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# STOCHASTIC SAMPLING METHODS

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## APPROXIMATING QUANTITIES OF INTEREST USING SAMPLING METHODS

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- Recall that quantities of interest often require the evaluation of stochastic integrals of functions of the solutions
- These integrals usually have to be approximated using quadrature rules, i.e.,

$$\int_{\Gamma} G(u(\mathbf{x}, \vec{y}); \mathbf{x}, \vec{y}) \rho(\vec{y}) d\vec{y} \approx \sum_{q=1}^Q w_q G(u(\mathbf{x}, \vec{y}_q); \mathbf{x}, \vec{y}_q))$$

or

$$\int_{\Gamma} G(u(\mathbf{x}, \vec{y}); \mathbf{x}, \vec{y}) \rho(\vec{y}) d\vec{y} \approx \sum_{q=1}^Q w_q \rho(\mathbf{y}_q) G(u(\mathbf{x}, \vec{y}_q); \mathbf{x}, \vec{y}_q))$$

- To use such a rule, one needs to know the solution  $u(\mathbf{x}, \vec{y})$  of the SPDE at each of the quadrature points  $\vec{y}_q$ ,  $q = 1, \dots, Q$ , in the probabilistic domain  $\Gamma$ 
  - for this purpose, one can use a stochastic Galerkin method to obtain an approximation to the the solution  $u(\mathbf{x}, \vec{y})$  and then evaluate that approximation at the quadrature points

- However, once a quadrature rule is chosen to approximate a quantity of interest,
  - i.e., once the quadrature points  $\{\vec{y}_q\}_{q=1}^Q$  are knownthe simplest and most direct means of determining  $u(\mathbf{x}, \vec{y}_q)$  is to simply solve the PDE  $Q$  times, once for each quadrature point  $\vec{y}_q$
- This approach is referred to as the **stochastic sampling method (SSM)** for SPDEs and for quantities of interest that depend on the solutions of SPDEs
- We have already encountered two SSMs
  - we have seen that SGMs based on Lagrange interpolating polynomials reduce to SSMs
  - we have also seen that non-intrusive polynomial chaos methods are essentially SSMs
    - although one does need the additional step of explicitly constructing the non-intrusive polynomial chaos approximation

- In an SSM, to determine an approximation to a quantity of interest,
  - one chooses a quadrature rule for the probabilistic integrals, i.e.,
    - one chooses quadrature weights and points  $\{w_q, \vec{y}_q\}_{q=1}^Q$
  - one chooses a finite element method, (i.e., a finite element space and a basis  $\{\phi_j\}_{j=1}^J$  for that space) and, for each  $q$ , one defines the finite element approximation of the solution at the quadrature points by

$$u_q(\mathbf{x}) = \sum_{j=1}^J b_{j,q} \phi_j(\mathbf{x}) \quad \text{for } q = 1, \dots, Q$$

- then, to determine  $b_{j,q}$  for  $j = 1, \dots, J$  and  $q = 1, \dots, Q$ , one separately, and if desired, in parallel, solves the  $Q$  deterministic problems: for  $q = 1, \dots, Q$ ,

$$\int_{\mathcal{D}} S\left(\sum_{j=1}^J b_{j,q} \phi_j, \vec{y}_q\right) T(\phi_{j'}) d\mathbf{x} = \int_{\mathcal{D}} \phi_{j'} f(\vec{y}_q) d\mathbf{x} \quad \text{for } j' = 1, \dots, J$$

- each of these can be discretized using a finite element method

⇒ one can use legacy codes as black boxes

⇒ i.e., without changing a single line of code

⇒ i.e., one just uses the legacy code  $Q$  times

– and finally, one just substitutes  $u_q(\mathbf{x})$  wherever  $u(\mathbf{x}; \vec{y}_q)$  is needed into the quadrature rule approximation of a quantity of interest

● The cost of determining an approximation to a quantity of interest using the SSM approach is dominated by

– the cost to determine  $Q$  finite element solutions, each of size  $J$

● This should be compared to the cost of using general SGM approaches for the same purpose that are dominated by

– the cost needed to determine the solution of a single system of size  $JK$

- Which approach wins, i.e., which one yields a desired accuracy in the statistics of quantities of interest for the lowest computational cost, depends on
  - the value of  $Q$ , the number of quadrature points in SSM approaches
  - the value of  $K$ , the number of probabilistic terms in the SGM approximation to the solution
  - the cost of solving the systems of discrete equations encountered
    - for nonlinear problems and time dependent problems, one may have to solve such systems many times
  - many implementation issues
- Of course, such comparisons do not factor in the relative programming cost for implementing the different approaches
  - SSM approaches allow for the easy use of legacy codes
  - general SGM approaches do not allow for this

- In most cases, and certainly due to some recent developments, SSMs win over SGMs
  - which is why polynomial chaos people are now doing non-intrusive polynomial chaos which is, as we have seen, practically a SSM
- Of course, there are many ways to sample points in parameter space other than at the quadrature points for some integration rule
  - so, we now take a more general view of SSMs

## STOCHASTIC SAMPLING METHODS ARE STOCHASTIC GALERKIN METHODS

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- From the previous discussions, it seems that we could have introduced stochastic sampling methods as a special case of stochastic Galerkin methods
  - in fact,

**every stochastic sampling method  
is a stochastic Galerkin method using  
Lagrange interpolating polynomials  
based on the sample points  
and quadrature rules also based on the sample points**

- However, stochastic sampling methods are easier to understand through the straightforward approach we have just taken
  - the straightforward approach also avoids difficult questions about the relations of the cardinality of the set of sample points and the construction of interpolating polynomials

# SURROGATE APPROXIMATIONS AND STOCHASTIC SAMPLING METHODS

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- Stochastic sampling methods (SSMs) for solving stochastic PDEs are based on
  - first determining a sample set of values  $\{\vec{y}_s\}_{s=1}^{N_{sample}}$  of the vector of random parameters  $\vec{y} \in \Gamma \subset \mathbb{R}^N$
  - then determining  $N_{sample}$  (approximate) solutions  $\{u(\mathbf{x}; \vec{y}_s)\}_{s=1}^{N_{sample}}$  of the PDE via, e.g., a finite element method

## Evaluating quantities of interest within the SSM framework

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- If we want to evaluate quantities of interest that involve integrals over the parameter set  $\Gamma$  using a  $Q$ -point quadrature rule involving the quadrature points  $\{\vec{y}_q\}_{q=1}^Q \subset \bar{\Gamma}$  and quadrature weights  $\{w_q\}_{q=1}^Q$ 
  - it is then natural to choose the set of sample points  $\{\vec{y}_s\}_{s=1}^{N_{sample}}$  that are used to solve the PDE  $N_{sample}$  times to be the same as the set of quadrature points  $\{\vec{y}_q\}_{q=1}^Q$  that are used to approximate the quantities of interest
- Alternately, we could choose  $\{\vec{y}_s\}_{s=1}^{N_{sample}}$  to be different (and presumably coarser) than the quadrature points  $\{\vec{y}_q\}_{q=1}^Q$ 
  - one would then use the sample points  $\{\vec{y}_s\}_{s=1}^{N_{sample}}$  to build a **surrogate** or **response surface**  $u_{surrogate}(\mathbf{x}, y)$  for the solution  $u(\mathbf{x}, y)$
  - surrogates/response surfaces for the solution  $u(\mathbf{x}, \vec{y})$  are (usually polynomial) functions of, in our case, the random parameters  $\vec{y}$

- in fact, they are simply representations, e.g., in terms of Lagrange interpolation polynomials, of the approximate solution in terms of the parameter vector  $\vec{y}$
- it is usually more efficient to build a surrogate/response surface **directly for** the integrand  $G(u(\mathbf{x}, \vec{y}); \mathbf{x}, \vec{y})$  of **the desired quantity of interest**
  - one solves for an approximation  $u_s(\mathbf{x})$  to the solution  $u(\mathbf{x}, \vec{y}_s)$  of the PDE for the sample parameter points  $\vec{y}_s, s = 1, \dots, N_{sample}$
  - one then evaluates the approximations to the integrand
 
$$G_s(\mathbf{x}) = G(u_s(\mathbf{x}); \mathbf{x}, \vec{y}_s) \quad \text{for } s = 1, \dots, N_{sample}$$
  - from these samplings of  $G$  at the sample points  $\vec{y}_s$ , one builds a surrogate  $G_{surrogate}(\mathbf{x}, \vec{y})$
- once a surrogate/response surface is built, it can be used to evaluate the integrand at the quadrature points  $\{\vec{y}_q\}_{q=1}^Q$

- To illustrate the different approaches, within the SSM framework, for computing approximations of quantities of interest, consider a quantity of the form

$$\mathcal{J}(u) = \int_{\Gamma} \int_{\mathcal{D}} G(u(\mathbf{x}, \vec{y})) \rho(\vec{y}) d\mathbf{x} d\vec{y}$$

- a spatial quadrature rule with the points  $\mathbf{x}_r$  and weights  $W_r$  for  $r = 1, \dots, R$  is used to approximate the spatial integral resulting in the approximation

$$\mathcal{J}(u) \approx \int_{\Gamma} \sum_{r=1}^R W_r G(u(\mathbf{x}_r, \vec{y})) \rho(\vec{y}) d\vec{y}$$

- a parameter-space quadrature rule with the points  $y_q$  and weights  $w_q$  for  $q = 1, \dots, Q$  is used to approximate the spatial integral resulting in the approximation

$$\mathcal{J}(u) \approx \sum_{q=1}^Q \sum_{r=1}^R w_q W_r \rho(\vec{y}_q) G(u(\mathbf{x}_r, \vec{y}_q))$$

- a set of points  $\{\vec{y}_s\}_{s=1}^{N_{sample}}$  is chosen in the parameter domain  $\Gamma$ 
  - these sample points are used to obtain the set of realizations  $\{u_s(\mathbf{x})\}_{s=1}^{N_{sample}}$  of a finite element discretization of the SPDE
  - each realization is determined by setting the parameters  $\vec{y} = \vec{y}_s$  in the discretized SPDE
  
- if the probabilistic quadrature points  $\{\vec{y}\}_{q=1}^Q$  are the same as the sample points  $\{\vec{y}\}_{s=1}^{N_{sample}}$ , we directly define the computable approximation

$$\mathcal{J}(u) \approx \sum_{q=1}^Q \sum_{r=1}^R w_q W_r \rho(\vec{y}_q) G(u_q(\mathbf{x}_r))$$

where we have, of course, renamed  $u_s(\mathbf{x})$  by  $u_q(\mathbf{x})$  since now they are one and the same

– if the the sample points  $\{\vec{y}\}_{s=1}^{N_{sample}}$  are coarser than the probalistic quadrature points  $\{\vec{y}\}_{q=1}^Q$ , we first build a surrogate  $G_{surrogate}(\mathbf{x}_r, \vec{y})$  for  $G(\mathbf{x}_r, \vec{y})$

- the simplest means for doing this is to use the set of Lagrange interpolating polynomials  $\{L_s(\vec{y})\}_{s=1}^{N_{sample}}$  corresponding to the sample points  $\{\vec{y}_s\}_{s=1}^{N_{sample}}$ , resulting in the surrogate approximation

$$G_{surrogate}(\mathbf{x}_r, \vec{y}) = \sum_{s=1}^{N_{sample}} G(u_s(\mathbf{x}_r)) L_s(\vec{y})$$

- other surrogate constructions may be used, e.g., least-squares fits to the data  $\{\vec{y}_s, G(u_s(\mathbf{x}_r))\}_{s=1}^{N_{sample}}$  using global orthogonal polynomials or even piecewise polynomials

- once the surrogate  $G_{surrogate}(\mathbf{x}_r, \vec{y})$  has been constructed, one defines the indirect computable approximation

$$\mathcal{J}(u) \approx \sum_{q=1}^Q \sum_{r=1}^R w_q W_r \rho(\vec{y}_q) G_{surrogate}(\mathbf{x}_r, \vec{y}_q)$$

by evaluating the surrogate at the probabilistic quadrature points  $\{\vec{y}_q\}_{q=1}^Q$

- for example, if the surrogate is constructed using Lagrange interpolating polynomials, we have the approximation

$$\mathcal{J}(u) \approx \sum_{s=1}^{N_{sample}} \sum_{r=1}^R W_r G(u_s(\mathbf{x}_r)) \sum_{q=1}^Q w_q \rho(\vec{y}_q) L_s(\vec{y}_q)$$

- of course, if the sample points  $\{\vec{y}_s\}_{s=1}^{N_{sample}}$  are the same as the probabilistic quadrature points  $\{\vec{y}_q\}_{q=1}^{N_q}$  so that  $L_s(\vec{y}_q) = \delta_{sq}$ , this approximation reduces to the one obtained before which, in this example, takes the simple form

$$\mathcal{J}(u) \approx \sum_{q=1}^Q w_q \rho(\vec{y}_q) \sum_{r=1}^R W_r G(u_q(\mathbf{x}_r))$$

- Note that if one uses the sample points directly as quadrature points, then one does not need to construct a representation of the approximate solution in terms of the random parameters
  - if one uses a coarser set of sampling points relative to the quadrature points, one does have to build such a representation since it needs to be evaluated at the quadrature points, and not just the sample points
  - of course, this is also unlike the case for general SGMs in which one does build such a representation, e.g., an intrusive polynomial chaos expansion

