Spectral Representation of Random Processes

Example: Represent u(t,x,Q) by

$$u^K(t,x,Q) = \sum_{k=0}^{K} u_k(t,x)\Psi_k(Q)$$

where $\Psi_k(Q)$ are orthogonal polynomials.

Single Random Variable:

Let $\psi_k(Q)$ be orthogonal with respect to $\rho_Q(q)$ with $\psi_0(Q) = 1$. Then

$$\mathbb{E}[\psi_0(Q)] = 1$$

and

$$\begin{aligned} \mathbb{E}[\psi_i(Q)\psi_j(Q)] &= \int_\Gamma \psi_i(q)\psi_j(q)\rho_Q(q)dq \\ &= \langle \psi_i, \psi_j \rangle_\rho \\ &= \delta_{ij}\gamma_i \end{aligned}$$

Normalization factor:

$$\gamma_i = \mathbb{E}[\psi_i^2(Q)] = \langle \psi_i, \psi_i \rangle_\rho$$

Spectral Representation of Random Processes

Random Process:

$$\begin{aligned}
\mathbb{E}\left[u^K(t,x,Q)\right] &= \mathbb{E}\left[\sum_{k=0}^{K} u_k(t,x)\psi_k(Q)\right] \\
&= u_0(t,x)\mathbb{E}[\psi_0(Q)] + \sum_{k=1}^{K} u_k(t,x)\mathbb{E}[\psi_k(Q)] \\
&= u_0(t,x)
\end{aligned}$$

$$\begin{aligned}
\mathrm{var}[u^K(t,x,Q)] &= \mathbb{E}\left[\left(u^K(t,x,Q) - \mathbb{E}[u^K(t,x,Q)]\right)^2\right] \\
&= \mathbb{E}\left[\left(\sum_{k=0}^{K} u_k(t,x)\psi_k(Q) - u_0(t,x)\right)^2\right] \\
&= \mathbb{E}\left[\left(\sum_{k=1}^{K} u_k(t,x)\psi_k(Q)\right)^2\right] \\
&= \sum_{k=1}^{K} u_k^2(t,x)\gamma_k
\end{aligned}$$

Spectral Representation of Random Processes

Hermite Polynomials: $\boldsymbol{Q \sim N(0,1)}$

$$H_0(Q) = 1 \quad , \quad H_1(Q) = Q \quad , \quad H_2(Q) = Q^2 - 1$$

$$H_3(Q) = Q^3 - 3Q \quad , \quad H_4(Q) = Q^4 - 6Q^2 + 3$$

with the weight

$$\rho_Q(q) = \frac{1}{\sqrt{2\pi}} e^{-q^2/2}$$

Normalization factor: $\gamma_i = \int_{\mathbb{R}} \psi^2(q) \rho_Q(q) dq = i!$

Legendre Polynomials: $\boldsymbol{Q \sim \mathcal{U}(-1,1)}$

$$P_0(Q) = 1 \quad , \quad P_1(Q) = Q \quad , \quad P_2(Q) = \frac{3}{2}Q^2 - \frac{1}{2}$$

$$P_3(Q) = \frac{5}{2}Q^3 - \frac{3}{2}Q \quad , \quad P_4(Q) = \frac{35}{8}Q^4 - \frac{15}{4}Q^2 + \frac{3}{8},$$

with the weight

$$\rho_Q(q) = \frac{1}{2}$$

Spectral Representation of Random Processes

Multiple Random Variables:

Definition: (p-Dimensional Multi-Index): a p-tuple

$$\mathbf{k}' = (k_1, \cdots, k_p) \in \mathbb{N}_0^p$$

of non-negative integers is termed a p-dimensional multi-index with magnitude $|\mathbf{k}'| = k_1 + k_2 + \cdots + k_p$ and satisfying the ordering $\mathbf{j}' \leq \mathbf{k}' \Leftrightarrow j_i \leq k_i$ for $i = 1, \cdots, p$.

