilde{z}_k)$

– *1000 samples of $U_i(Z)$ and $\tilde{U}_i(Z)$ with $m = 20$:* (left and right panels)



– *Extensions to arbitrary random matrices:*
(M. Grigoriu, *Monte Carlo Methods & Applications*, 2014)

- *Asymmetric matrices*, i.e., $A(Z) \neq A(Z)^T$
$\Longrightarrow$ Construct surrogate models for both right & left eigenvectors of $A(Z)$ defined by

$$\begin{aligned} A(Z)\, U_i(Z) &= \Lambda_i\, U_i(Z) \quad \text{(right vectors)} \\ A(Z)^T\, V_i(Z) &= \Lambda_i\, V_i(Z) \quad \text{(left vectors)} \end{aligned}$$

- *Multiple eigenvalues*, e.g., $\Lambda_1(Z)$ has multiplicity $q \geq 1$
$\Longrightarrow$ Construct surrogate models for $U_1(Z)$ and the generalized eigenvectors $\{U_r(Z), r = 2, \ldots, q\}$ defined by

$$\begin{aligned} A(Z)\, U_1(Z) &= \Lambda_1(Z)\, U_1(Z) \\ A(Z)\, U_2(Z) &= \Lambda_1(Z)\, U_2(Z) + U_1(Z) \\ &\vdots \\ A(Z)\, U_q(Z) &= \Lambda_1(Z)\, U_q(Z) + U_{q-1}(Z) \end{aligned}$$

EXTREMES OF SOLUTIONS OF SEs

Objective: *Estimate the distribution of extreme stresses in an elastic system*

Stress/strain relation: $S(x), A(x), \Sigma(x) =$ *matrix-valued random fields*

$$S(x) = \begin{bmatrix} S_{11}(x) \\ S_{22}(x) \\ S_{12}(x) \end{bmatrix} = \begin{bmatrix} A_{11}(x) & A_{12}(x) & A_{13}(x) \\ A_{12}(x) & A_{22}(x) & A_{23}(x) \\ A_{13}(x) & A_{23}(x) & A_{33}(x) \end{bmatrix} \begin{bmatrix} \Sigma_{11}(x) \\ \Sigma_{22}(x) \\ \Sigma_{12}(x) \end{bmatrix} = A(x)\,\Sigma(x), \quad x \in D,$$

- **Model for the compliance tensor:** $\boxed{A(x) = R(x)\,\Lambda(x)\,R(x)'}$, $x \in D$,

$$\Lambda(x) = \begin{bmatrix} \Lambda_1(x) & 0 & 0 \\ 0 & \Lambda_2(x) & 0 \\ 0 & 0 & \Lambda_3(x) \end{bmatrix} \quad \text{and} \quad R(x) = R_1\big(\Theta_1(x)\big)\, R_2\big(\Theta_2(x)\big)\, R_3\big(\Theta_3(x)\big),$$

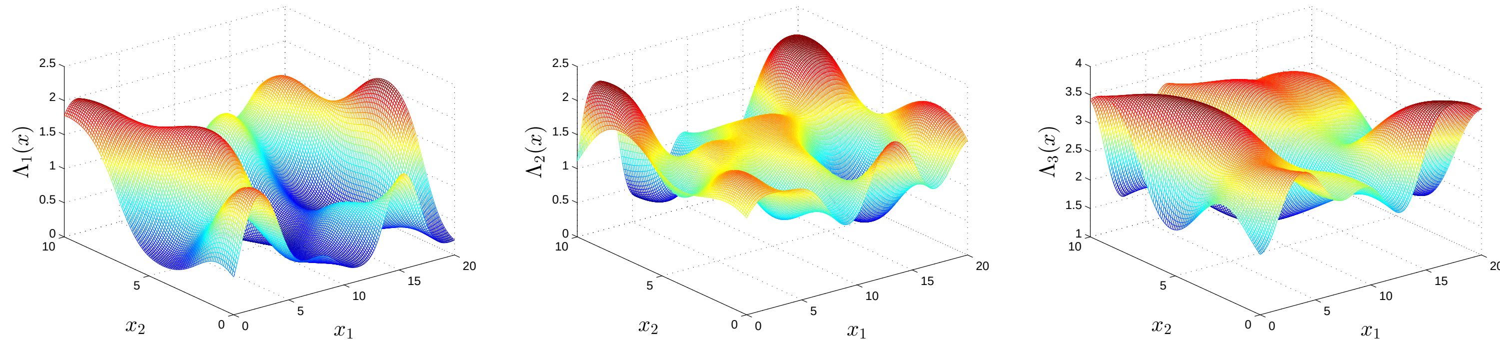
and

$$R_1(\theta_1) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\theta_1) & -\sin(\theta_1) \\ 0 & \sin(\theta_1) & \cos(\theta_1) \end{bmatrix}, \qquad R_2(\theta_2) = \begin{bmatrix} \cos(\theta_2) & 0 & \sin(\theta_2) \\ 0 & 1 & 0 \\ -\sin(\theta_2) & 0 & \cos(\theta_2) \end{bmatrix},$$