- We will concentrate on the case where the sample points are used directly as quadrature points
- So, we next discuss quadrature rules that can be used to approximate quantities of interest
  - (coarser) versions of **some** of these rules can also supply sample points that can be used to build surrogates or response surfaces
- We will discuss quadrature rules for the  **$N$ -dimensional hypercube**, the case that most often arises in practice
  - other rectangular regions, i.e., bounding boxes, can be mapped in the obvious way to the unit hypercube
- Unfortunately, we do not have time to discuss sampling in **unbounded domains** or **in general, non-rectangular domains**

# QUADRATURE RULES FOR HYPERCUBES

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- One is tempted to use well-known quadrature rules to define the sample points for SSMs
- We will discuss two classes of quadrature rules for the  $N$ -dimensional hypercube
  - sampling and simple averaging rules
    - the canonical example is Monte Carlo integration
  - weighted quadrature rules based on standard one-dimensional rules
    - ultimately, we consider sparse grid Smolyak quadrature rules
- Recall that in the SSM framework we are using, the quadrature points are also the points used to sample the solutions of the SPDE

## Sampling and simple averaging quadrature rules

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- We consider **sampling + simple averaging-based quadrature rules** that are based on
  - determining a set of quadrature points  $\{y_q\}_{q=1}^Q$
  - approximating integrals of a function  $G(y)$  by an equal weight rule

$$\int_{\Gamma} G(\vec{y})\rho(y) dy \approx \frac{1}{Q} \sum_{q=1}^Q G(\vec{y}_q) \quad \text{if one samples the points according to the PDF } \rho(\vec{y})$$

or by

$$\int_{\Gamma} G(\vec{y})\rho(y) dy \approx \frac{1}{Q} \sum_{q=1}^Q \rho(y_q)G(y_q) \quad \text{if one samples the points uniformly}$$

- The second approach seems simpler, but is wasteful
  - the density of points is the same in regions where  $\rho(\cdot)$  is small as where it is large
    - unfortunately, many sampling methods can only be used to sample uniformly or have difficulty, i.e., they are much less efficient, when sampling nonuniformly
- Note that the weights do not depend on the position of the points  $\{\vec{y}_q\}_{q=1}^Q$  or on other geometric quantities

## Monte Carlo sampling

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- As has already been said, the simplest quadrature rule is based on **Monte Carlo**, i.e., random, **sampling** of the hypercube
  - random sampling could be done uniformly in the hypercube
    - in which case  $w_q = \frac{\rho(\vec{y}_q)}{Q}$
  - random sampling could instead be done according to the density function  $\rho(\vec{y})$  by, e.g., a rejection method
    - in which case  $w_q = \frac{1}{Q}$
- Monte Carlo integration has one very great virtue (other than its simplicity)
  - its convergence behavior is independent of the dimension  $N$ , i.e., of the number of parameters

- Unfortunately, it also has one great fault

- its convergence behavior is slow

$$\text{Error} = O\left(\frac{\sigma}{\sqrt{Q}}\right)$$

- The slow convergence of Monte Carlo integration has motivated the huge amount of effort devoted to improving or replacing Monte Carlo sampling as an integration rule
  - it has also motivated the development of stochastic Galerkin methods

## “Improved” sampling + simple averaging-based quadrature rules

- There have been many sampling + simple averaging-based quadrature rules proposed as replacements for Monte Carlo quadrature, including

variance reduction Monte Carlo methods

quasi-Monte Carlo methods (Halton, Sobol, Faure, Hammersley, . . .)

stratified sampling

Latin hypercube sampling and its many “improved” versions

orthogonal arrays

lattice rules

importance sampling

etc.

- In general, these “improved” rules have, in theory, improved rates of convergence, **at least for not too large  $N$**

- the best theoretical result is of the type

$$\text{Error} = O\left(\frac{(\ln Q)^N}{Q}\right) \quad \Leftarrow \text{note the dependence on } N$$

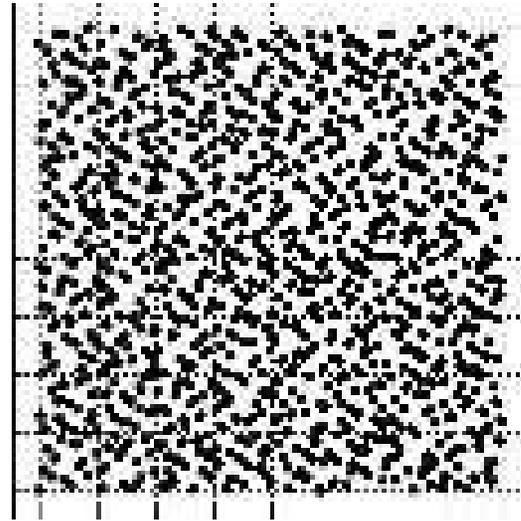
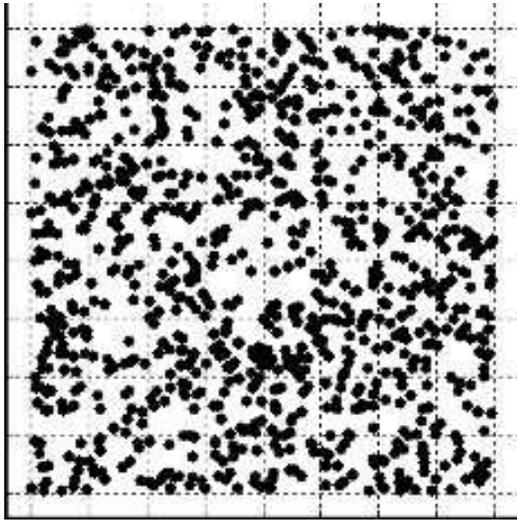
- this is often a pessimistic estimate

- for large  $N$ , the  $(\ln Q)^N$  term dominates

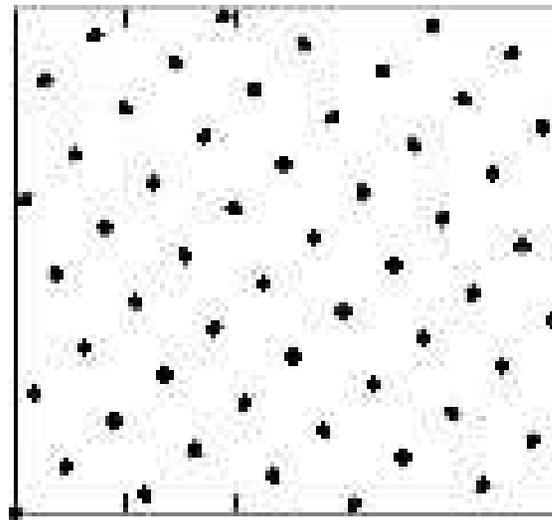
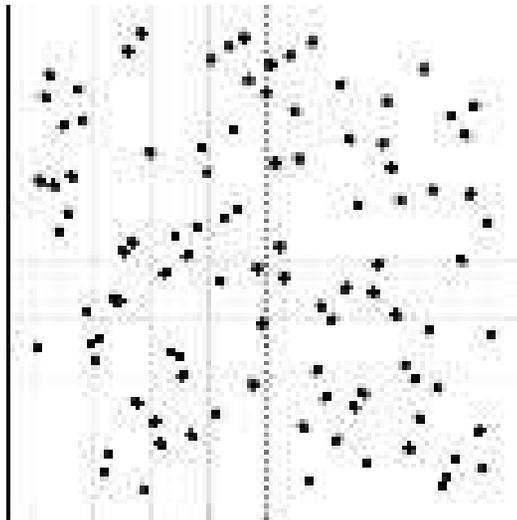
- the curse of dimensionality is still with us

- also, in many cases, biasing problems exist, especially for a large number of sample points

- However, if one is careful when using them, the “improved” sampling and averaging methods often can indeed improve on Monte-Carlo sampling



Monte Carlo and quasi-Monte Carlo point sets



Latin hypercube and lattice rule point sets

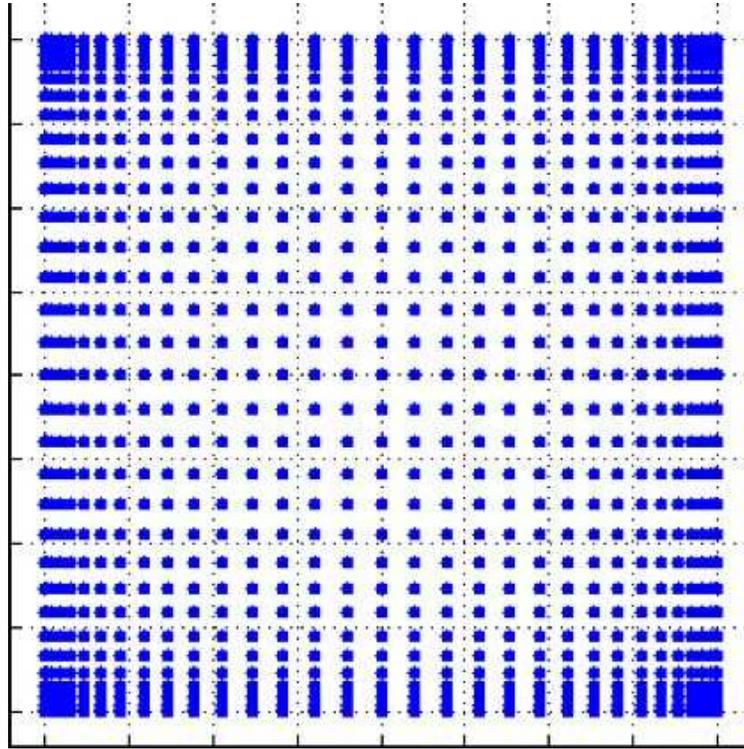
## Tensor products of standard 1-D quadrature rules

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- One is familiar with many quadrature rules in 1D
- On the hypercube, one can easily define multiple integration rules as tensor products of 1D rules
- As we have already seen, tensor products really suffer from [the curse of dimensionality](#)
- Tensor product rules integrate tensor products of polynomials exactly
- Just as was the case for interpolation and approximation, one can get the same rate of convergence using quadrature rules that integrate complete polynomials exactly
- The same table of numbers used before applies here

## Quadrature rules in hypercubes

$N =$ no. random parameters	number of quadrature points in each direction	$Q =$ number of quadrature points	
		using complete polynomial rule	using a tensor product rule
3	4	20	64
	6	56	216
5	4	56	1,024
	6	252	7,776
10	4	286	1,048,576
	6	3,003	60,046,176
20	4	1,771	$> 1 \times 10^{12}$
	6	53,130	$> 3 \times 10^{15}$
100	4	176,851	$> 1 \times 10^{60}$
	6	96,560,646	$> 6 \times 10^{77}$



A tensor product set of quadrature points in 2D

- On the other hand, tensor product rules are easy to define
  - the quadrature points are tensor products of the quadrature points of the 1D rules
  - the quadrature weights are products of the weights of the 1D rules

- High-dimensional rules based on complete polynomials are not so easy to define
  - determining a good set of quadrature points and the corresponding quadrature weights is difficult
  - these difficulties further motivated interest in SGM methods
- But now, there is available an intermediate means of defining quadrature rules
  - the number of points is much less than that for tensor product rules, but is somewhat greater than that for complete polynomial rules
  - these rules are constructed through **judicious sparsifications of tensor product rules**
  - they are known as **Smolyak** or **sparse grid** quadrature rules

# SPARSE (SMOLYAK) QUADRATURE RULE-BASED STOCHASTIC SAMPLING METHODS

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- Let  $I$  be a positive integer and for each  $i = 1, \dots, I$ , let  $m_i$  denote a positive integer
- For each  $i = 1, \dots, I$ , let  $\Theta^{(i)} = \{y_1^{(i)}, \dots, y_{m_i}^{(i)}\}$  denote a set of points in  $[-1, 1]$ 
  - note that for convenience, we will be looking at the hypercube  $[-1, 1]^N$
- Let  $N > 1$  denote the number of parameters
- Let  $p = (p_1, p_2, \dots, p_N)$  denote a multi-index,
  - in this case, an  $N$ -vector whose components are **positive** integersand let  $|p| = \sum_{n=1}^N p_n$

- Let  $M$  denote a positive integer

- Let  $\mathcal{I}(M, N) = \{p : M + 1 \leq |p| \leq N + M\}$

- Then,

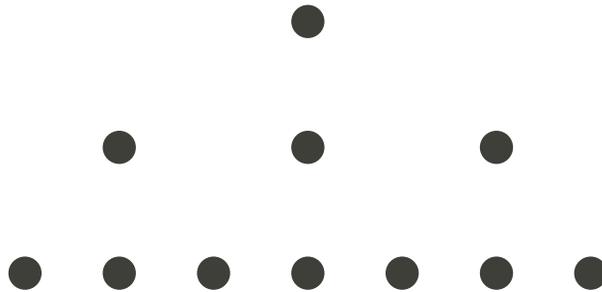
$$\mathcal{S}(M, N) = \bigcup_{p \in \mathcal{I}(M, N)} \Theta^{(p_1)} \otimes \Theta^{(p_2)} \otimes \dots \otimes \Theta^{(p_N)}$$

defines a **sparse grid**

- Example

- let  $I = 3$ ,  $m_1 = 1$ ,  $m_2 = 3$ , and  $m_3 = 7$

- let  $\Theta^{(i)}$ ,  $i = \dots, I = 3$  be given by the three one-dimensional nested point sets



