Modeling Techniques and Numerical Solution Algorithms for Discrete Partial Differential Equations with Random Data

I. Problem Statement and Discretization

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Stochastic Differential Equations with Random Data

Example: diffusion equation

 $-\nabla \cdot (a\nabla u) = f \quad \text{in } \mathcal{D} \subset \mathbb{R}^d \\ u = g_D \text{ on } \partial \mathcal{D}_D, \quad (a\nabla u) \cdot n = 0 \text{ on } \partial \mathcal{D}_N = \partial \mathcal{D} \setminus \partial \mathcal{D}_D$

Uncertainty / randomness:

 $a = a(x,\omega)$ a *random field* For each fixed *x*, $a(x,\omega)$ a random variable

1

Other possibly uncertain quantities : Forcing function fBoundary data g_D Viscosity v in Navier-Stokes equations $-v \nabla^2 u + (u \cdot \text{grad})u + \text{grad } p = f$ - div u = 0

Depictions: Random Data on Unit Square





Diffusion Equation with Random Diffusion Coefficient $-\nabla \cdot (a\nabla u) = f$ in \mathcal{D}

Assumptions:

1. Spatial correlation of random field: For $x, y \in \mathcal{D}$:

Random field $a(x,\omega)$ Mean $\mu(x) = E(a(x,\cdot))$ Variance $\sigma(x) = E(a(x,\cdot)^2) - \mu^2$ Covariance function $c(x,y) = E((a(x,\cdot) - \mu(x))(a(y,\cdot) - \mu(y))))$ is finitevs. white noise, where c is a δ -function

2. Coercivity $0 < \alpha_1 \le a \le \alpha_2 < \infty$

 \implies Problem is well-posed

Monte-Carlo Simulation

Sample $a(x, \omega)$ at all $x \in \mathcal{D}$, solve in usual way

Standard weak formulation: find $u \in H^1_E(\mathcal{D})$ such that

$$a(u,v) = \ell(v)$$

for all $v \in H^1_{E_0}(\mathcal{D})$,

$$a(u,v) = \int_{\mathcal{D}} a \nabla u \cdot \nabla v \, dx, \qquad \ell(v) = \int_{\mathcal{D}} f \, v \, dx$$

Multiple realizations (samples) of $a(x, \cdot) \rightarrow$ Multiple realizations of $u \rightarrow$ Statistical properties of u

Problem: convergence is slow, requires many solves

Another Point of View

$$-\nabla \cdot (a\nabla u) = f \quad \text{in } \mathcal{D}$$

Covariance function is finite \implies random field (diffusion coefficient) has *Karhunen-Loève* expansion:

$$a(x,\omega) = a_0(x) + \sigma \sum_{r=1}^{\infty} \sqrt{\lambda_r} a_r(x) \xi_r(\omega)$$

$$a_0(x) = \mu(x) = E(a(x, \cdot))$$
 mean

 $a_r(x), \lambda_r =$ eigenfunctions/eigenvalues of covariance operator $(Ca)(x) = \lambda a(x), \quad (Ca)(x) = \int_D c(x, y) a(y) dy$

 $\xi_r(\omega)$ = identically distributed uncorrelated random variables with mean 0 and variance 1

Finite Noise Assumption

 $-\nabla \cdot (a\nabla u) = f \quad \text{in } \mathcal{D}$

Truncated Karhunen-Loève expansion:

$$a(x,\omega) = a_0(x) + \sigma \sum_{r=1}^m \sqrt{\lambda_r} a_r(x)\xi_r(\omega)$$

~ Principal components analysis Requires: *m* large enough so that the fluctuation of *a* is well-represented, i.e. $\lambda_{m+1} / \lambda_1$ is small

More precisely: error from truncation is

$$\frac{\left|\mathcal{D}\right|\sigma^2 - \sum_{j=1}^m \lambda_j}{\left|\mathcal{D}\right|\sigma^2}$$

Choose *m* to make this small

Two Ways to Use This

$$a(x,\omega) = a_0(x) + \sigma \sum_{r=1}^m \sqrt{\lambda_r} a_r(x)\xi_r(\omega)$$

 Stochastic Finite Element (Galerkin) Method: Introduce a weak formulation analogous to finite elements in space that handles the "stochastic" component of the problem