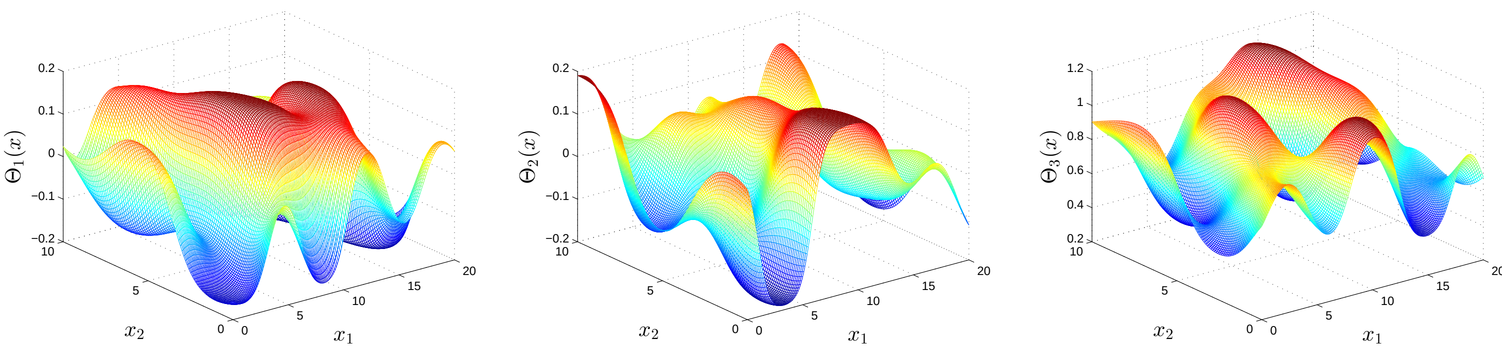
$$R_3(\theta_3) = \begin{bmatrix} \cos(\theta_3) & -\sin(\theta_3) & 0 \\ \sin(\theta_3) & \cos(\theta_3) & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \text{and} \qquad \Lambda = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix}.$$

- **Samples of eigenvalue and rotation fields:**

  - Samples of $\{\Lambda_k(x)\}$

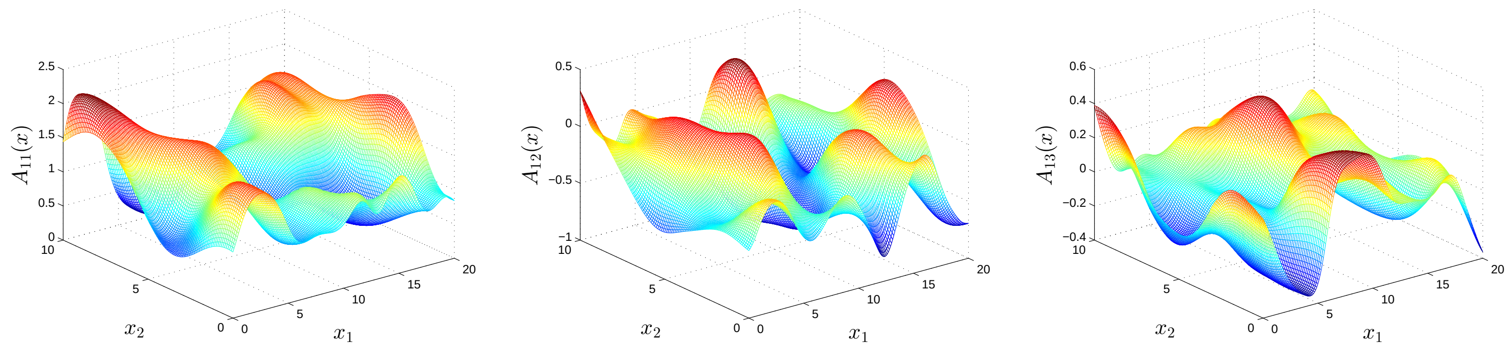


  - Samples of $\{\Theta_k(x)\}$

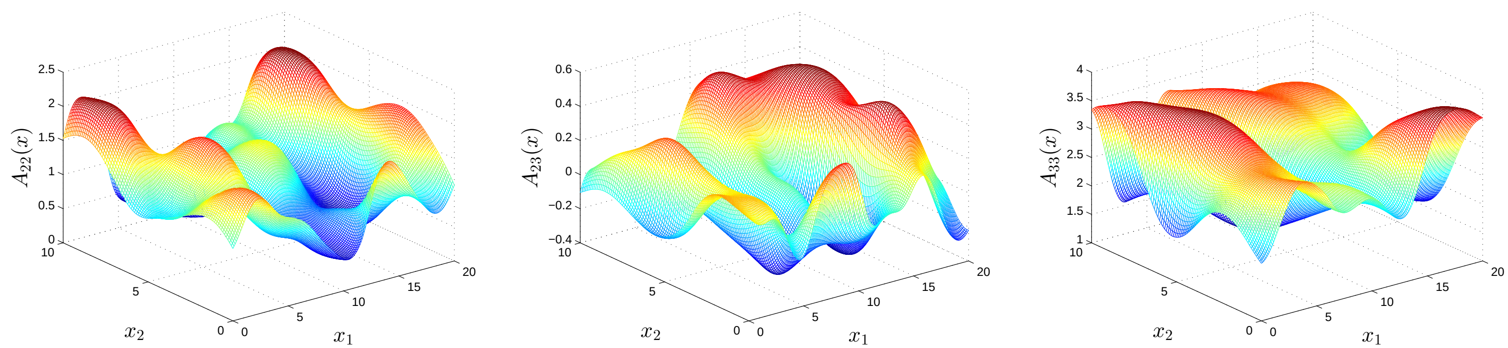


• Samples of compliances:

$A_{11}(x)$, $A_{12}(x)$, $A_{13}(x)$



$A_{22}(x)$, $A_{23}(x)$, $A_{33}(x)$



- **Objective:** *Estimate large strains/stresss* in random microstructures
- **Solution:** *Monte Carlo and extreme value theory* (EVT)
- **Why EVT:**
  - Maxima $M_n = \max(X_1, \ldots, X_n)$, $\{X_i\} \sim$ iid, follow generalized extreme value (GEV) distributions for a sufficiently large n under mild conditions, i.e.,

$$P(M_n \leq x) \simeq G(y) = \exp\left\{ - \left[1 + \xi \left(\frac{x - \mu}{\sigma}\right)\right]^{-1/\xi} \right\},$$

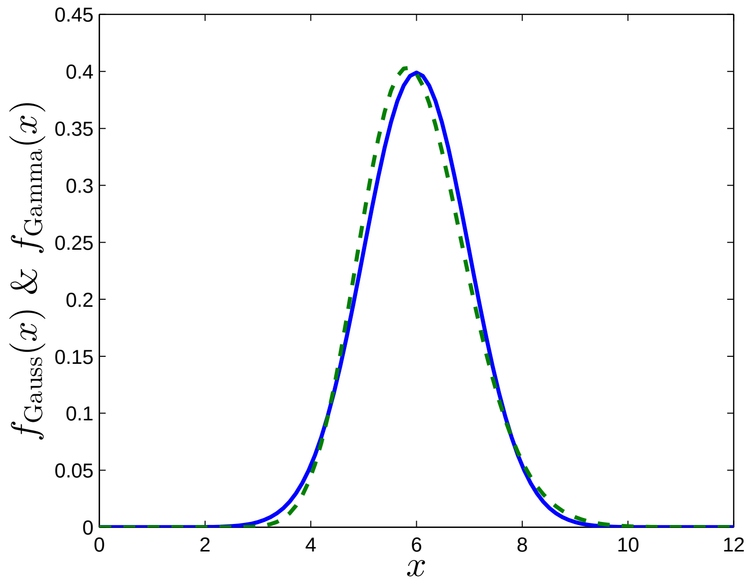
    with support $\{x : 1 + \xi\,(x - \mu)/\sigma > 0\}$ and location, scale, and shape parameters $\mu \in \mathbb{R}$, $\sigma > 0$, and $\xi \in \mathbb{R}$
  - To find $P(M_n \leq x)$, we need to estimate (μ, σ, ξ)
    (The functional form of $P(M_n \leq x)$ is known)

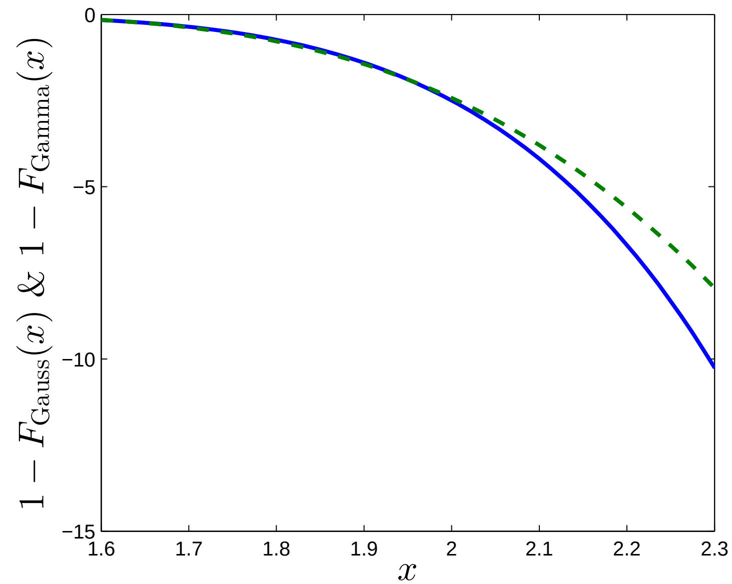
- **Why not direct calculations**, i.e., $P(M_n \leq x) = F(x)^n$, where $F =$ CDF of X_i
  - Potential numerical errors for $F(x) \sim 1$ and n large
  - Sensitivity of $P(M_n \leq x)$ to the tail of F

- **Example:**

  – *Data:* $\Longrightarrow \hat{\mu} = 0, \hat{\sigma} = 1, \hat{\gamma}_3 \in [0, 1/3], \hat{\gamma}_4 =?$

  – *Two distributions consistent with data:*
  Gauss (solid lines) & Gamma with $\gamma_3 = 1/3$ (dash lines)