- let  $N = 2$  and  $M = 2$  so that  $\mathcal{I}(2, 2) = \{p : 3 \leq |p| \leq 4\}$

- $\mathcal{I}(2, 2)$  then contains the combinations

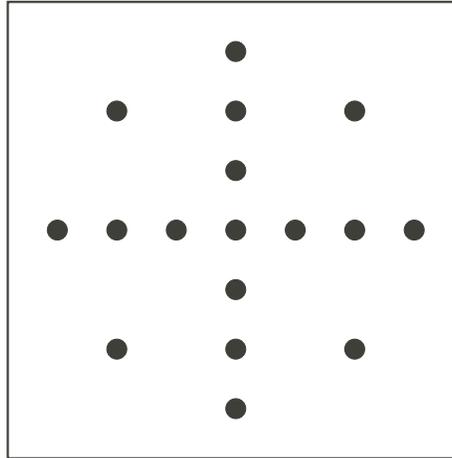
$$(p_1, p_2) = (1, 1), (1, 2), (2, 1), (3, 1), (1, 3), (2, 2)$$

but not the combinations

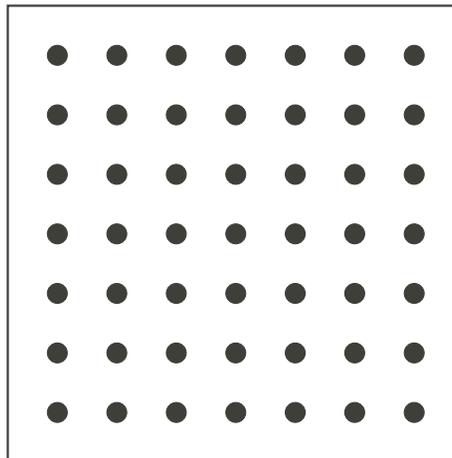
$$(p_1, p_2) = (2, 3), (3, 2), (3, 3)$$

- for nested point sets, it is enough to include the combinations for which  $|p| = N + M$ , i.e.,  $(3, 1)$ ,  $(1, 3)$ ,  $(2, 2)$  in the example

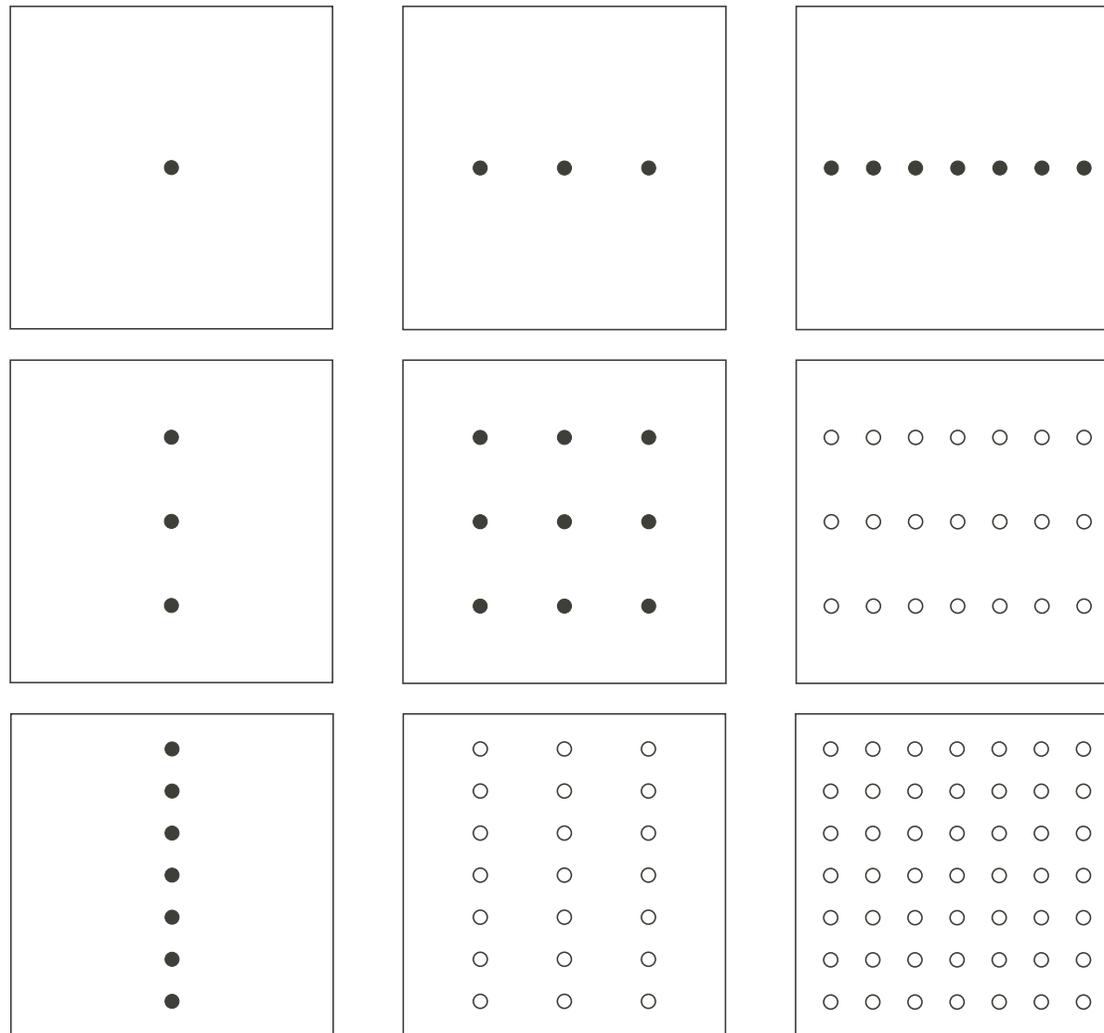
– then,  $\mathcal{S}(2, 2)$  is given by



– this should be contrasted with the **full tensor-product** point set



- the following diagram shows how the sparse grid comes about



● point sets included in  $\mathcal{S}(2, 2)$

○ point sets not included in  $\mathcal{S}(2, 2)$

- What Smolyak showed is that
  - if one chooses the underlying one-dimensional grids to be the quadrature points for some integration rulethen
  - the accuracy of the full tensor product point set can be preserved with point sets with much fewer points
- Along the way, Smolyak also showed how to systematically compute the weights of the resulting sparse quadrature rule
- The use of Smolyak grids in the SPDE setting has been rigorously analyzed for some simple linear and nonlinear elliptic PDEs

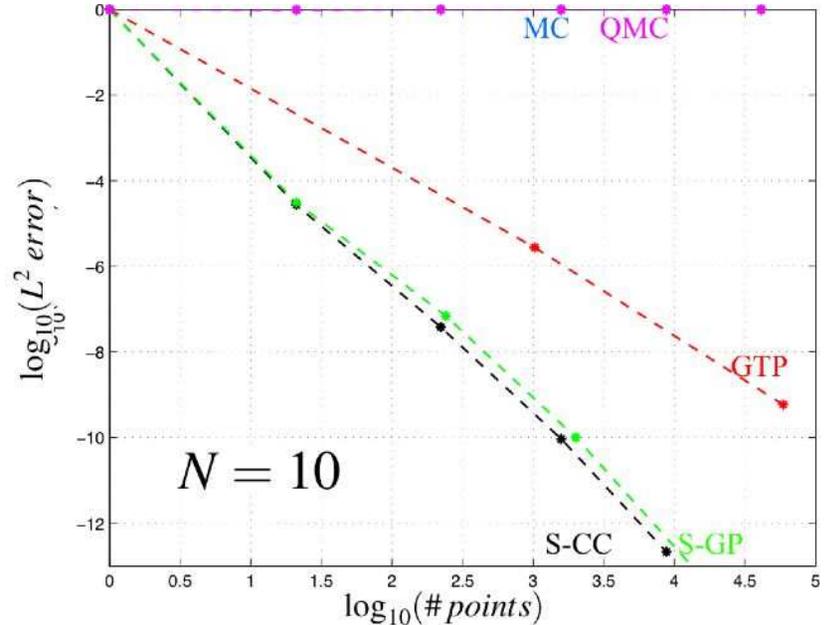
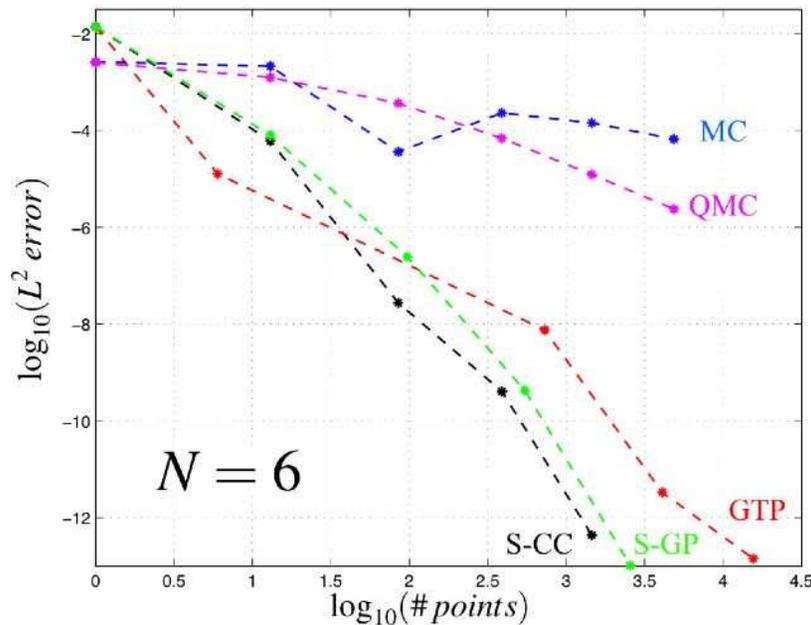
- Some choices of one-dimensional quadrature rules upon which the Smolyak grids can be constructed
  - **Newton-Cotes**: nested equidistant abscissas by taking  $m_1 = 1$  and  $m_i = 2^{i-1} + 1$  for  $i > 1$ 
    - maximum degree of exactness is  $m_I - 1$
    - can have (highly) negative weights causing numerical inaccuracies
  - **Clenshaw-Curtis**: nested (same growth as above) Chebyshev points
    - maximum degree of exactness is  $m_I - 1$
    - nested grids keep the number of points down
  - **Gauss**: non-nested abscissas
    - maximum degree of exactness is  $2m_I - 1$
  - **Gauss-Patterson**: seems to have good promise

**Results that follow are from papers of Nobile, Tempone, and Webster**

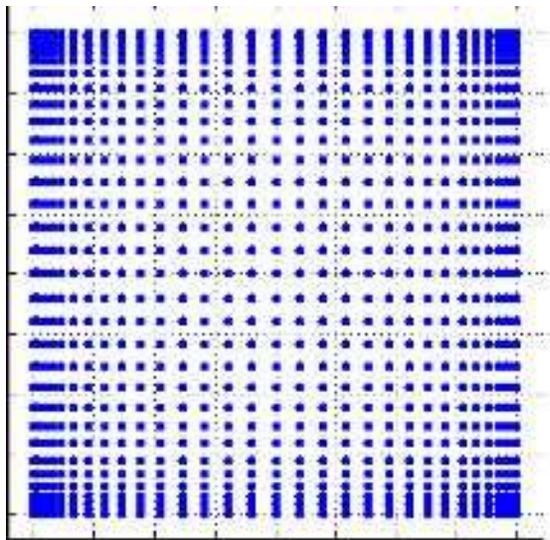
- For the integral

$$\int_{\mathbb{R}^N} \exp \left( - \sum_{n=1}^N a_n^2 (y_n - b_n)^2 \right) d\vec{y}$$

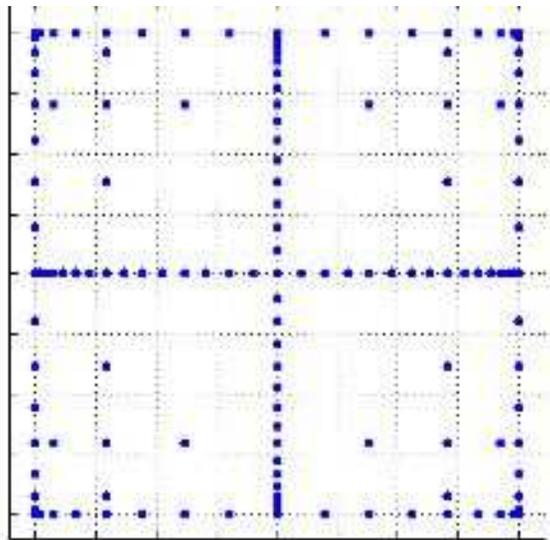
where  $a_n$  and  $b_n$  are randomly sampled uniformly in  $(0, 1)$ , we have the following errors for different quadrature rules