2. Stochastic Collocation Method:

Devise a special strategy for sampling $\underline{\xi}$ that converges more quickly than Monte Carlo simulation ; derived from interpolation

Ghanem, Spanos, Babuška, Deb, Oden, Matthies, Keese, Karniadakis, Xiu, Hesthaven, Tempone, Nobile, Webster, Schwab, Todor, Ernst, Powell, Furnival, E., Ullmann, Rosseel, Vandewalle

Stochastic Finite Element (Stochastic Galerkin) Method

Probability space (Ω, \mathcal{F}, P) $L_P^2(\Omega) \equiv \{ \text{square integrable functions wrt } dP(\omega) \}$

Inner product on
$$L_P^2(\Omega): \langle v, w \rangle = E(vw) = \int_{\Omega} v(\omega)w(\omega)dP(\omega)$$

Use to concoct weak formulation on product space $H^1_E(\mathcal{D}) \otimes L^2_P(\Omega)$

Find
$$u \in H^1_E(\mathcal{D}) \otimes L^2_P(\Omega)$$
 such that
 $\langle a(u,v) \rangle = \langle \ell(v) \rangle$
for all $v \in H^1_{E_0}(\mathcal{D}) \otimes L^2_P(\Omega)$
 $\int_{\Omega D} a \nabla u \cdot \nabla v \, dx \, dP(\omega)$

Solution $u=u(x,\omega)$ is itself a random field

For Computation: Return to Finite Noise Assumption

Truncated Karhunen-Loève expansion

$$a(x,\xi(\omega)) = a_0(x) + \sigma \sum_{r=1}^m \sqrt{\lambda_r} a_r(x)\xi_r(\omega)$$

Stochastic weak formulation uses

$$\langle a(u,v) \rangle = \iint_{\Omega D} a \,\nabla u \cdot \nabla v \, dx \, dP(\omega) = \iint_{\xi(\Omega) D} a(x,\xi) \nabla u \cdot \nabla v \, dx \, \rho(\xi) d\xi$$

Bilinear form entails
integral over *image* of
random variables ξ
Require joint
density function
associated with ξ

Statement of Problem Becomes

Find
$$u \in H^1_E(\mathcal{D}) \otimes L^2_P(\Gamma)$$
 such that

$$\iint_{\Gamma \mathcal{D}} a(x, \underline{\xi}) \nabla u \cdot \nabla v \, dx \, \rho(\underline{\xi}) d\underline{\xi} = \iint_{\Gamma \mathcal{D}} fv \, dx \, \rho(\underline{\xi}) d\underline{\xi}$$
for all $v \in H^1_{E_0}(\mathcal{D}) \otimes L^2_P(\Gamma)$ $(\Gamma = \underline{\xi}(\Omega))$

Like an ordinary Galerkin (or Petrov-Galerkin) problem on a (d+m)-dimensional "continuous" space

d = dimension of spatial domain m = dimension of stochastic space

Discretization

$$\iint_{\Gamma \mathcal{D}} a(x, \underline{\xi}) \nabla u \cdot \nabla v \, dx \, \rho(\underline{\xi}) d\underline{\xi} = \iint_{\Gamma \mathcal{D}} f \, v \, dx \, \rho(\underline{\xi}) d\underline{\xi}$$

Finite dimensional spaces:

- spatial discretization: $S_h \subset H_0^1(\mathcal{D})$, spanned by $\{\varphi_j\}_{j=1}^{N_x}$ for example: piecewise linear on triangles
- stochastic discretization: $T_p \subset L^2(\Gamma)$, spanned by $\{\psi_l\}_{l=1}^{N_{\xi}}$ for example: polynomial chaos = *m*-variate Hermite polynomials (orthogonal wrt Gaussian measure)

Discrete weak formulation:

$$a(u_{hp}, v_{hp}) = \ell(v_{hp}) \quad \text{for all } v_{hp} \in S_h \otimes T_p$$
$$u_{hp} = \sum_{j=1}^{N_x} \sum_{l=1}^{N_\xi} u_{jl} \varphi_j(x) \psi_l(\xi)$$