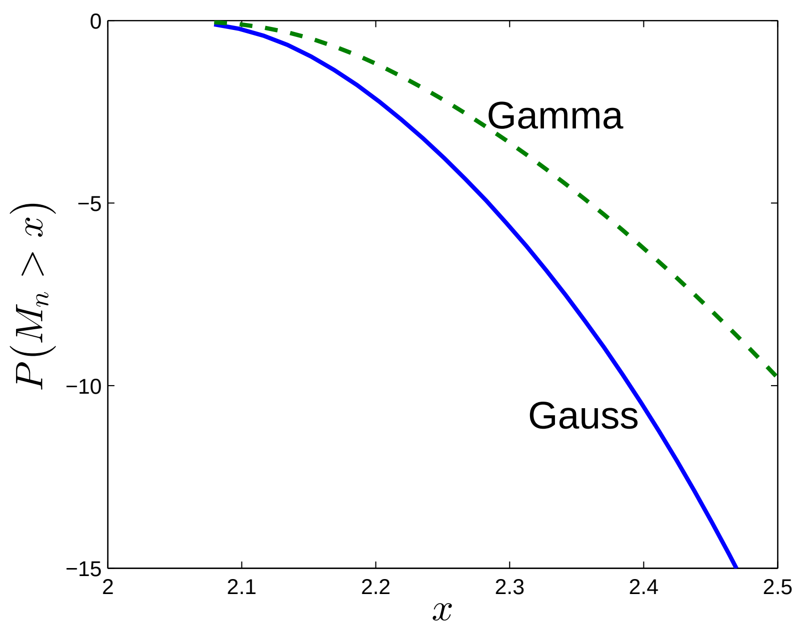




– *Probability $P\big(M_n > x\big)$, $n = 100$:*

– Solid line: $P\big(M_n > x\big) = 1 - F_{\text{Gauss}}(x)^n$

– Dash line: $P\big(M_n > x\big) = 1 - F_{\text{Gamma}}(x)^n$



– *Note:*

- $F_{\text{Gauss}}(x)$ and $F_{\text{Gamma}}(x)$ are consistent with data
- Available information is insufficient to identify the correct tail of $F(\cdot)$
- The distributions of M_n based on $F_{\text{Gauss}}(x)$ and $F_{\text{Gamma}}(x)$ differ significantly

- **Implementation of GEV approximation:**

  – *Data:* $\Longrightarrow$ Find estimates $\left(\hat{\mu}, \hat{\sigma}, \hat{\xi}\right)$ of the GEV parameters (μ, ξ, σ)

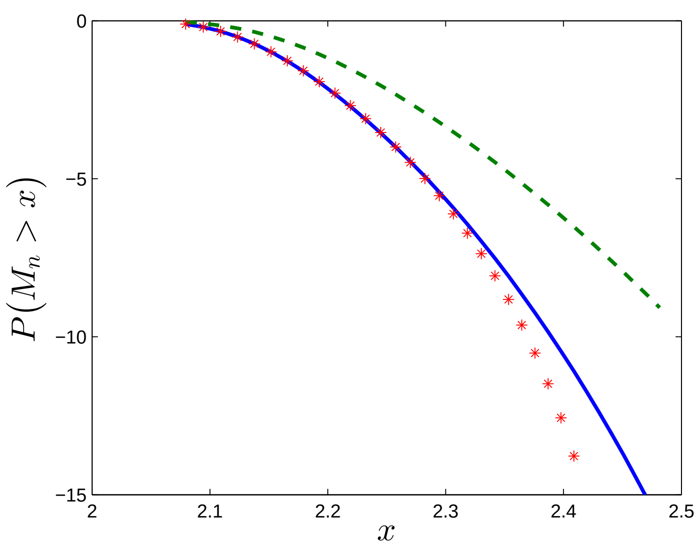
  – *GEV approximation:*

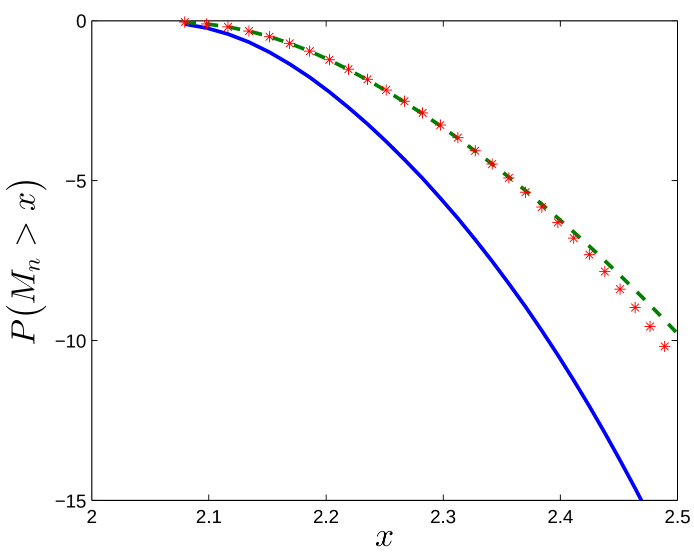
$$P\left(M_n \le x\right) \simeq GEV\left(x; \hat{\mu}, \hat{\sigma}, \hat{\xi}\right) = \exp\left\{ - \left[1 + \hat{\xi}\left(\frac{x - \hat{\mu}}{\hat{\sigma}}\right)\right]^{-1/\hat{\xi}} \right\}$$

- **Exact & GEV approximations of $P(M_n > x)$:**

  – *Exact:* $\{X_i\} \sim$ Gauss (solid lines) and $\{X_i\} \sim$ Gamma (dash lines)