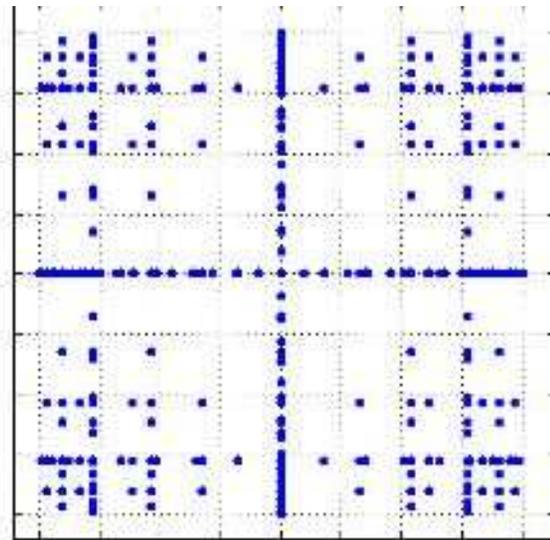
Comparisons of errors vs. number of quadrature points for different integration rules



Isotropic FT



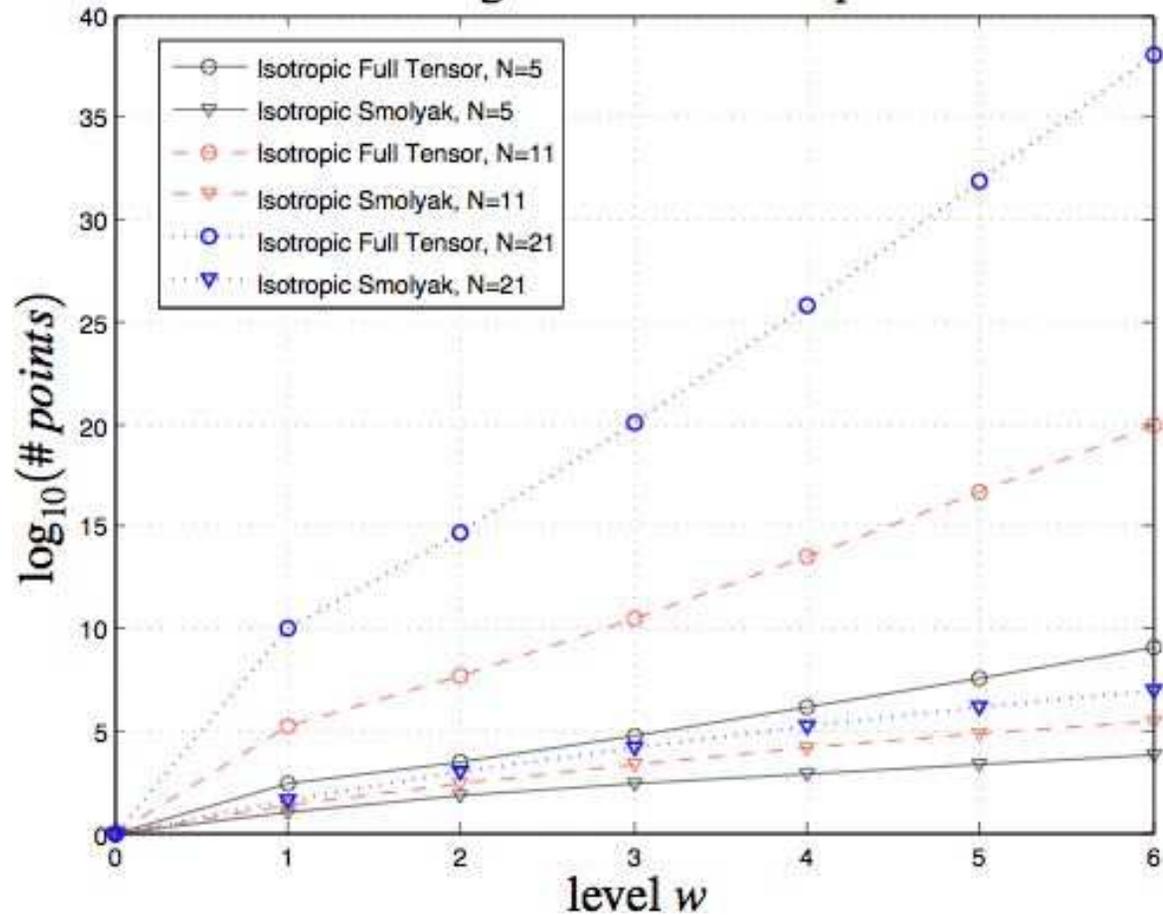
Smolyak C-C



Smolyak Gauss

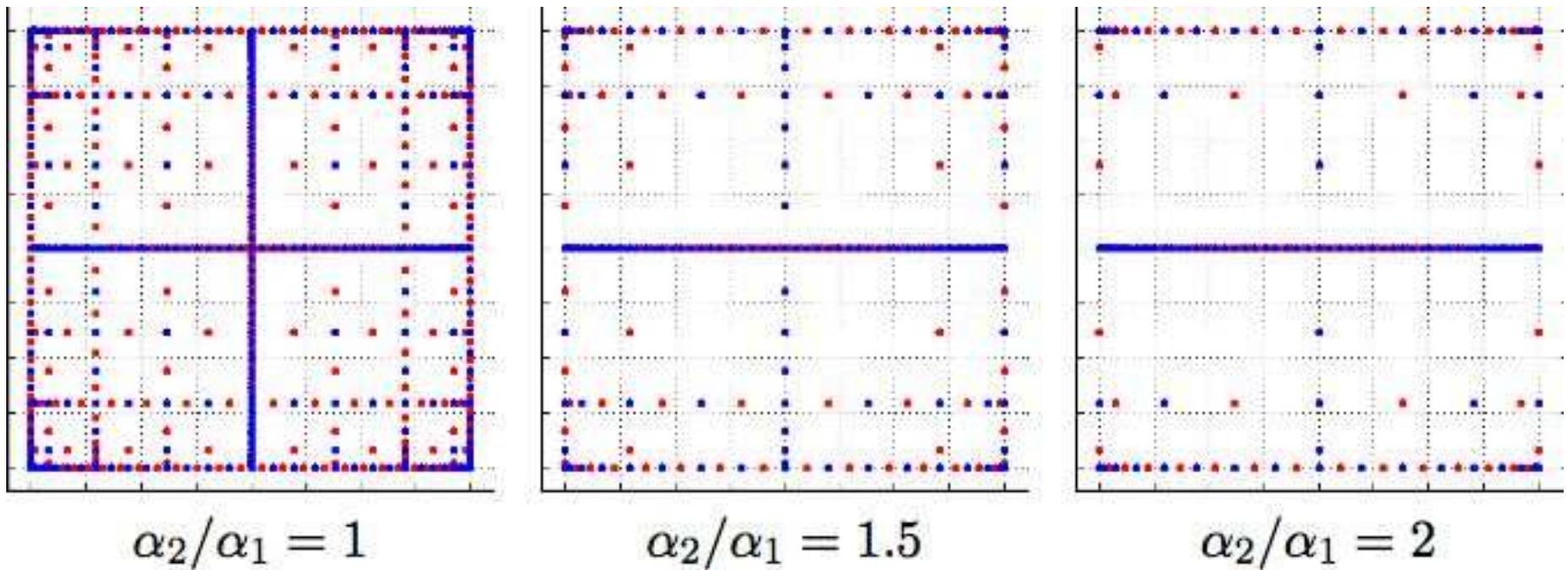
For  $N = 2$  and  $M = 5$ : comparison of full tensor product grids with two Smolyak grids

## Counting the Collocation points

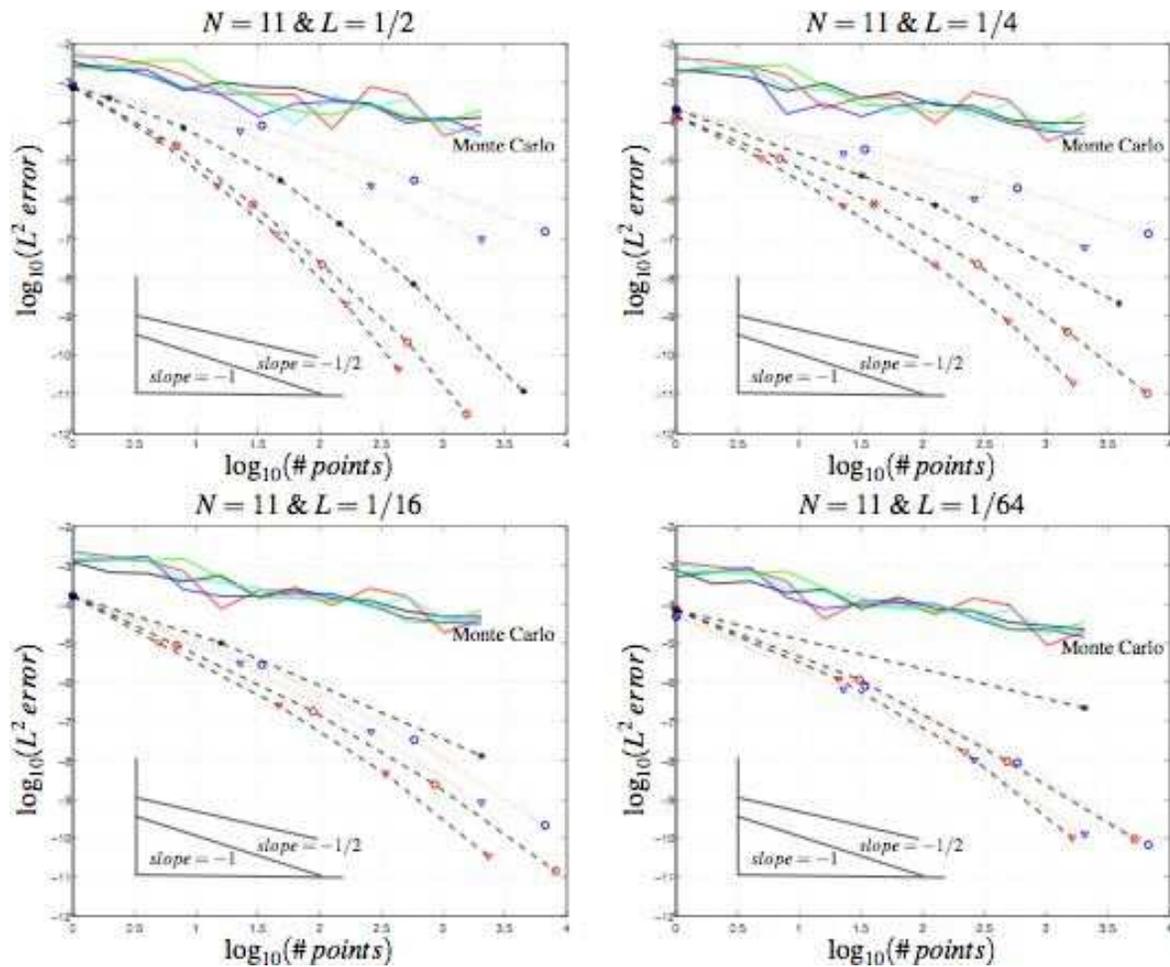


For  $N = 5, 11,$  and  $21$ : comparison of full tensor product grids with Clenshaw-Curtis-Smolyak grids for different levels, i.e., for different maximum number of points in each direction

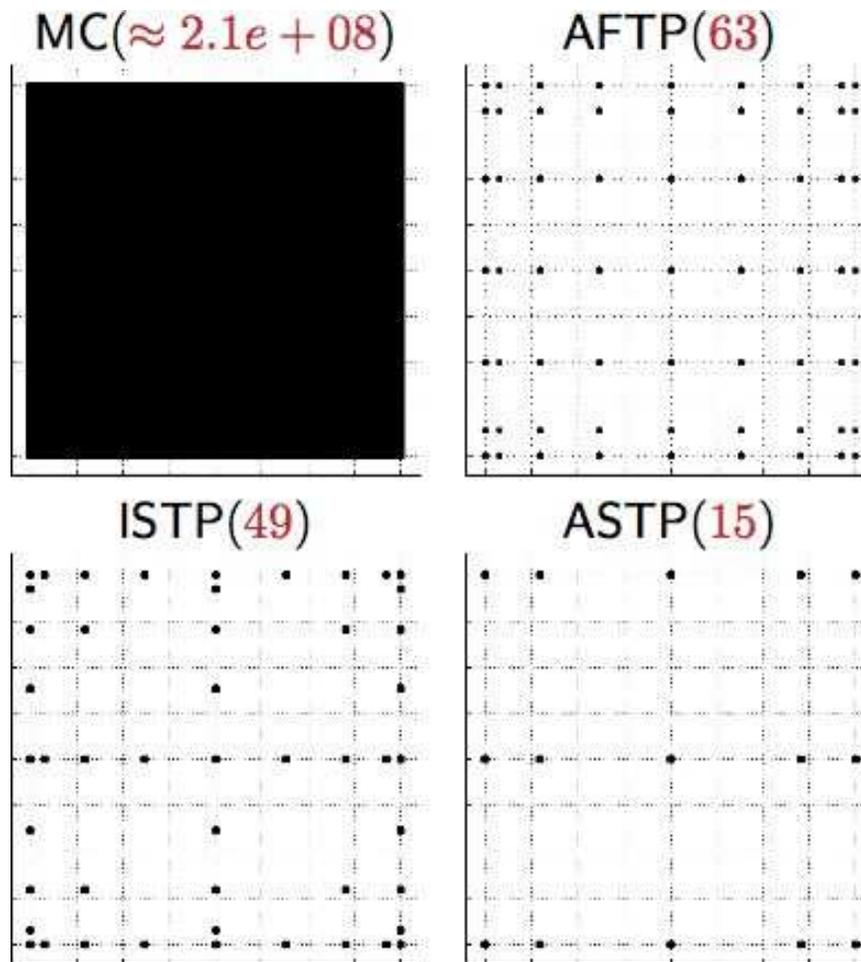
- There is more good news about Smolyak grids
- Recently, **anisotropic** Smolyak grids have been developed to take advantage of anisotropies in the relative importance of random parameters
- For example, in the Karhunen-Loève expansion for the colored noise case, the random variables  $y_1, y_2, \dots$  are increasingly less influential
- Adaptive strategies have been developed to determine how to take advantage of such anisotropies