Basis Functions for Stochastic Space

Underlying space:
$$L^{2}(\Gamma) = \left\{ v(\underline{\xi}) \Big| \int_{\Gamma} v(\underline{\xi})^{2} \rho(\underline{\xi}) d\underline{\xi} < \infty \right\}$$

 $\rho(\underline{\xi}) = \rho_{1}(\xi_{1}) \rho_{2}(\xi_{2}) \cdots \rho_{M}(\xi_{M})$

Let $q_j^{(k)}(\xi_k)$ = polynomial of degree *j* orthogonal wrt ρ_k

Examples: if $\rho_k \sim Gaussian measure \longrightarrow$ Hermite polynomials $\rho_k \sim uniform \, distribution \longrightarrow$ Legendre polynomials Any ρ_k can be handled computationally (Gautschi) \longrightarrow Rys polynomials

$$T_p \subset L^2(\Gamma)$$
 spanned by $\{q_{j_1}^{(1)}(\xi_1)q_{j_2}^{(2)}(\xi_2)\cdots q_{j_m}^{(m)}(\xi_m)\}$

Orthogonality of basis functions —> sparsity of coefficient matrix

Matrix Equation Au = f $a(x,\xi(\omega)) = a_0(x) + \sigma \sum_{r=1}^m \sqrt{\lambda_r} a_r(x)\xi_r(\omega)$ $A = G_0 \otimes A_0 + \sum_{r=1}^m G_r \otimes A_r$ $[A_0]_{jk} = \int a_0(x) \nabla \varphi_j(x) \cdot \nabla \varphi_k(x) dx$ $[A_r]_{jk} = \sqrt{\lambda_r} \int_{\sigma} \sigma(x) a_r(x) \nabla \varphi_j(x) \cdot \nabla \varphi_k(x) dx$ $[G_0]_{lq} = \langle \psi_l, \psi_q \rangle, \quad [G_r]_{lq} = \langle \xi_r \psi_l, \psi_q \rangle$ $[f]_{kq} = \iint f(x,\xi)\varphi_k(x)\psi_q(\xi)dx\rho(\xi)d\xi$

Properties of *A*:

- order = $N_x \times N_{\xi}$ = (size of spatial basis) \times (size of stochastic basis)
- sparsity: inherited from that of $\{G_r\}$ and $\{A_r\}$

Dimensions of Discrete Stochastic Space

$$T_p \subset L^2(\Gamma)$$
 spanned by $\{q_{j_1}^{(1)}(\xi_1)q_{j_2}^{(2)}(\xi_2)\cdots q_{j_m}^{(m)}(\xi_m)\}$

Full tensor product basis: $0 \le j_i \le p$, i = 1, ..., mDimension: $(p+1)^m$ Too large

"Complete" polynomial basis:
$$j_1 + j_2 + \dots + j_m \le p$$

Dimension: $\binom{m+p}{p} = \frac{(m+p)!}{m! p!}$

More manageable

Order these in a systematic way \longrightarrow

$$\psi_1(\underline{\xi}), \psi_2(\underline{\xi}), \dots, \psi_{N_{\xi}}(\underline{\xi})$$

Example

$$T_{p} \subset L^{2}(\Gamma) \text{ spanned by } \{q_{j_{1}}^{(1)}(\xi_{1})q_{j_{2}}^{(2)}(\xi_{2})\cdots q_{j_{m}}^{(m)}(\xi_{m})\}$$

"Complete" polynomial basis: $j_{1} + j_{2} + \cdots + j_{m} \leq p$
 $m=2, p=3 \longrightarrow {\binom{m+p}{p}} = {\binom{5}{2}} = 10$

Orthogonal (Hermite) polynomials in 1D:

$$H_0(\xi) = 1, \ H_1(\xi) = \xi, H_2(\xi) = \xi^2 - 1, \ H_3(\xi) = \xi^3 - 3\xi$$

Gives basis set:

$$\begin{split} \psi_{1}(\underline{\xi}) &= 1 & \psi_{6}(\underline{\xi}) = \xi_{1}\xi_{2} \\ \psi_{2}(\underline{\xi}) &= \xi_{1} & \psi_{7}(\underline{\xi}) = (\xi_{1}^{2} - 1)\xi_{2} \\ \psi_{3}(\underline{\xi}) &= \xi_{1}^{2} - 1 & \psi_{8}(\underline{\xi}) = (\xi_{2}^{2} - 1) \\ \psi_{4}(\underline{\xi}) &= \xi_{1}^{3} - 3\xi_{1} & \psi_{9}(\underline{\xi}) = (\xi_{2}^{2} - 1)\xi_{1} \\ \psi_{5}(\underline{\xi}) &= \xi_{2} & \psi_{10}(\xi) = \xi_{2}^{3} - 3\xi_{2} \end{split}$$