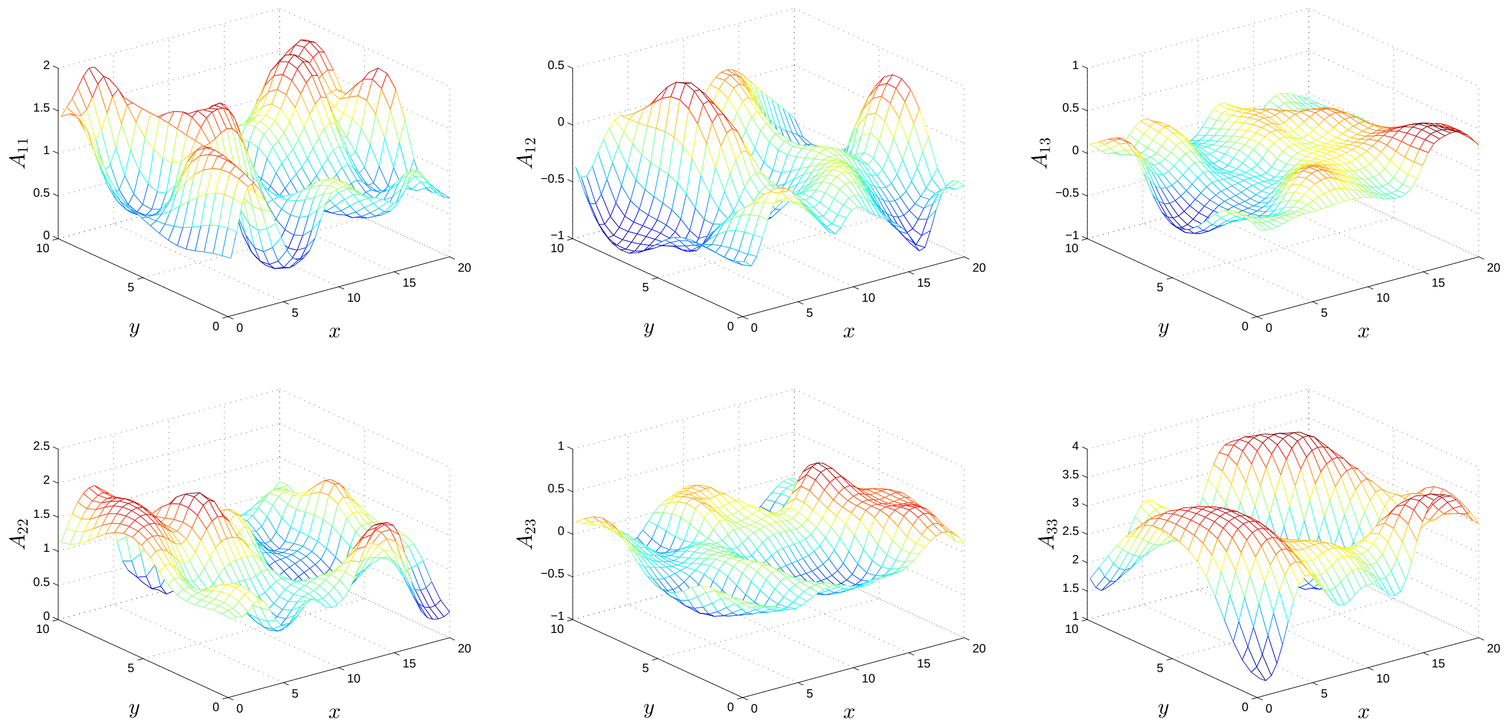
  – *GEV approximation:* Gauss data (left) and Gamma data (right), $n = 100$