Anisotropic Clenshaw-Curtis sparse grids for different levels of anisotropy; on the left is the isotropic case; the anisotropic grids will yield the same accuracy as the isotropic one, provided the integrand possesses the necessary anisotropy



$L^2$  errors in the expected values of the solution of an SPDE using different sampling strategies; Monte Carlo is always worst, anisotropic Smolyak best, with Clenshaw-Curtis being better than Gauss;  $L$  is a correlation length for the colored noise



Number of points needed to reduce the  $L^2$  errors in the expected values of the solution of an SPDE by a factor of  $10^4$

- This shows the effectiveness of using stochastic sampling methods along with modern sparse grid techniques

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**LOCAL POLYNOMIAL APPROXIMATING SPACES  
IN STOCHASTIC GALERKIN METHODS**

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# PIECEWISE POLYNOMIAL APPROXIMATING SPACES FOR PARAMETER SPACE DISCRETIZATION

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- Emulating finite element spatial discretization methods, one is led to locally-supported piecewise polynomial spaces for approximating functions of the random parameters
- One starts by “triangulating”  $\Gamma$ , the set of all possible values for the random parameters  $\{y_1, \dots, y_N\}$ 
  - of course, unless one wants to get fancy, i.e.,
    - use infinite elements or other methods for treating unbounded domainswe have to assume that  $\Gamma$  is bounded
  - thus, we consider problems for which the  $\Gamma_n$ ,  $n = 1, \dots, N$ , themselves are bounded
    - e.g., we cannot consider  $y_1$  to be a Gaussian random parameter since, in this case,  $\Gamma_1 = (-\infty, \infty)$
    - of course, we can consider truncated Gaussian parameters

- One then chooses  $Z_K$  to be a space of piecewise polynomial functions of degree less than or equal to  $M$ , defined with respect to the triangulation
  - since  $Z_K \subset L^q_\rho(\Gamma)$ , one can choose  $M = 0$ , i.e., **piecewise constant functions**
  - however, one can choose higher degree piecewise polynomials as well
  - one is free to choose **discontinuous finite element spaces**
- Unfortunately, the number of parameters  $N$  cannot be large
  - even for a subdivision with two elements in each direction,  $N$  cannot be big, e.g.,  $K = 2^N$  becomes prohibitively large very quickly

- Also, triangulating in high dimensions is not an easy task
  - unless  $N$  is small, one can in practice only consider the case of  $\Gamma$  being rectangular domain in  $\mathbb{R}^N$  that is “triangulated” into smaller rectangular domains
- One can choose a standard “finite element”-type basis set
  - $\{\psi_k(\vec{y})\}_{k=1}^K$  consists of compactly supported piecewise polynomials
  - if  $Z_K$  is a discontinuous (with respect to the triangulation of  $\Gamma$ ) finite element space, then each basis function can be chosen to have support over only a single element
  - if  $Z_K$  is a continuous (with respect to the triangulation of  $\Gamma$ ) finite element space, then each basis function can be chosen to have support over a small patch of elements

- There is a really big difference between using discontinuous and continuous finite element-type spaces to discretize in parameter space
- First, consider an example of a **continuous** finite element-type space
  - $\Gamma$  is a hypercube in  $N$ -dimensions ( $N =$  number of random parameters)
  - $\Gamma$  is subdivided into  $N_{\text{hypercubes}}$  smaller hypercubes
  - $Z_K$  consists of tensor products of **continuous** piecewise polynomials of degree less than or equal to  $M \geq 1$  in each parameter direction
  - then, the number of probabilistic degrees of freedom is given by
 
$$K = \left( M N_{\text{hypercubes}}^{1/N} + 1 \right)^N$$
  - as always, the discrete problem involves  $JK$  degrees of freedom  $c_{j,k}$

- If we look at the  $JK \times JK$  coefficient matrix for the discrete system (emanating from a linear Poisson problem)

$$\int_{\Gamma} \int_{\mathcal{D}} a(\mathbf{x}; \vec{y}) \nabla \phi_j(\mathbf{x}) \cdot \nabla \phi_{j'}(\mathbf{x}) \psi_k(\vec{y}) \psi_{k'}(\vec{y}) \rho(\vec{y}) d\mathbf{x} d\vec{y}$$

we see that it is sparse with respect to both the spatial and probabilistic indices

- if the support of  $\phi_j(\mathbf{x})$  and  $\phi_{j'}(\mathbf{x})$  do not overlap, then the corresponding matrix entry vanishes for all  $k$  and  $k'$
- if the support of  $\psi_k(\mathbf{x})$  and  $\psi_{k'}(\mathbf{x})$  do not overlap, then the corresponding matrix entry vanishes for all  $j$  and  $j'$
- this sparsity can be taken advantage of when one solves the system, especially if one uses an iterative method
- however, we still have a **coupled (albeit sparse)  $JK \times JK$  system to solve**

- Now, consider an example of using **discontinuous** finite element-type spaces to discretize in parameter space
  - $\Gamma$  is a hypercube in  $N$ -dimensions ( $N =$  number of random parameters)
  - $\Gamma$  is subdivided into  $N_{\text{hypercubes}}$  smaller hypercubes
  - in each element,  $Z_K$  consists of complete polynomials of degree less than or equal to  $M \geq 0$ 
    - no continuity is required across element boundaries
  - then, the number of probabilistic degrees of freedom is given by
 
$$K = N_{\text{hypercubes}} \left( \frac{(N + M)!}{N!M!} \right)$$
 which can be larger than that obtained using continuous finite element-type spaces
  - as always, the discrete problem involves  $JK$  degrees of freedom  $c_{j,k}$

Piecewise polynomial approximation in parameter space

$N =$ no. random parameters	$M =$ maximal degree of polynomials	$N_{\text{hypercubes}}^{1/N} =$ no. of intervals in each direction	$K =$ no. of probabilistic degrees of freedom	
			continuous tensor product basis	discontinuous basis
3	0	5	–	125
		10	–	1,000
	1	5	216	500
		10	1,331	4,000
	2	5	1,331	1,250
		10	9,261	10,000
5	0	5	–	3,125
		10	–	100,000
	1	5	7,776	18,750
		10	161,051	600,000
	2	5	161,051	65,625
		10	4,084,101	2,100,000

- But, let's examine the  $JK \times JK$  coefficient matrix for the discrete system in the discontinuous finite element case

$$\int_{\Gamma} \int_{\mathcal{D}} a(\mathbf{x}; \vec{y}) \nabla \phi_j(\mathbf{x}) \cdot \nabla \phi_{j'}(\mathbf{x}) \psi_k(\vec{y}) \psi_{k'}(\vec{y}) \rho(\vec{y}) d\mathbf{x} d\vec{y}$$

- again, we have the usual sparsity with respect to both the spatial indices
- but now, since the support of the probabilistic basis functions  $\{\psi_k(\vec{y})\}_{k=1}^K$  is restricted to a single element in parameter space, we have that
  - with respect to parameter space, the matrix is block diagonal
  - there is a complete uncoupling of the probabilistic degrees of freedom

- Let  $\Gamma_{hypercube}$  denote one of the  $N_{hypercubes}$  elements in the subdivision of  $\Gamma$  into smaller hypercubes
- Let  $K_{hypercube}$  denote the probabilistic degrees of freedom in each element  $\Gamma_{hypercube}$ , i.e.,

$$K_{hypercube} = \frac{(N + M)!}{N!M!} = \frac{K}{N_{hypercubes}}$$

- For each of the  $N_{hypercubes}$  elements  $\Gamma_{hypercube}$ , let

$$I_{hypercube} = \left\{ k \in \{1, \dots, K\} \mid \text{supp}(\psi_k(\vec{y})) \subset \Gamma_{hypercube} \right\}$$

- note that the cardinality of the index set  $I_{hypercube}$  is  $K_{hypercube}$

- Then, the coupled  $JK \times JK$  system for the degrees of freedom  $c_{j,k}$  uncouples into  $N_{\text{hypercubes}}$  systems, each of size  $JK_{\text{hypercube}} \times JK_{\text{hypercube}}$

$$\int_{\mathcal{D}} \int_{\Gamma} \rho(\vec{y}) S \left( \sum_{j=1}^J \sum_{k=1}^K c_{jk} \phi_j(\mathbf{x}) \psi_k(\vec{y}), \vec{y} \right) T \left( \phi_{j'}(\mathbf{x}) \right) \psi_{k'}(\vec{y}) d\mathbf{x} d\vec{y}$$

$$= \int_{\mathcal{D}} \int_{\Gamma} \rho(\vec{y}) \phi_{j'}(\mathbf{x}) \psi_{k'}(\vec{y}) f(\vec{y}) d\mathbf{x} d\vec{y}$$

for  $j' \in \{1, \dots, J\}$  and  $k' \in \{1, \dots, K\}$

$$\sum_{j=1}^J \sum_{k \in I_{\text{hypercube}}} c_{j,k} \int_{\Gamma_{\text{hypercube}}} \int_{\mathcal{D}} a \nabla \phi_j(\mathbf{x}) \cdot \nabla \phi_{j'}(\mathbf{x}) \psi_k(\vec{y}) \psi_{k'}(\vec{y}) \rho(\vec{y}) d\mathbf{x} d\vec{y}$$

$$= \int_{\Gamma_{\text{hypercube}}} \int_{\mathcal{D}} f \phi_{j'}(\mathbf{x}) \psi_{k'}(\vec{y}) \rho(\vec{y}) d\mathbf{x} d\vec{y}$$

for all  $j' = 1, \dots, J$  and  $k' \in I_{\text{hypercube}}$

- The moral of the story is that, in practice, one pretty much has to settle for piecewise constant approximations in parameter space
- Even for this case,  $N$  cannot be too large

## PIECEWISE CONSTANT APPROXIMATING SPACES

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- Let  $\cup_{k=1}^K \Gamma_k$  denote a subdivision of  $\Gamma$  into disjoint, non-overlapping subsets

— we have that

$$\cup_{k=1}^K \bar{\Gamma}_k = \bar{\Gamma} \quad \text{and} \quad \Gamma_k \cap \Gamma_{k'} = \emptyset \quad \text{if } k \neq k'$$

- Let

$$\psi_k(\vec{y}) = \begin{cases} 1 & \text{if } \vec{y} \in \Gamma_k \\ 0 & \text{otherwise} \end{cases} \quad \text{for } k \in \{1, \dots, K\}$$

and let

$$Z_K = \text{span} \{ \psi_k \}_{k=1}^K$$

- thus,  $Z_K$  is the space of **piecewise constant functions** with respect to the partition  $\cup_{k=1}^K \Gamma_k$  of  $\Gamma$

- Clearly,  $Z_K \subset L^p_\rho(\Gamma)$  so that it can be used as an approximating space for discretizing parameter dependences of solution of an SPDE
- Recall that, after the invocation of the piecewise constant basis functions and of a parameter-space quadrature rule, the stochastic Galerkin method has the form

$$\begin{aligned}
& \sum_{r=1}^R w_r \rho(\vec{y}_r) \psi_{k'}(\vec{y}_r) \int_{\mathcal{D}} S\left(\sum_{j=1}^J \sum_{k=1}^K c_{jk} \phi_j(\mathbf{x}) \psi_k(\vec{y}_r), \vec{y}_r\right) T\left(\phi_{j'}(\mathbf{x})\right) d\mathbf{x} \\
&= \sum_{r=1}^R w_r \rho(\vec{y}_r) \psi_{k'}(\vec{y}_r) \int_{\mathcal{D}} \phi_{j'}(\mathbf{x}) f(\vec{y}_r) d\mathbf{x} \\
&\quad \text{for } j' \in \{1, \dots, J\} \text{ and } k' \in \{1, \dots, K\}
\end{aligned}$$

where  $\{w_r, \vec{y}_r\}_{r=1}^R$  denotes the quadrature rule used to approximate integrals over parameter space  $\Gamma$

- Suppose we choose the quadrature rule so that

$$R = K \quad \text{and} \quad \vec{y}_r \in \Gamma_r \quad \text{for } r \in \{1, \dots, R = K\}$$

– thus,

- each quadrature point  $\vec{y}_r$  belongs to one of the subsets  $\Gamma_k$

and

- each subset contains one and only one of the quadrature points

– Clearly, we then have that

$$\psi_k(\vec{y}_r) = \delta_{kr} \quad \text{for all } k, r \in \{1, \dots, K = R\}$$