Example of Sparsity Pattern

For *m*-variate polynomials of total degree *p*:





Uses of the Computed Solution:

$$u_{hp} = \sum_{l=1}^{N_{\xi}} \underbrace{\sum_{j=1}^{N_x} u_{jl} \varphi_j(x) \psi_l(\underline{\xi})}_{u_l(x)} = \underbrace{\sum_{l=1}^{N_{\xi}} u_l(x) \psi_l(\underline{\xi})}_{u_l(x)}$$

1. Moments: First moment of *u* (expected value):

$$E(u_{hp}) = \sum_{l=1}^{M} u_l(x) \int_{\Gamma} \psi_l(\underline{\xi}) \rho(\underline{\xi}) d\underline{\xi}$$

= $u_1(x) = \sum_{j=1}^{N} u_{j1} \varphi_j(x)$ Free!

using orthogonality of stochastic basis functions Similarly for second moment / covariance **Uses of the Computed Solution:**

$$u_{hp} = \sum_{l=1}^{N_{\xi}} \underbrace{\sum_{j=1}^{N_x} u_{jl} \varphi_j(x) \psi_l(\underline{\xi})}_{u_l(x)} = \underbrace{\sum_{l=1}^{N_{\xi}} u_l(x) \psi_l(\underline{\xi})}_{u_l(x)}$$

2. Cumulative distribution functions

E.g.: $P(u_{hp}(x,\xi) > \alpha)$ at some point x

Sample
$$\underline{\xi}$$

Evaluate $u_{hp}(x,\underline{\xi}) = \sum_{l=1}^{N_{\xi}} u_l(x) \psi_l(\underline{\xi})$
Repeat Precomputed

Not free, but **no solves required**

Stochastic Collocation Method

Given
$$a(x,\xi) = a_0(x) + \sigma \sum_{r=1}^m \sqrt{\lambda_r} a_r(x)\xi_r$$
 as above

Let $\underline{\xi}$ be a specified realization (~ Monte Carlo) \longrightarrow

Weak formulation:

$$\int_{\mathcal{D}} (a_0(x) + \sigma \sum_{r=1}^m \sqrt{\lambda_r} a_r(x)\xi_r) \nabla u \cdot \nabla v \, dx = \int_{\mathcal{D}} f \, v \, dx$$

Discretize in space in usual way.

Stochastic collocation: choose special set $\xi^{(1)}, \xi^{(2)}, \dots, \xi^{(N_{\xi})}$ from considerations of interpolation

Advantage: Spatial systems are decoupled

Multi-Dimensional Interpolation

Given $\underline{\xi}^{(1)}, \underline{\xi}^{(2)}, \dots, \underline{\xi}^{(N_{\xi})}, \text{ and } v(\underline{\xi}), \text{ consider an interpolant}$ $(Iv)(\underline{\xi}) \equiv \sum_{k=1}^{N_{\xi}} v(\underline{\xi}^{(k)}) L_k(\underline{\xi}) \approx v(\underline{\xi}),$

where $L_k(\underline{\xi}^{(j)}) = \delta_{jk}$, Lagrange interpolating polynomial

If $u_h^{(k)}$ solves the discrete (in space) version of $\int_{\mathcal{D}} (a_0(x) + \sigma \sum_{r=1}^m \sqrt{\lambda_r} a_r(x)\xi_r) \nabla u \cdot \nabla v \, dx = \int_{\mathcal{D}} f \, v \, dx$ with $\underline{\xi} = \underline{\xi}^{(k)}$, then the *collocated* solution is $u_{hp}(x,\underline{\xi}) = \sum_{k=1}^{N_{\xi}} u_h^{(k)}(x) L_k(\underline{\xi})$