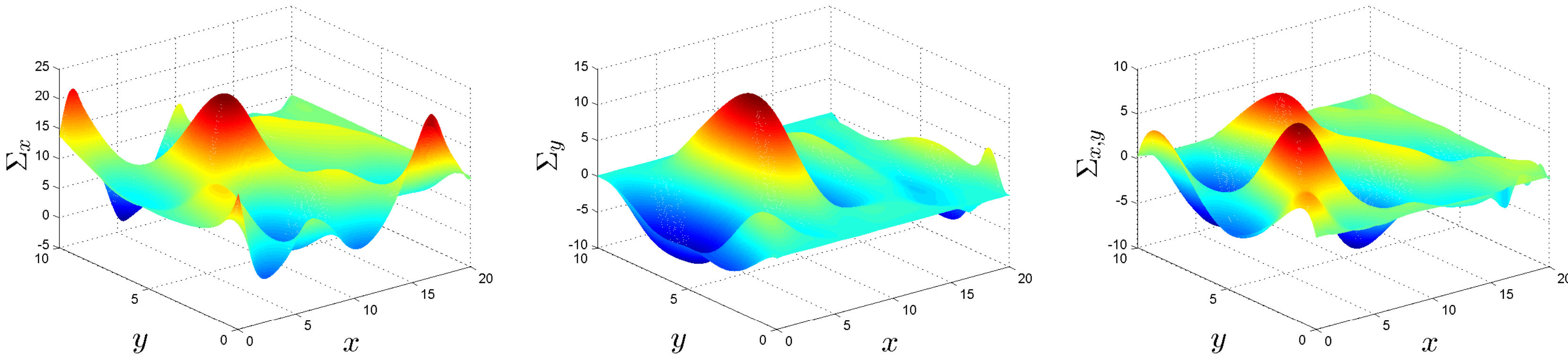


Numerical illustration

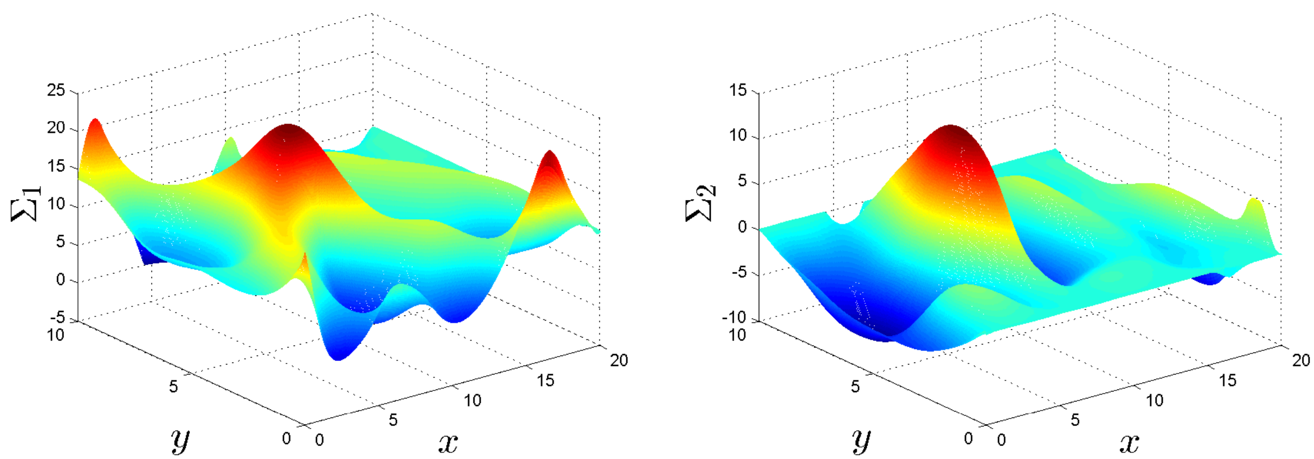
- **Specimen:** *Rectangular plate (20 × 10) under uniform tension in the long direction*
- **Compliance tensor $A(x, y)$:** *Matrix-valued, positive definite, non-Gaussian field*
- **A sample of random compliance tensor $A(x, y)$:**



- **A sample of the stress field:**



- **A sample of principal stresses:**



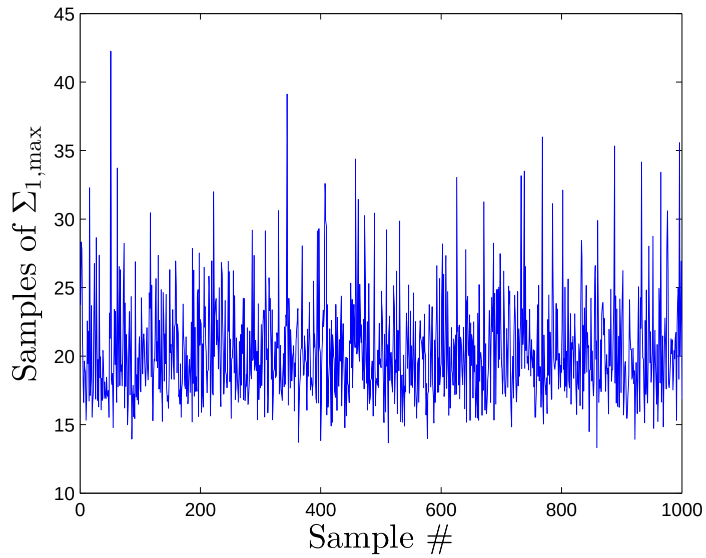
- **Notations:**

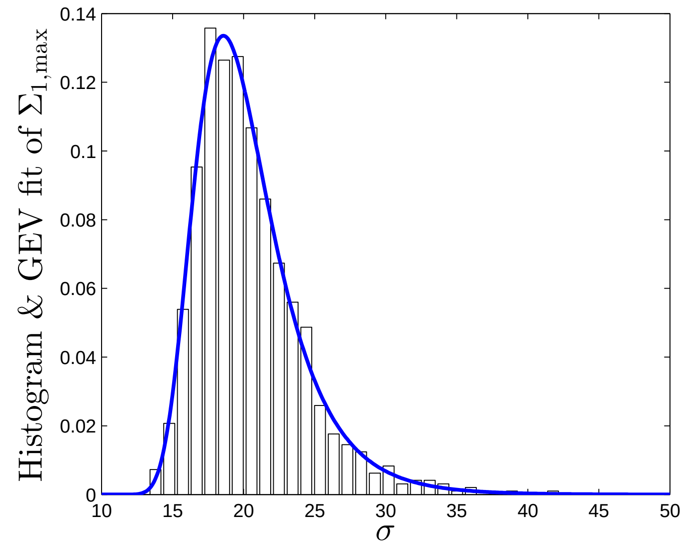
  $\Sigma_1(x,y) = \text{first principal stress at } (x,y) \in D$