- Then, the discretized stochastic Galerkin system reduces to

$$\int_{\mathcal{D}} S\left(u_r(\mathbf{x}), \vec{y}_r\right) T\left(\phi_{j'}(\mathbf{x})\right) d\mathbf{x} = \int_{\mathcal{D}} \phi_{j'}(\mathbf{x}) f(\vec{y}_r) d\mathbf{x}$$

$$\text{for } j' \in \{1, \dots, J\} \quad \text{and} \quad r \in \{1, \dots, R = K\}$$

where  $u_r(\mathbf{x}) = \sum_{j=1}^J c_{jr} \phi_j(\mathbf{x})$

- thus, we have total uncoupling of the spatial and parameter problems
- we solve a sequence of  $R = K$  problems of size  $J$  to determine  $\{u_r(\mathbf{x})\}_{r=1}^R$
- then, the stochastic Galerkin-piecewise constant approximation of the solution of the SPDE is simply given by

$$u(\mathbf{x}; \vec{y}) = u_r(\mathbf{x}) \quad \text{for } \vec{y} \in \Gamma_r$$

- Note that to determine the  $u_r(\mathbf{x})$  one does not have to explicitly know the weights  $w_r$  or the subregions  $\Gamma_k$ 
  - one need only know the point set  $\{\vec{y}_k\}_{k=1}^K$
- Note also that there is no restrictions on the point set  $\{\vec{y}_k\}_{k=1}^K$ 
  - one can, in fact, use any of the point sets we have encountered in discussing stochastic sampling or stochastic collocation or stochastic Galerkin methods
- Clearly,  
**any stochastic sampling method can be viewed  
as a stochastic Galerkin method**

## Approximations of quantities of interest

---

- It is natural to use the same quadrature rule
  - to approximate a quantity of interestas was used to
  - approximate the integrals in discretized SPDE,i.e., we choose

$$K = R = Q$$

$$\{\vec{y}_k\}_{k=1}^K = \{\vec{y}_r\}_{r=1}^R = \{\vec{y}_q\}_{q=1}^Q \quad \text{and} \quad \{w_r\}_{r=1}^R = \{w_q\}_{q=1}^Q$$

- We then have that

$$\psi_r(\vec{y}_q) = \delta_{rq} \quad \text{for all } r, q \in \{1, \dots, K = R = Q\}$$

- Using this in the expression for the approximation of a quantity of interest results in

$$\begin{aligned} \int_{\Gamma} G(u(\mathbf{x}; \vec{y})) \rho(\vec{y}) d\vec{y} &\approx \sum_{q=1}^Q w_q \rho(\vec{y}_q) G(u_{SC}(\mathbf{x})) \\ &= \sum_{q=1}^Q w_q \rho(\vec{y}_q) G\left(\sum_{r=1}^R u_r(\mathbf{x}) \psi_r(\vec{y}_q)\right) = \sum_{q=1}^Q w_q \rho(\vec{y}_q) G(u_q(\mathbf{x})) \end{aligned}$$

i.e.,

$$\int_{\Gamma} G(u(\mathbf{x}; \vec{y})) \rho(\vec{y}) d\vec{y} \approx \sum_{q=1}^Q w_q \rho(\vec{y}_q) G(u_q(\mathbf{x}))$$

where, for  $q \in \{1, \dots, Q = R = K_{LI}\}$ ,  $u_q(\mathbf{x}) = \sum_{j=1}^J c_{jq} \phi_j(\mathbf{x})$

is determined from

$$\int_{\mathcal{D}} S(u_q(\mathbf{x}), \vec{y}_q) T(\phi_{j'}(\mathbf{x})) d\mathbf{x} = \int_{\mathcal{D}} \phi_{j'}(\mathbf{x}) f(\vec{y}_q) d\mathbf{x} \quad \text{for } j' \in \{1, \dots, J\}$$

- This all looks very familiar:
  - it looks just the same as when we discussed stochastic collocation methods
  - in fact, there is very little distinction between stochastic sampling and stochastic collocation methods
  - and, as we have seen, all stochastic sampling and stochastic collocation methods can be derived from the stochastic Galerkin framework

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**ECONOMIES IN POLYNOMIAL CHAOS METHODS  
FOR LINEAR SPDES**

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- Suppose that the SPDE is **linear in the solution  $u$**
- For example, consider the case for which one has, after using a polynomial chaos expansion method, the SPDE<sup>†</sup>

$$\int_{\mathcal{D}} \int_{\Gamma} \rho(\vec{y}) a(\mathbf{x}; \vec{y}) S \left( \sum_{j=1}^J \sum_{k=1}^{K_{PC}} c_{jk} \phi_j(\mathbf{x}) \Psi_k(\vec{y}) \right) T \left( \phi_{j'}(\mathbf{x}) \right) \Psi_{k'}(\vec{y}) d\mathbf{x} d\vec{y}$$

$$= \int_{\mathcal{D}} \int_{\Gamma} \rho(\vec{y}) \phi_{j'}(\mathbf{x}) \Psi_{k'}(\vec{y}) f(\mathbf{x}; \vec{y}) d\mathbf{x} d\vec{y},$$

where now both  $S(\cdot)$  and  $T(\cdot)$  are **linear**

---

<sup>†</sup>Here, it is useful to follow the explicit dependences of the data functions  $a$  and  $f$  on the spatial variable  $\mathbf{x}$

- Since,  $S(\cdot)$  is linear and does not involve derivatives with respect to the components of  $\vec{y}$ , we have that

$$\begin{aligned} \sum_{j=1}^J \sum_{k=1}^{K_{PC}} c_{jk} \int_{\mathcal{D}} S(\phi_j(\mathbf{x})) T(\phi_{j'}(\mathbf{x})) \int_{\Gamma} a(\mathbf{x}; \vec{y}) \rho(\vec{y}) \Psi_k(\vec{y}) \Psi_{k'}(\vec{y}) d\vec{y} d\mathbf{x} \\ = \int_{\mathcal{D}} \phi_{j'}(\mathbf{x}) \int_{\Gamma} f(\mathbf{x}; \vec{y}) \rho(\vec{y}) \Psi_{k'}(\vec{y}) d\vec{y} d\mathbf{x} \end{aligned}$$

- In this **linear SPDE** case, there are two economies possible in the implementation of PC methods

## PC-expansions of data functions

---

- We approximate the data functions  $a$  and  $f$  in the same way one approximates the solution, i.e., using PC-expansions
  - thus, we assume we have in hand the approximations

$$a(\mathbf{x}; \vec{y}) \approx \sum_{k''=1}^{K_{PC}} a_{k''}(\mathbf{x}) \Psi_{k''}(\vec{y})$$

and

$$f(\mathbf{x}; \vec{y}) \approx \sum_{k''=1}^{K_{PC}} f_{k''}(\mathbf{x}) \Psi_{k''}(\vec{y})$$

- substituting into the PC-discretization of the SPDE results in

$$\begin{aligned}
& \sum_{k''=1}^{K_{PC}} \sum_{j=1}^J \sum_{k=1}^{K_{PC}} c_{jk} \left( \int_{\mathcal{D}} a_{k''}(\mathbf{x}) S(\phi_j(\mathbf{x})) T(\phi_{j'}(\mathbf{x})) d\mathbf{x} \right) \\
& \qquad \qquad \qquad \left( \int_{\Gamma} \rho(\vec{y}) \Psi_k(\vec{y}) \Psi_{k'}(\vec{y}) \Psi_{k''}(\vec{y}) d\vec{y} \right) \\
& = \sum_{k''=1}^{K_{PC}} \left( \int_{\mathcal{D}} f_{k''}(\mathbf{x}) \phi_{j'}(\mathbf{x}) d\mathbf{x} \right) \left( \int_{\Gamma} \rho(\vec{y}) \Psi_{k'}(\vec{y}) \Psi_{k''}(\vec{y}) d\vec{y} \right) \\
& = \int_{\mathcal{D}} f_k(\mathbf{x}) \phi_{j'}(\mathbf{x}) d\mathbf{x}
\end{aligned}$$

where the last equality follows from the orthonormality of the PC-basis functions  $\{\Psi_k(\vec{y})\}_{k=1}^{K_{PC}}$

- orthogonality also results in some **sparsity** in the left-hand side that may be taken advantage of when using iterative linear system solution methods
  - for example, whenever  $k + k' \neq k''$  (and for similar situations involving reversal of indices), the summand on the left-hand side vanishes

- Determining the PC-approximations of the data functions  $a$  and  $f$  may be costly since one has to determine a different expansion for every spatial quadrature point used in the finite element spatial discretization
  - of course, if the data is independent of  $\mathbf{x}$ , then only one expansion for each data function is needed
- We again point out that the economies resulting from the use of PC-expansions of the data functions are realizable only for **linear SPDEs**

## KL-expansions of random data fields

---

- Now, suppose that the data functions  $a$  and  $f$  are **Gaussian** correlated random fields

- then, we may determine the approximate KL-expansions

$$a(\mathbf{x}; \vec{y}) \approx \sum_{n=1}^N \sqrt{\lambda_n} a_n(\mathbf{x}) y_n$$

and

$$f(\mathbf{x}; \vec{y}) \approx \sum_{n=1}^N \sqrt{\sigma_n} f_n(\mathbf{x}) y_n,$$

- $\{\lambda_n, a_n(\mathbf{x})\}_{n=1}^{\infty}$  and  $\{\sigma_n, f_n(\mathbf{x})\}_{n=1}^{\infty}$  are the eigenpairs of the covariance functions for  $a$  and  $f$ , respectively
- recall that we have to assume (spherical) Gaussian variables since otherwise  $\vec{y}$  is not a set of independent parameters

– substituting into the PC-discretization of the **linear** SPDE results in

$$\begin{aligned} & \sum_{j=1}^J \sum_{k=1}^{K_{PC}} c_{jk} \sum_{n=1}^N \sqrt{\lambda_n} \left( \int_{\mathcal{D}} a_n(\mathbf{x}) S(\phi_j(\mathbf{x})) T(\phi_{j'}(\mathbf{x})) d\mathbf{x} \right) \\ & \qquad \qquad \qquad \left( \int_{\Gamma} y_n \rho(\vec{y}) \Psi_k(\vec{y}) \Psi_{k'}(\vec{y}) d\vec{y} \right) \\ & = \sum_{n=1}^N \sqrt{\sigma_n} \left( \int_{\mathcal{D}} f_n(\mathbf{x}) \phi_{j'}(\mathbf{x}) d\mathbf{x} \right) \left( \int_{\Gamma} y_n \rho(\vec{y}) \Psi_{k'}(\vec{y}) d\vec{y} \right) \end{aligned}$$

• **Doubly** orthogonal polynomials can be constructed<sup>†</sup> such that

$$\int_{\Gamma} \Psi_k(\vec{y}) \Psi_{k'}(\vec{y}) \rho(\vec{y}) d\vec{y} = 0 \quad \text{and} \quad \int_{\Gamma} \vec{y} \Psi_k(\vec{y}) \Psi_{k'}(\vec{y}) \rho(\vec{y}) d\vec{y} = 0$$

whenever  $k \neq k'$

---

<sup>†</sup>The construction involves solving an eigenvalue problem for each polynomial

- As a result, **the probabilistic and spatial degrees of freedom uncouple**
  - one can solve for the  $c_{ij}$ 's by solving  $K_{PC}$  deterministic finite element problems of size  $J$  instead of the single problem of size  $JK_{PC}$
- We again point out that the economies resulting from the use of KL-expansions of the data random fields are realizable only for **linear SPDEs**
- Moreover, even for linear SPDEs, they are only possible for **Gaussian random fields** since it is only in this case that the KL expansions are linear in independent random parameters
- This should be contrasted with stochastic collocation methods and the non-intrusive polynomial chaos methods for which the uncoupling of the parameter and spatial degrees of freedom occurs for general, nonlinear SPDEs
  - for stochastic collocation methods, the uncoupling also occurs for general, non-Gaussian probability distributions

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**OPTIMAL CONTROL PROBLEMS FOR  
STOCHASTIC PARTIAL DIFFERENTIAL EQUATIONS**

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## Optimization problems

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- The state system

$$-\nabla \cdot (\kappa(\omega, \mathbf{x}) \nabla u(\omega, \mathbf{x})) = f(\omega, \mathbf{x}) \quad \text{in } \Omega \times D$$

$$u(\omega, \mathbf{x}) = 0 \quad \text{on } \Omega \times \partial D$$

- $\omega$  is an elementary event in a probability space  $\Omega$
- $\mathbf{x}$  is a point in the spatial domain  $D$
- $\kappa(\omega, \mathbf{x})$  and  $f(\omega, \mathbf{x})$  are correlated random fields
- the solution  $u(\omega, \mathbf{x})$  is also a random field

- Optimal control problem

- $\kappa(\omega, \mathbf{x})$  is given

- $f(\omega, \mathbf{x})$  to be determined

- given target function  $\hat{u}(\omega, \mathbf{x})$  may be deterministic or may be a random field

- cost functional ( $E(\cdot)$  denotes the expected value)

$$\mathcal{F}(u, f; \hat{u}) = E\left(\|u(\omega, \cdot) - \hat{u}(\omega, \cdot)\|_{L^2(D)}^2 + \alpha \|f(\omega, \cdot)\|_{L^2(D)}^2\right)$$

⇒

find a state  $u$  and a control  $f$  such that  $\mathcal{F}(u, f; \hat{u})$  is minimized subject to the state system being satisfied

- Parameter identification problem

- $f(\omega, \mathbf{x})$  is given

- $\kappa(\omega, \mathbf{x})$  to be determined

- given target function  $\hat{u}(\omega, \mathbf{x})$  may be deterministic or may be a random field