Consider the p-variate basis functions

$$\Psi_{\mathbf{i}'}(Q) = \psi_{i_1}(Q_1), \cdots, \psi_{i_p}(Q_p)$$

which satisfy

$$\begin{aligned}
\mathbb{E}[\Psi_{\mathbf{i}'}(Q)\Psi_{\mathbf{j}'}(Q)] &= \int_\Gamma \Psi_{\mathbf{i}'}(q)\Psi_{\mathbf{j}'}(q)\rho_Q(q)dq \\
&= \left\langle \Psi_{\mathbf{i}'}, \Psi_{\mathbf{j}'} \right\rangle_\rho \\
&= \delta_{\mathbf{i}'\mathbf{j}'}\gamma_{\mathbf{i}'}
\end{aligned}$$

Spectral Representation of Random Processes

Multi-Index Representation:

$$u^K(t,x,Q) = \sum_{|\mathbf{k}'|=0}^{K} u_{\mathbf{k}'}(t,x)\Psi_{\mathbf{k}'}(Q)$$

Single Index Representation:

$$u^K(t,x,Q) = \sum_{k=0}^{K} u_k(t,x)\Psi_k(Q)$$

k	$\|\mathbf{k}'\|$	Multi-Index	Polynomial
0	0	$(0,0,0)$	$\psi_0(Q_1)\psi_0(Q_2)\psi_0(Q_3)$
1	1	$(1,0,0)$	$\psi_1(Q_1)\psi_0(Q_2)\psi_0(Q_3)$
2		$(0,1,0)$	$\psi_0(Q_1)\psi_1(Q_2)\psi_0(Q_3)$
3		$(0,0,1)$	$\psi_0(Q_1)\psi_0(Q_2)\psi_1(Q_3)$
4	2	$(2,0,0)$	$\psi_2(Q_1)\psi_0(Q_2)\psi_0(Q_3)$
5		$(1,1,0)$	$\psi_1(Q_1)\psi_1(Q_2)\psi_0(Q_3)$
6		$(1,0,1)$	$\psi_1(Q_1)\psi_0(Q_2)\psi_1(Q_3)$
7		$(0,2,0)$	$\psi_0(Q_1)\psi_2(Q_2)\psi_0(Q_3)$
8		$(0,1,1)$	$\psi_0(Q_1)\psi_1(Q_2)\psi_1(Q_3)$
9		$(0,0,2)$	$\psi_0(Q_1)\psi_0(Q_2)\psi_2(Q_3)$

Scalar Initial Value Problem

Problem:

$$\frac{du}{dx} = f(t, Q, u) \ , \ t > 0$$

$$u(0, Q) = u_0$$

Quantity of Interest:

$$y(t) = \int_\Gamma u(t,q)\rho_Q(q)dq$$

Finite-Dimensional Representation:

$$u^K(t, Q) = \sum_{k=0}^{K} u_k(t)\Psi_k(Q)$$

where

$$u_k(t) = \frac{1}{\gamma_k}\int_\Gamma u(t,q)\Psi_k(q)\rho_Q(q)dq$$

Stochastic Galerkin Method

Weak Stochastic Formulation: For i=0, …, K

$$
\begin{aligned}
0 &= \left\langle \frac{du^K}{dt} - f, \Psi_i \right\rangle_\rho \\
&= \int_\Gamma \left[\sum_{k=0}^{K} \frac{du_k}{dt}(t)\Psi_k(q) - f\left(t, q, \sum_{k=0}^{K} u_k(t)\Psi_k(q)\right)\right] \Psi_i(q)\rho_Q(q)dq
\end{aligned}
$$

which is equivalent to

$$
\mathbb{E}\left[\frac{du^K(t,Q)}{dt}\Psi_i(Q)\right] = \mathbb{E}\left[f\left(t, Q, u^K\right)\Psi_i(Q)\right]
$$

Quadrature yields

$$
\sum_{r=1}^{R} \Psi_i(q^r)\rho_Q(q^r)w^r \left[\sum_{k=0}^{K} \frac{du_k}{dt}(t)\Psi_k(q^r) - f\left(t, q^r, \sum_{k=0}^{K} u_k(t)\Psi_k(q^r)\right)\right] = 0
$$