  $\Sigma_{1,\max} = \max_{(x,y)\in D}\{\Sigma_1(x,y)\}$

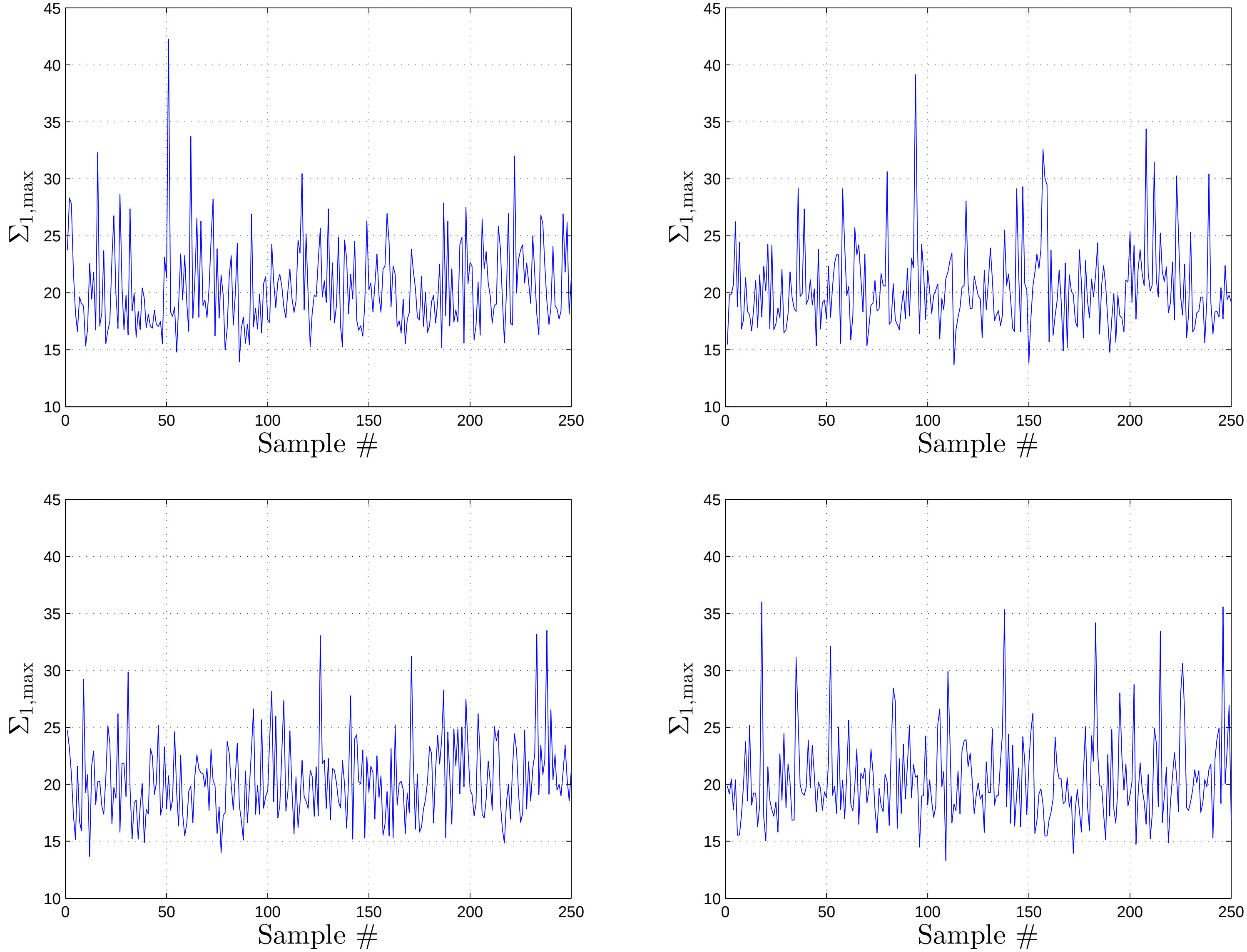
  $\{\sigma_{1,\max}^{(i)},\ i = 1,\ldots,N\} = N \text{ independent samples of } \Sigma_{1,\max}$

- **1000 samples of** $\Sigma_{1,\max}$ (left panel) and **histogram/GEV fit** (right panel)