- cost functional

$$\mathcal{K}(u, \kappa; \hat{u}) = \mathbf{E} \left( \|u(\omega, \cdot) - \hat{u}(\omega, \cdot)\|_{L^2(D)}^2 + \beta \|\nabla \kappa(\omega, \cdot)\|_{L^2(D)}^2 \right)$$

⇒

find a state  $u$  and a coefficient function  $\kappa$  such that  $\mathcal{K}(u, \kappa; \hat{u})$  is minimized subject to the state system being satisfied

## Results

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- Existence of optimal solutions
- Existence of Lagrange multipliers
- Derivation of optimality system

– the adjoint or co-state system

$$-\nabla \cdot (\kappa(\omega, \mathbf{x}) \nabla \xi(\omega, \mathbf{x})) = -(u(\omega, \mathbf{x}) - \hat{u}(\omega, \mathbf{x})) \quad \text{in } \Omega \times D$$

$$\xi(\omega, \mathbf{x}) = 0 \quad \text{on } \Omega \times \partial D$$

– optimality condition

$$\mathbb{E}(-\beta \Delta \kappa + \nabla u \cdot \nabla \xi) = 0$$

- Discretization of noise so that  $\kappa$ ,  $f$ ,  $\hat{u}$ , and  $u$  depend on a parameter vector  $\vec{y}(\omega) = (y_1(\omega), \dots, y_N(\omega))^T$ 
  - these parameters may be “knobs” in an experiment
  - alternately, they could result from an approximation, e.g., a truncated Karhunen-Loevy expansion, of a correlated random field
- finite element analyses of stochastic collocation method (in progress)
  - isotropic and anisotropic Smolyak sparse grids are used as collocation points
- development of gradient method to effect optimization

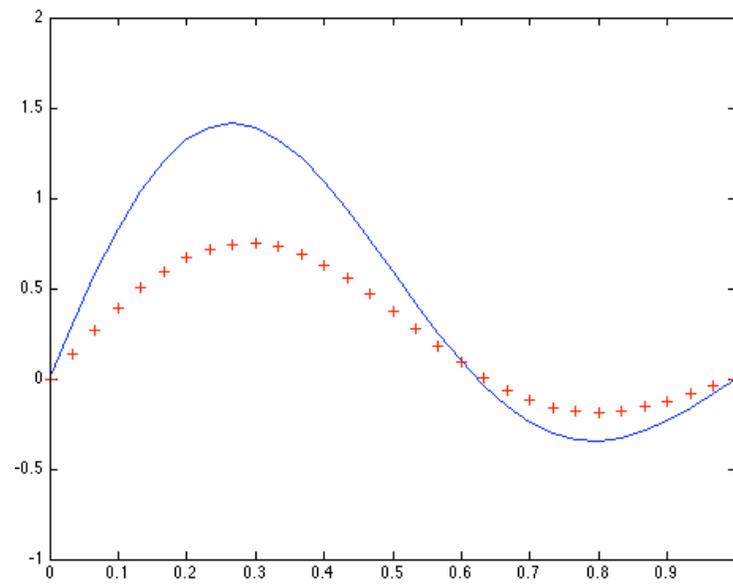
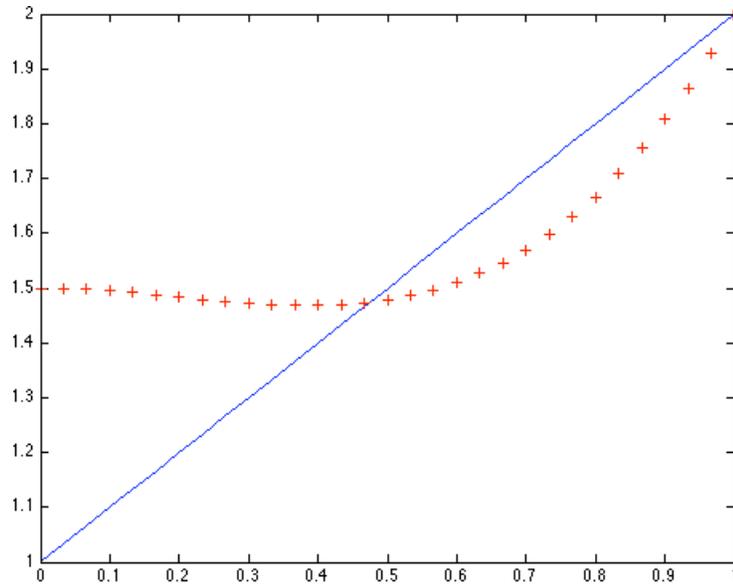
## Computational results

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- choose target  $\hat{u} = x(1 - x^2) + \sum_{i=1}^N \sin\left(\frac{n\pi x}{L}\right) y_n(\omega)$
- choose optimal  $\kappa = (1 + x^3) + \sum_{i=1}^N \cos\left(\frac{n\pi x}{L}\right) y_n(\omega)$
- set  $f = -\nabla \cdot (\kappa \nabla \hat{u})$
- choose initial  $\kappa = 1 + x$
- assume  $y_i$  uniform on  $[-1, 1]$  with  $E(y_i) = 0$  and  $E(y_i y_j) = \delta_{ij}$



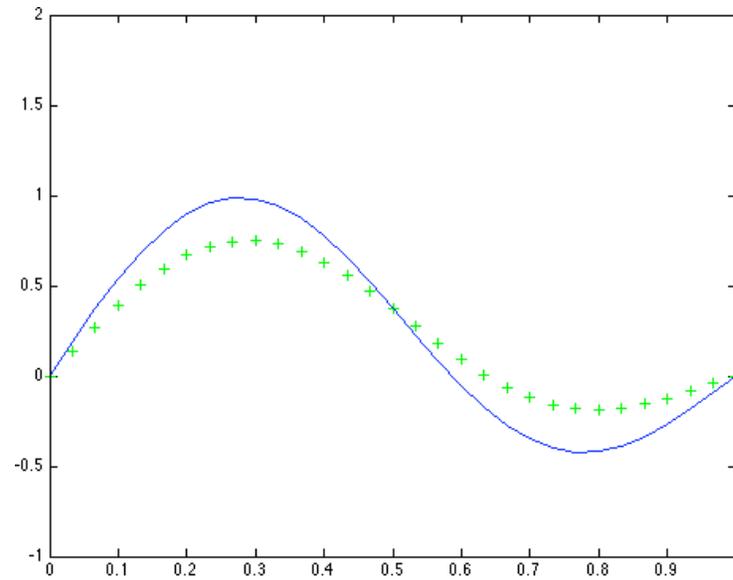
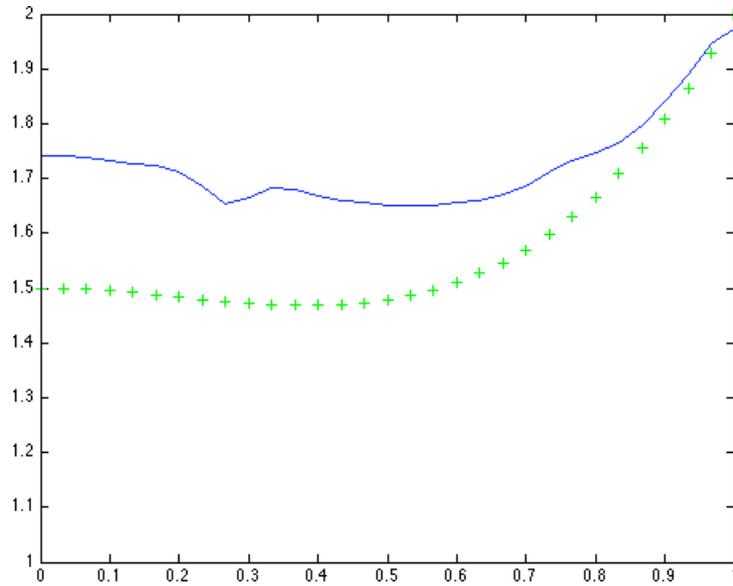
given random  $f$  and  $\hat{u}$ , identify the expectation of both the control  $E(\kappa)$  and the state  $E(u)$  and compare with the exact statistical quantities



Left: expected value of initial (blue) and target (red) coefficient  $\kappa$

Right: expected value of initial and target solution  $u$

Number of random variables =  $N = 1$

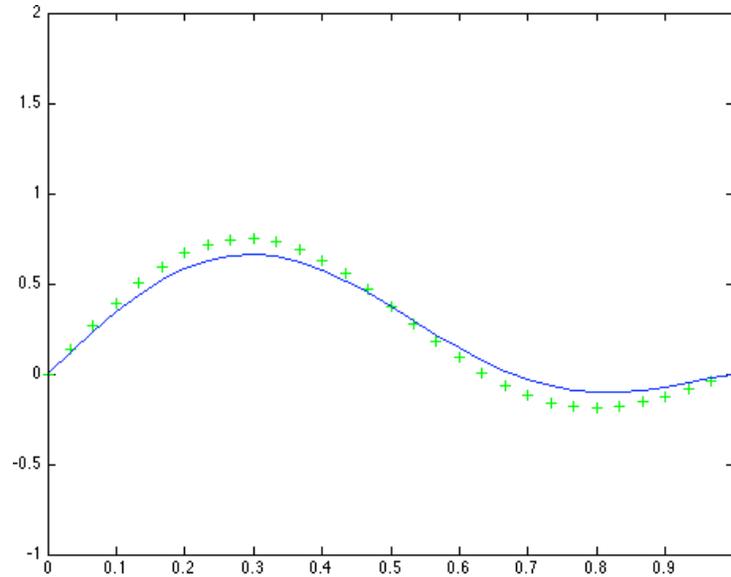
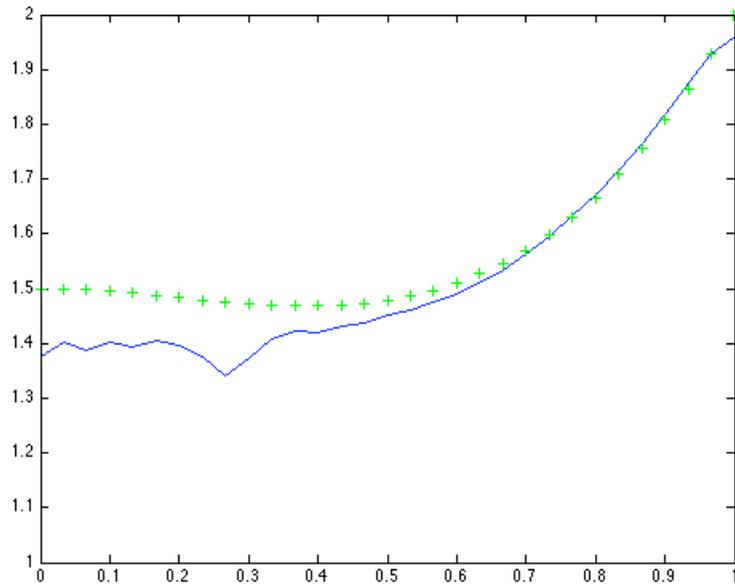


Left: expected value of optimal and target coefficient  $\kappa$

Right: expected value of optimal and target solution  $u$

Number of random variables =  $N = 1$

Number of Monte Carlo samples =  $M = 1$

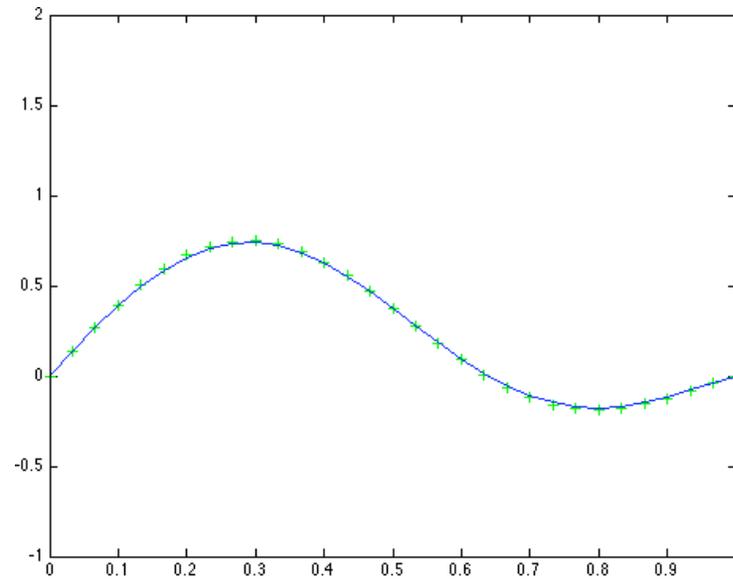
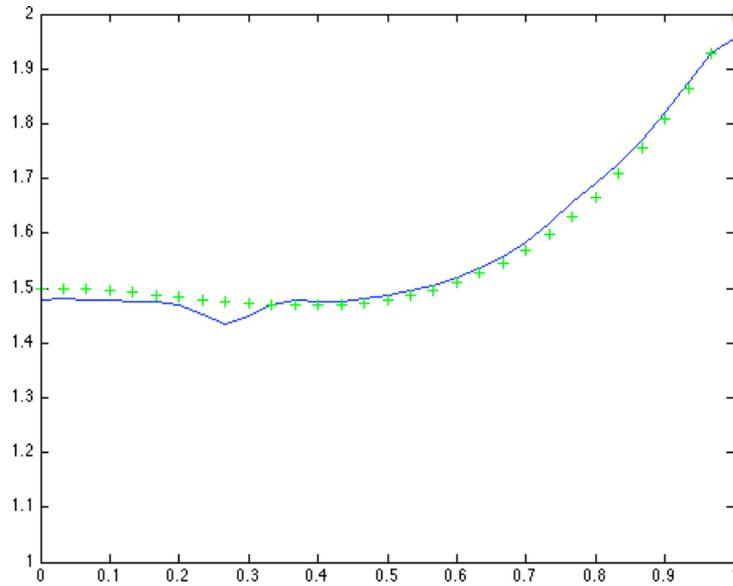