20

To Compute Statistical Quantities

Solution
$$u_{hp}(x,\underline{\xi}) = \sum_{k=1}^{N_{\xi}} u_h^{(k)}(x) L_k(\underline{\xi})$$

1. Moments

$$E(u_{hp})(x) = \sum_{k=1}^{N_{\xi}} u_h^{(k)}(x) \int_{\Gamma} L_k(\underline{\xi}) \rho(\underline{\xi}) d\underline{\xi}$$

Not free but can be precomputed

2. Distribution functions

Obtained by sampling, cheap

Strategy for Interpolation

$$(Iv)(\underline{\xi}) \equiv \sum_{k=1}^{N_{\xi}} v(\underline{\xi}^{(k)}) L_k(\underline{\xi}) \approx v(\underline{\xi}),$$

One choice of $\{L_k\}$: $L_k(\underline{\xi}) = \ell_{k_1}(\xi_1)\ell_{k_2}(\xi_2)\cdots\ell_{k_m}(\xi_m)$ $\ell_{k_j} = 1D$ interpolating polynomial $0 \le k_j \le p$

Advantage: easy to construct

Disadvantage: "curse of dimensionality," dimension = $(p+1)^{m}$

Detour: Sparse Grids

Given: 1D interpolation rule $(U^{(k)}v)(y^{(k)}) = \sum_{j=1}^{m_k} v(y_j^{(k)})\ell_j(y^{(k)})$

Derived from (1D) grid $Y^{(k)} = \{y_1^{(k)}, \dots, y_{m_k}^{(k)}\}$

Multidimensional rule above is induced by *fully populated* multidimensional grid $Y^{(1)} \times Y^{(2)} \times \cdots \times Y^{(m)}$. $|Y^{(k)}| = m_k = p + 1$

Alternative: multidimensional *sparse grid* (Smolyak)

$$\mathcal{H}(m+p,m) \equiv \bigcup_{p-m+1 \le i_1 + \dots + i_m \le p} (Y^{(i_1)} \times Y^{(i_2)} \times \dots \times Y^{(i_m)})$$

Sparse Grid Interpolation



For v of the form $v(\xi) = v_1(\xi_1)v_2(\xi_2)\cdots v_m(\xi_m)$, interpolating function takes the form

$$(Iv)(\underline{\xi}) = \sum_{i_1 + \dots + i_m \le p} (U^{(i_1)} - U^{(i_1 - 1)}) v_1(\xi_1) \otimes (U^{(i_2)} - U^{(i_2 - 1)}) v_2(\xi_2) \otimes \dots \otimes (U^{(i_m)} - U^{(i_m - 1)}) v_m(\xi_m)$$

d=2, *p*=5

Sparse Grid Interpolation

Theorem (Novak, Ritter, Wasilkowski, Wozniakowski) For $\underline{\xi} \in$ sparse grid and $v(\underline{\xi})$ a tensor product polynomial of total degree at most *p*,

 $v(\underline{\xi}) = q_{j_1}^{(1)}(\xi_1) q_{j_2}^{(2)}(\xi_2) \cdots q_{j_m}^{(m)}(\xi_m), \quad j_1 + j_2 + \cdots + j_m \le p$ $(Iv)(\underline{\xi}) = v(\underline{\xi}).$

That is: sparse grid interpolation evaluates the set of complete *m*-variate polynomials exactly

Overhead: number of sparse grid points to achieve this (= # stochastic dof) is larger than for Galerkin

$$2^{p}\binom{m+p}{p}$$
 vs. $\binom{m+p}{p}$

Sparse Grid Interpolation

Choice of (1D) points to define sparse grids dictated by interpolation error

Choices studied:

Clenshaw-Curtis
$$\xi_j^k = \cos(\frac{\pi(j-1)}{i_k-1})$$

Gaussian nodes

Analysis (Babuška, Tempone, Zouraris, Nobile, Webster)

Monte-Carlo:
$$E(u) - E_s(u_h) = (E(u) - E(u_h)) + (E(u_h) - E_s(u_h))$$

 $\leq c_1 h E(|u|_2) + (E(u_h) - E_s(u_h)) - \frac{1}{\sqrt{s}}$

Convergence is slow wrt number of samples but independent of number of random variables *m*