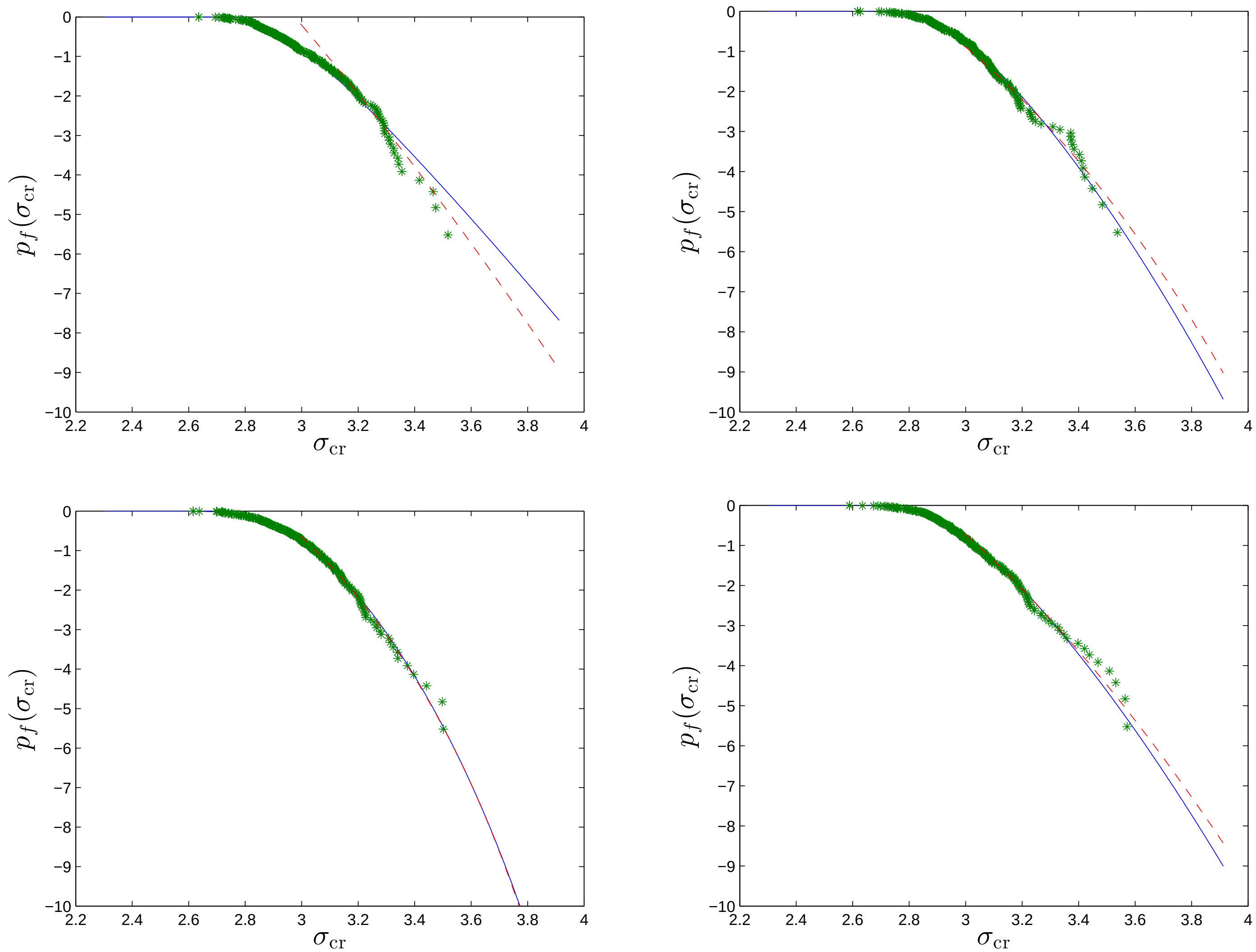




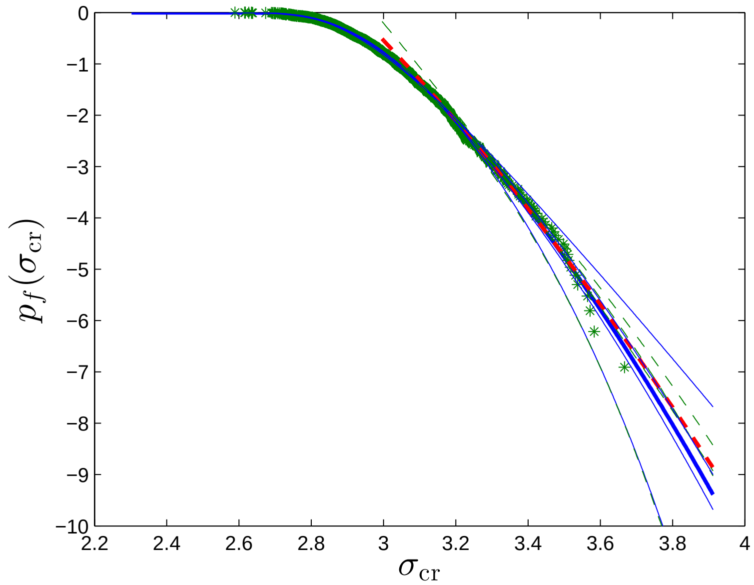
• **Four sets of 250 samples of $\Sigma_{1,\max}$:**



- **Estimates of** $p_f(\sigma_{\mathrm{cr}}) = P\big(\Sigma_{1,\max} > \sigma_{\mathrm{cr}}\big)$**:**
  Empirical (stars) and GEV/GP based on subsets of $\{\sigma_{1,\max}^{(i)}\}$ with size 250



- **Estimates of $p_f(\sigma_{\rm cr}) = P\big(\Sigma_{1,\max} > \sigma_{\rm cr}\big)$:**
  From the previous figures and estimate based on all data (heavy lines)



- **Comments:**
  – *Significant sample-to-sample variability* for $\Sigma_{1,\max}$
  – *Estimates of failure probability $p_f(\sigma) = P\big(\max\{\Sigma_1\} > \sigma\big)$:*
    – *Stars:* 1000 independent samples of $\max\{\Sigma_1\}$
    – *Heavy solid line:* GEV estimate of $p_f(\sigma)$ based on 1000 samples
    – *Thin solid lines:* GEV estimate of $p_f(\sigma)$ based on distinct sets of 250 samples

COMMENTS:

- **Solutions of stochastic equations** require
  - *Discretization* of physical and probability spaces
  - *Discretization of probability space* involves
    - Parametric models for random fields $\Longrightarrow$ finite stochastic dimension
    - SROMs

- **Surrogate models:**
  - *Non-intrusive*
  - *Accurate:*
    - Numerical examples
    - Error bounds are available

- **Extremes of solutions of SEs:**
  - *Solution by EVT*
  - *Example:* Distribution of extreme stresses in an elastic body