Left: expected value of optimal and target coefficient  $\kappa$

Right: expected value of optimal and target solution  $u$

Number of random variables =  $N = 1$

Number of Monte Carlo samples =  $M = 10$

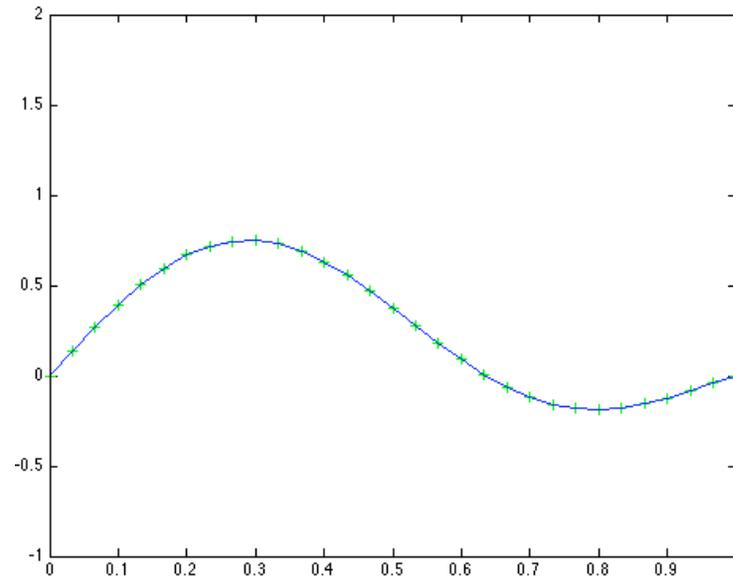
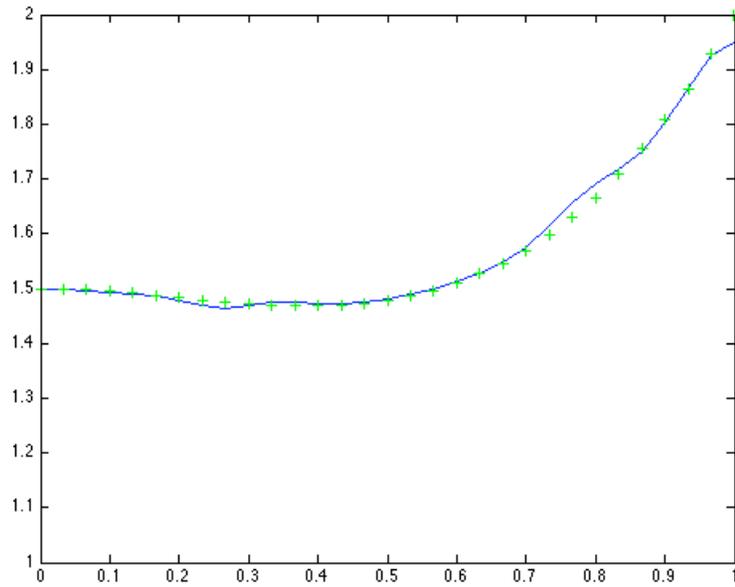


Left: expected value of optimal and target coefficient  $\kappa$

Right: expected value of optimal and target solution  $u$

Number of random variables =  $N = 1$

Number of Monte Carlo samples =  $M = 100$

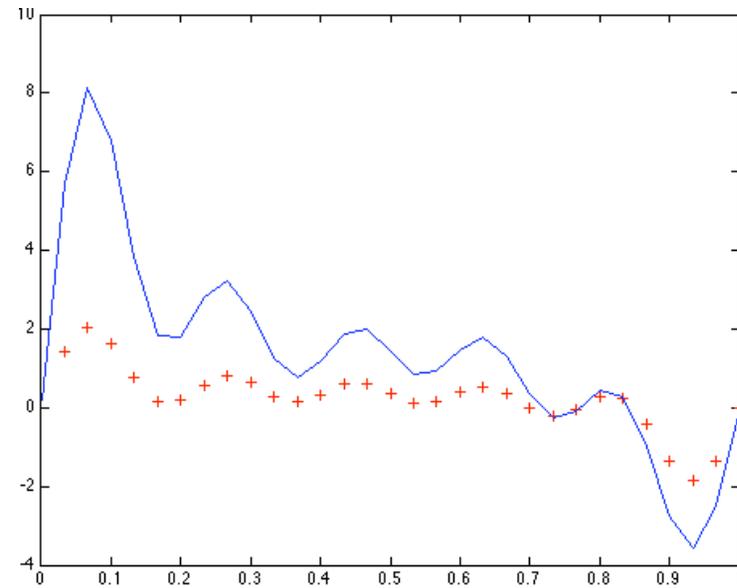
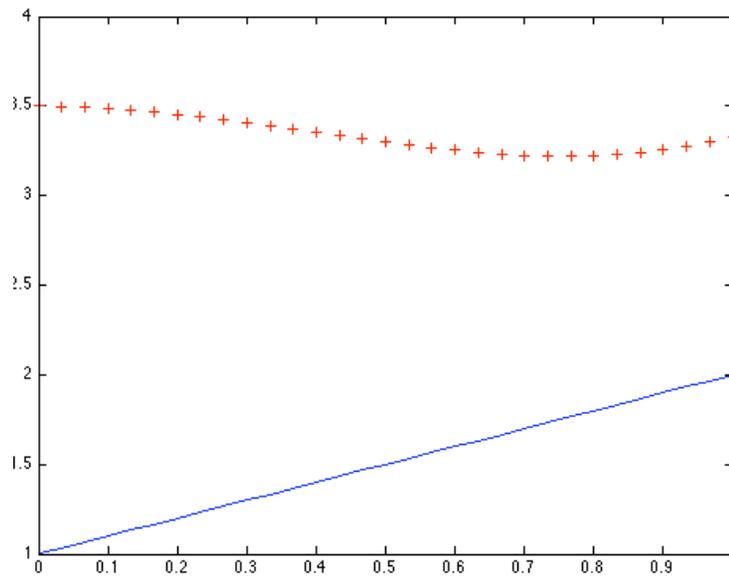


Left: expected value of optimal and target coefficient  $\kappa$

Right: expected value of optimal and target solution  $u$

Number of random variables =  $N = 1$

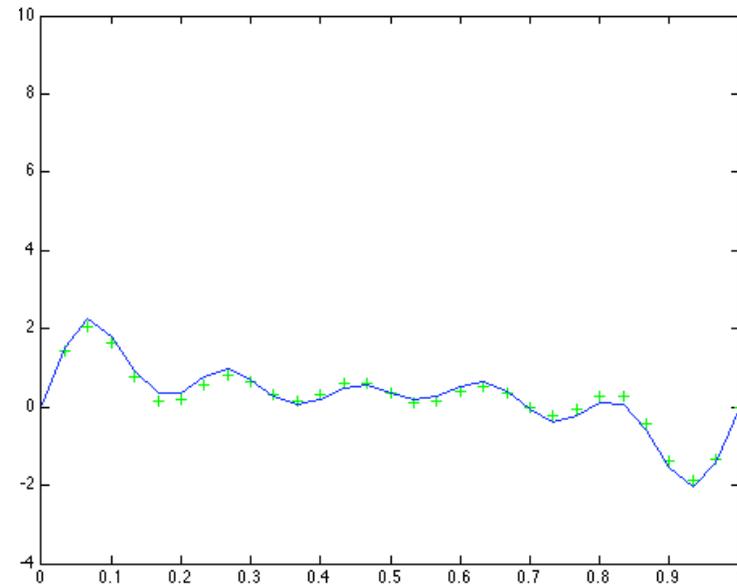
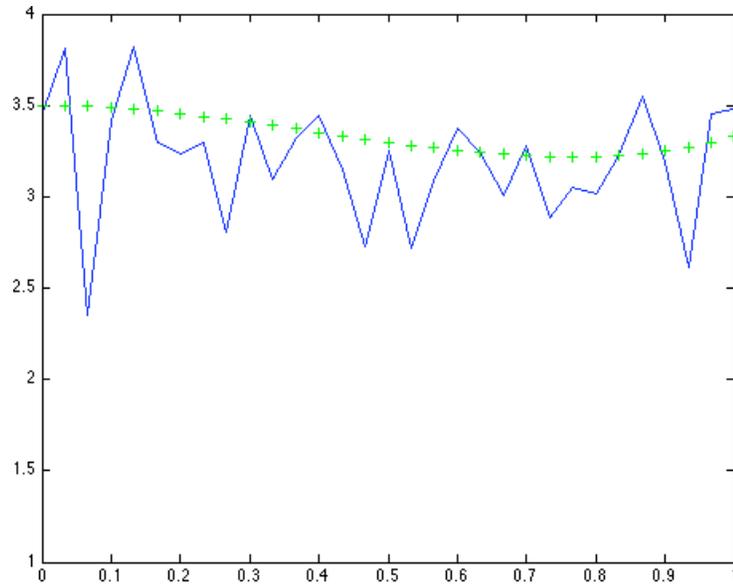
Number of anisotropic Smolyak collocation points =  $M = 1$



Left: expected value of initial (blue) and target (red) coefficient  $\kappa$

Right: expected value of initial and target solution  $u$

Number of random variables =  $N = 5$

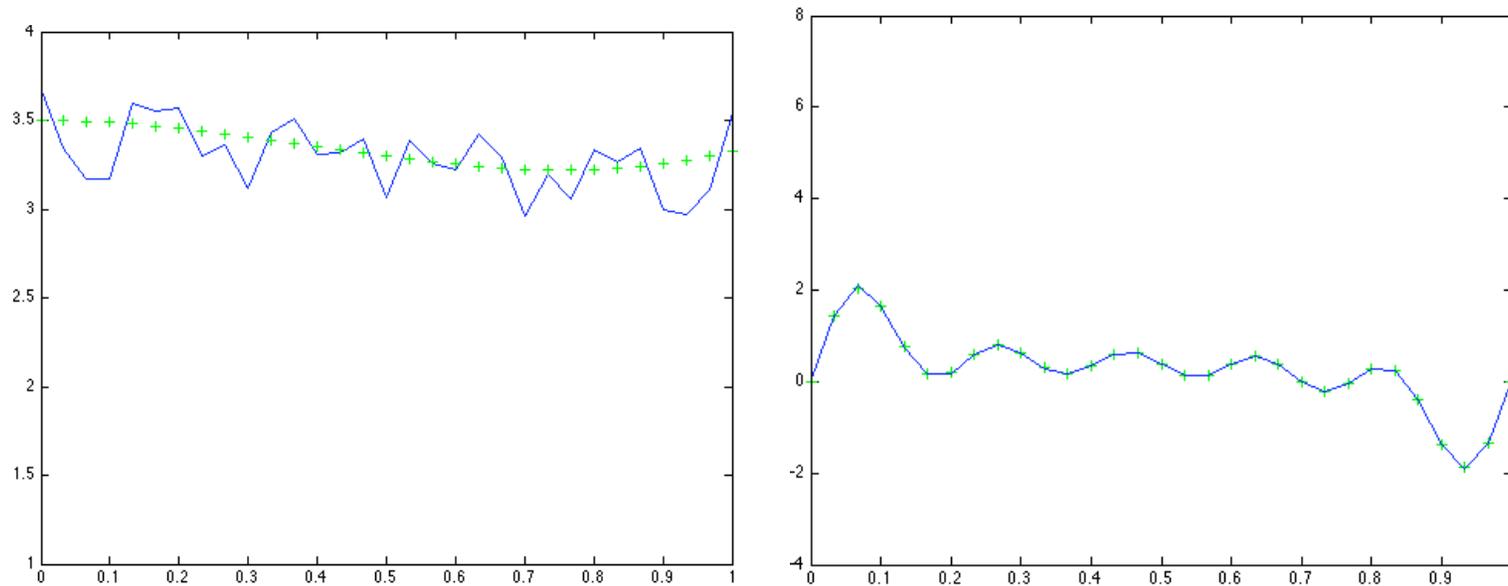


Left: expected value of optimal and target coefficient  $\kappa$

Right: expected value of optimal and target solution  $u$

Number of random variables =  $N = 5$

Number of Monte Carlo samples =  $M = 11$



Left: expected value of optimal and target coefficient  $\kappa$

Right: expected value of optimal and target solution  $u$

Number of random variables =  $N = 5$

Number of anisotropic Smolyak collocation points =  $M = 11$

$N$	MC	AS
5	7e+03	801
10	9e+06	1581
20	8e+09	11561

For  $N$  random parameters, the number of Monte Carlo samples and the number of anisotropic Smolyak collocation points required to reduce the original error in the expected values of both the solution  $u$  and coefficient  $\kappa$  by a factor of  $10^6$