Stochastic Galerkin Method

Example: Consider

$$\frac{du}{dt} = -\alpha(\omega)u$$
$$u(0,\omega) = \bar{\beta}$$

where $\bar{\beta}$ is fixed and $\alpha \sim N(\bar{\alpha}, \sigma_\alpha^2)$ with $\bar{\alpha} > 0$. Here

$$\alpha = \alpha^N = \sum_{n=0}^{N} \alpha_n \psi_n(Q) \quad , \ \alpha_0 = \bar{\alpha}, \alpha_1 = \sigma_\alpha, \alpha_n = 0, n > 1$$

$$\beta = \beta^N = \sum_{n=0}^{N} \beta_n \psi_n(Q) \quad , \ \beta_0 = \bar{\beta}, \beta_n = 0, n > 0$$

Analytic solution:

$$u(t,Q) = \bar{\beta} e^{-(\bar{\alpha}+\sigma_\alpha Q)t}$$

Stochastic Galerkin Method

Approximate solution: Find

$$u^K(t,Q) = \sum_{k=0}^{K} u_k(t)\psi_k(Q)$$

subject to

$$0 = \left\langle \frac{du^K}{dt} + \alpha^N u^K, \psi_i \right\rangle_\rho$$

$$= \int_{\mathbb{R}} \sum_{k=0}^{K} \frac{du_k}{dt}(t)\psi_k(q)\psi_i(q)\rho_Q(q)dq + \int_{\mathbb{R}} \alpha^N \sum_{k=0}^{K} u_k(t)\psi_k(q)\psi_i(q)\rho_Q(q)dq$$

which is equivalent to

$$\frac{du_i}{dt} = -\gamma_i \sum_{n=0}^{N}\sum_{k=0}^{K} \alpha_n u_k(t) e_{ink}$$

where

$$\gamma_i = \mathbb{E}[\psi_i^2(Q)] = \int_{\mathbb{R}} \psi_i^2(q)\rho_Q(q)dq$$

$$e_{ink} = \mathbb{E}[\psi_i(q)\psi_n(q)\psi_k(q)] = \int_{\mathbb{R}} \psi_i(q)\psi_n(q)\psi_k(q)\rho_Q(q)dq$$

Initial Conditions:

$$u_k(0) = \beta_k \ , \ k = 0, \cdots, K$$

since

$$u^K(0,Q) = \sum_{k=0}^{K} u_k(0)\psi_k(Q) = \beta = \sum_{n=1}^{N} \beta_n \psi_n(q)$$

Stochastic Galerkin Method

Note: To evaluate QoI, we observe that

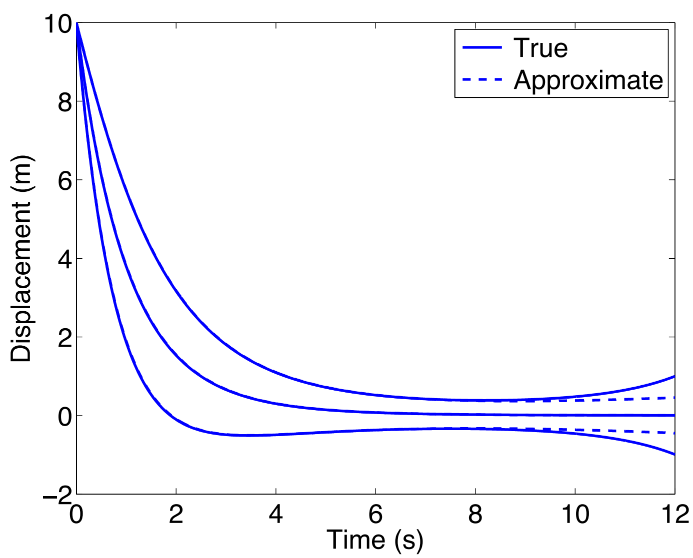
$$\mathbb{E}\left[u^K(t,Q)\right] = u_0(t)$$