Stochastic Galerkin and Collocation:

$$E(u) - E(u_{hp}) = (E(u) - E(u_{h})) + (E(u_{h}) - E(u_{hp}))$$

$$\leq c_{1}h E(|u|_{2}) \qquad \leq c_{2}r^{p}, \ r < 1$$

Exponential in polynomial degree pConstants (c_2 , r) depend on m

Rule of thumb: the same p gives the same error
(for all versions of SG and collocation)More dof for collocation than SG27

Recapitulating

Monte-Carlo methods:

Many samples needed for statistical quantities Many systems to solve Systems are independent Statistical quantities are free (once data is accumulated) With *s* realizations: $E_s(u_h) = \frac{1}{s} \sum_{r=1}^{s} u_h^{(r)}(x)$

Convergence is slow but independent of *m*

Stochastic Galerkin methods:

One large system to solve Statistical quantities are free or (relatively) cheap

Stochastic collocation methods:

Systems are independent Fewer systems than Monte Carlo More degrees of freedom than Galerkin Statistical quantities are (relatively) cheap Similar convergence behavior Faster than MC Depends on *m*

Computing with the Stochastic Galerkin and Collocation Methods

For both: compute a discrete solution, a random field $u_{hp}(x,\xi)$

Stochastic Galerkin:

$$u_{hp}(x,\underline{\xi}) = \sum_{l=1}^{N_{\xi}} \sum_{j=1}^{N_{x}} u_{jl} \varphi_{j}(x) \psi_{l}(\underline{\xi}) = \sum_{l=1}^{N_{\xi}} u_{l}(x) \psi_{l}(\underline{\xi})$$

Stochastic Collocation:

$$u_{hp}(x,\underline{\xi}) = \sum_{l=1}^{N_{\xi}} \sum_{j=1}^{N_{x}} u_{jl} \varphi_{j}(x) L_{l}(\underline{\xi}) = \sum_{l=1}^{N_{\xi}} u_{l}(x) L_{l}(\underline{\xi})$$

Postprocess to get statistics

Computational Issues

Stochastic Galerkin: Solve one large system of order $N_x \times N_{\xi}$



$$N\xi = \binom{m+p}{p}$$

Frequently cited as a problem for this methodology

Stochastic Collocation: Solve N_{ξ} "ordinary" algebraic systems (of order N_x), one for each sparse grid point

Here: $N_{\xi}^{(collocation)} \sim 2^p N_{\xi}^{(Galerkin)}$

Some savings possible

What is Involved?

Stochastic Galerkin:

$$A = G_0 \otimes A_0 + \sum_{r=1}^{m} G_r \otimes A_r$$
$$[A_0]_{jk} = \int_{\mathcal{D}} a_0(x) \nabla \varphi_j(x) \cdot \nabla \varphi_k(x) dx$$
$$[A_r]_{jk} = \sqrt{\lambda_r} \int_{\mathcal{D}} \sigma(x) a_r(x) \nabla \varphi_j(x) \cdot \nabla \varphi_k(x) dx$$
$$[G_0]_{lq} = \langle \psi_l, \psi_q \rangle, \quad [G_r]_{lq} = \langle \xi_r \psi_l, \psi_q \rangle$$

Assembly of m+1 matrices A_r of ordinary finite element structure Construction of m matrices G_r with at most two nonzeros per row

For Krylov subspace iteration: matrix-vector product can be done implicitly

What is Involved?

Stochastic Collocation: solve discrete version of

$$\int_{\mathcal{D}} (a_0(x) + \sigma \sum_{r=1}^m \sqrt{\lambda_r} a_r(x) \xi_r^{(k)}) \nabla u \cdot \nabla v \, dx = \int_{\mathcal{D}} f \, v \, dx$$

One system for each (sparse) grid point $\underline{\xi}^{(k)}$

Coefficient matrix:
$$A^{(k)} = A_0 + \sum_{r=1}^m A_r \xi_r^{(k)}$$

Now there is a choice:

- 1. Assembly of $N\xi$ coefficient matrices of ordinary finite element structure, one for each grid point, or
- 2. Assembly of m+1 matrices A_r

For (1): mvp is cheaper, preprocessing is more expensive For (2): cumulative cost of mvp ~ 2^p (cost for SG)

Comparison: Depends on Solution Algorithms

Next Topic