$$\text{var}[u^K(t,Q)] = \sum_{k=1}^{K} u_k^2(t)\gamma_k.$$

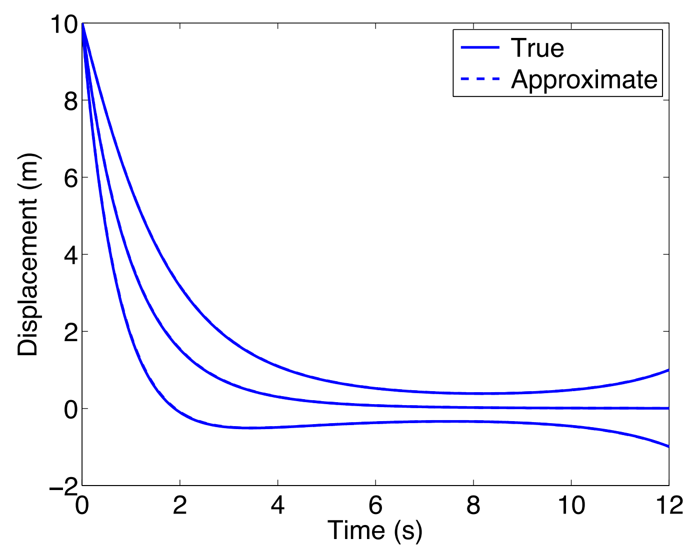
Exact Mean and Variance:

$$\bar{u}(t) = \int_{\mathbb{R}} \bar{\beta} e^{-(\bar{\alpha}+\sigma_\alpha q)t} \cdot \frac{1}{\sqrt{2\pi}} e^{-q^2/2} dq$$
$$= \bar{\beta} e^{-\bar{\alpha}t} e^{\sigma_\alpha^2 t^2/2}$$

$$\text{var}[u] = \mathbb{E}\left[u^2(t)\right] - \bar{u}^2(t)$$
$$= e^{-2\bar{\alpha}t}\bar{\beta}^2 \left(e^{2\sigma_\alpha^2 t^2} - e^{-\sigma_\alpha^2 t^2}\right)$$



K = 8



K = 16

Stochastic Galerkin Method

Properties:

- Accuracy is optimal in L2 sense.
- Disadvantages
  - Method is intrusive and hence difficult to implement with legacy codes or codes for which only executable is available.
  - Method requires densities with associated orthogonal polynomials. These can sometimes be constructed from empirical histograms.
  - Method requires mutually independent parameters.

Stochastic Collocation

Strategy: Using either deterministic or stochastic techniques, generate M samples from parameter space and enforce

$$u(t, q^m) = u^K(t, q^m)$$

Vandemonde System:

$$\begin{bmatrix} \Psi_0(q^1) & \cdots & \Psi_K(q^1) \\ \vdots & & \vdots \\ \Psi_0(q^M) & \cdots & \Psi_K(q^M) \end{bmatrix} \begin{bmatrix} u_0(t) \\ \vdots \\ u_K(t) \end{bmatrix} = \begin{bmatrix} u(t, q^1) \\ \vdots \\ u(t, q^M) \end{bmatrix}$$

Issues: System typically ill-conditioned and dense

Alternative Strategy: Employ Lagrange basis functions which yield identity and

$$u_m(t) = u(t, q^m) \;\; \text{for} \;\; m = 1, \cdots M$$

Equivalent Formulation: Employ $\Psi_i(q) = L_k(q)$ and take $q^m = q^r$ to get

$$\frac{du_m}{dt}(t) = f(t, q^m, u_m) \; , \; m = 1, \cdots, M$$

Stochastic Collocation

Properties:

- Whereas motivated in the context of a Galerkin method, collocation is based on interpolation theory.
- Advantages
    - Method is nonintrusive in the sense that once M collocation points are specified, one solves M deterministic problems using existing software.
    - Method is applicable to general parameter distributions with correlated parameters.
    - Algorithms available in Sandia Dakota package.
- Disadvantages
    - Evaluation of QoI typically requires sampling from joint distribution, which may not be available.

Discrete Projection Method

Problem:

$$\frac{du}{dx} = f(t, Q, u) \ , \ t > 0$$

$$u(0, Q) = u_0$$

Finite-Dimensional Representation:

$$u^K(t, Q) = \sum_{k=0}^{K} u_k(t)\Psi_k(Q)$$

where

$$u_k(t) = \frac{1}{\gamma_k}\int_\Gamma u(t,q)\Psi_k(q)\rho_Q(q)dq$$

Discrete Projection (Pseudo-spectral):

$$u_k(t) = \frac{1}{\gamma_k}\sum_{r=1}^{R} u(t,q^r)\Psi_k(q^r)\rho_Q(q^r)w^r$$

Discrete Projection Method

Example: We revisit the spring model

$$m\frac{d^2z}{dt^2} + c\frac{dz}{dt} + kz = f_0\cos(\omega_F t)$$

$$z(0) = z_0\ , \ \frac{dz}{dt}(0) = z_1$$

with the response

$$y(\omega_F, Q) = \frac{1}{\sqrt{(k - m\omega_F^2)^2 + (c\omega_F)^2}}$$

where $Q \sim N(\bar{q}, V)$

Parameters:

$$m = \bar{m}\,\Psi_0(Q) + \sigma_m\Psi_1(Q) = \bar{m} + \sigma_m Q_1$$

$$c = \bar{c}\,\Psi_0(Q) + \sigma_c\Psi_2(Q) = \bar{c} + \sigma_c Q_2$$

$$k = \bar{k}\,\Psi_0(Q) + \sigma_k\Psi_3(Q) = \bar{k} + \sigma_k Q_3$$

where $\Psi_k(Q) = \psi_{k_1}(Q_1)\psi_{k_2}(Q_2)\psi_{k_3}(Q_3)$ are tensored Hermite polynomials.

Discrete Projection Method

Approximated Response:

$$y^K(\omega_F, Q) = \sum_{k=0}^{K} y_k(\omega_F)\Psi_k(Q)$$

where

$$y_k(\omega_F) = \frac{1}{\gamma_k}\int_{\mathbb{R}^3} y(\omega_F, q)\Psi_k(q)\rho_Q(q)dq$$

$$\approx \frac{1}{\gamma_k}\sum_{r_1=1}^{R_{\ell_1}}\sum_{r_2=1}^{R_{\ell_2}}\sum_{r_3=1}^{R_{\ell_3}} y(\omega_F, q^r)\Psi_k(q^r)\rho_Q(q^r)w_\ell^r$$

and

$$\rho_Q(q) = \left(\frac{1}{\sqrt{2\pi}}\right)^3 e^{-m^2/2}e^{-c^2/2}e^{-k^2/2}$$

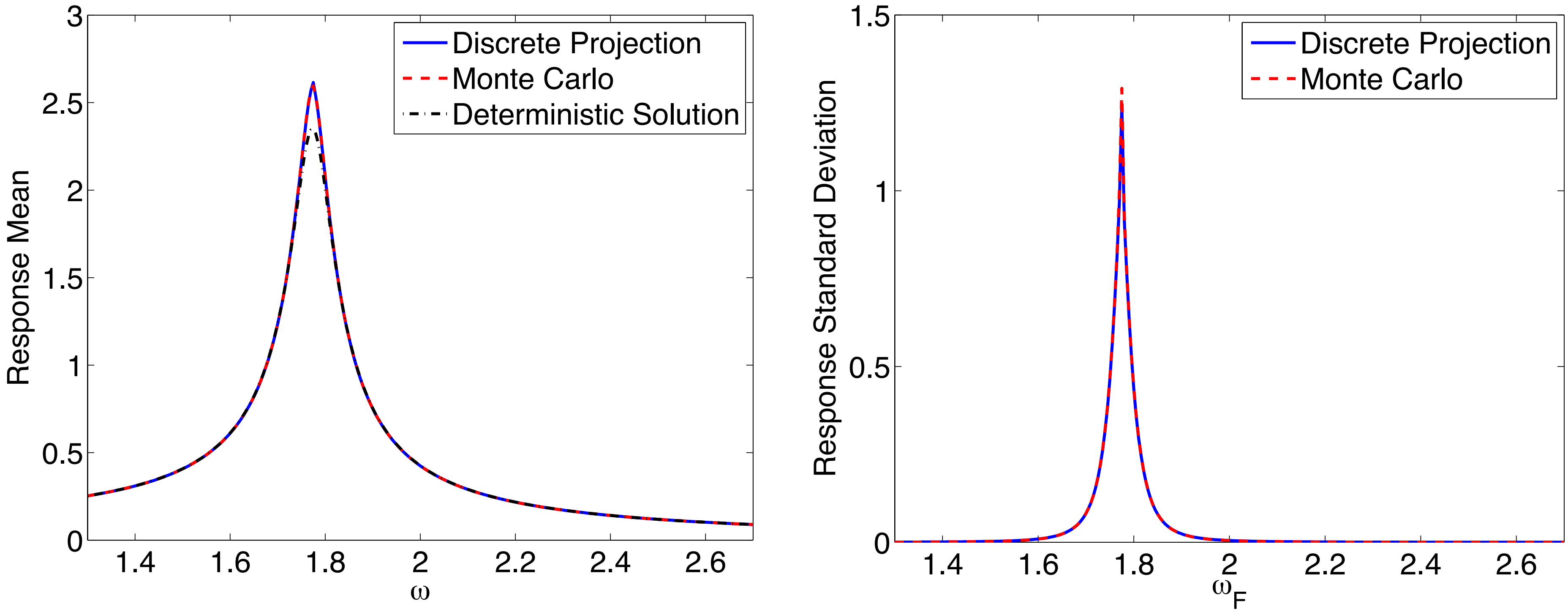
Note:

$$\bar{y}(\omega_F) = y_0(\omega_F)$$

$$\text{var}\left[y^K(\omega_F, Q)\right] = \sum_{k=1}^{K} y_k(\omega_F)\gamma_k$$

Discrete Projection Method

Results:



Discrete Projection

Properties:

- Advantages
  - Like collocation, the method is nonintrusive and hence can be employed with post-processing to existing codes. The method is often referred to as nonintrusive PCE.
  - Algorithms available in Sandia Dakota package.
- Disadvantages
  - Requires the construction of the joint density which often relies on mutually independent parameters.

Boundary Value Problems and Elliptic PDE

Model:

$$\mathcal{N}(u, Q) = F(Q) \quad , \; x \in \mathcal{D}$$

$$B(u, Q) = G(Q) \quad , \; x \in \partial\mathcal{D}$$

Quantity of Interest:

$$y(x) = \int_\Gamma u(x,q)\rho_Q(q)dq$$

Deterministic Weak Formulation: Find $u \in V$, which satisfies

$$\int_\mathcal{D} N(u,Q)S(v)dx = \int_\mathcal{D} F(Q)vdx \quad \text{for all } v \in V$$

Stochastic Weak Formulation: Find $u \in V \otimes Z$ that satisfies

$$\int_\Gamma \int_\mathcal{D} N(u,q)S(v(x))z(q)\rho_Q(q)dxdq = \int_\Gamma \int_\mathcal{D} F(q)v(x)z(q)\rho_Q(q)dxdq$$

for all test functions $v \in V, z \in Z$

Boundary Value Problems and Elliptic PDE

Approximated Solution:

$$u^K(x, Q) = \sum_{k=0}^{K} u_k(x)\Psi_k(Q)$$
$$= \sum_{k=0}^{K}\sum_{j=1}^{J} u_{jk}\phi_j(x)\Psi_k(Q).$$

Galerkin Method:

$$\sum_{r=1}^{R} \Psi_i(q^r)\rho_Q(q^r)w^r \int_{\mathcal{D}} N\Big(\sum_{k=0}^{K}\sum_{j=1}^{J} u_{jk}\phi_j(x)\Psi_k(q^r), q^r\Big) S(\phi_\ell(x))dx$$
$$= \sum_{r=1}^{R} \Psi_i(q^r)\rho_Q(q^r)w^r \int_{\mathcal{D}} F(q^r)\phi_\ell(x)dx$$

Quantity of Interest:

$$y(x) = \sum_{r=1}^{R} w^r \rho_Q(q^r) \sum_{k=0}^{K}\sum_{j=1}^{J} u_{jk}\phi_j(x)\Psi_k(q^r)$$

Boundary Value Problems and Elliptic PDE

Collocation: Enforce

$$u(x, q^m) = u^K(x, q^m) = \sum_{j=1}^{J} u_{jm}\phi_j(x)$$

at M collocation points to yield M relations

$$\int_{\mathcal{D}} N\left(\sum_{j=1}^{J} u_{jm}\phi_j(x), q^m\right) S(\phi_\ell(x))dx = \int_{\mathcal{D}} F(q^m)\phi_\ell(x)dx$$

for $\ell = 1, \cdots, J$

Quantity of Interest:

$$\begin{aligned} y &= \sum_{r=1}^{R} w^r \rho_Q(q^r) \sum_{j=1}^{J} u_{jr}\phi_j(x) \\ &= \sum_{r=1}^{R} w^r \rho_Q(q^r)\hat{u}_r(x) \end{aligned}$$