CVOD-based Reduced-order Modeling for Stochastic PDEs

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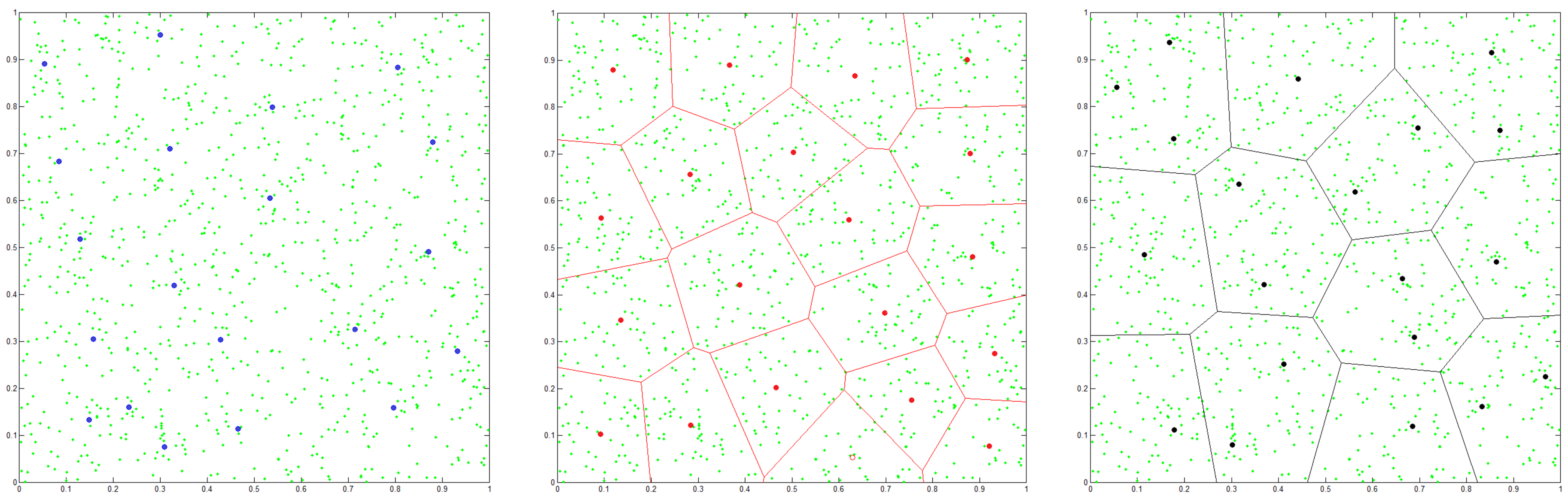
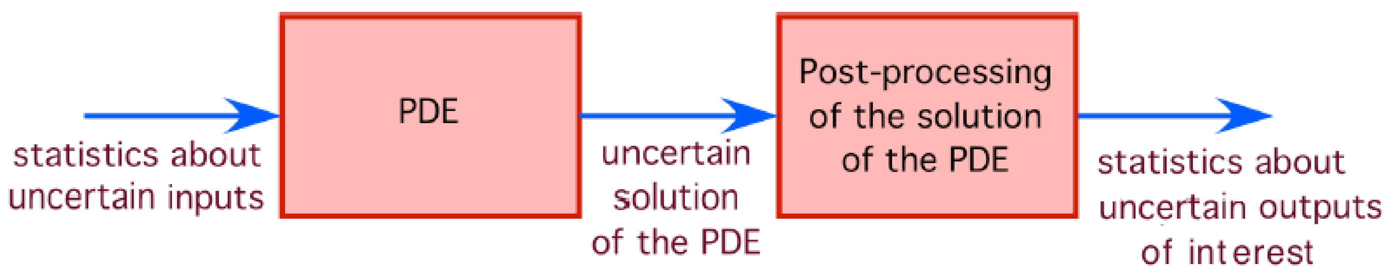
Introduction: Today, model reduction plays an important role in the approximation of complex dynamical system. We briefly review the proper orthogonal decomposition (POD) and centroidal Voronoi tessellation (CVT) techniques for low-dimensional approximations of a snapshot set. Then we compare their advantages and disadvantages and come up with an idea of combing CVT and POD into a hybrid method CVOD that inherits favorable characteristics from both its parents. Detailed properties and algorithm are proposed, along with a comparison of CVOD with POD and CVT.



From left to right are POD, CVT and CVOD reduced basis of 20 (colored points) for a snapshot set of 1000 (green points).

Uncertainty Model

Uncertainty Model for PDEs with Random Inputs



Uncertainty quantification is the task of determining statistical information about the uncertainty in an output of interest that depends on the solution of a PDE, given statistical information about the uncertainty in the inputs of the PDE.

A realization of the random system is a solution $u(\mathbf{x}, t; \vec{y})$ of a PDE for specific discrete random parameters $\vec{y} = \{y_{n_1}\}_{n_1=1}^{N_1}$ All realizations generate snapshot set $\mathcal{W}$ to determine statistical quantity of interest (QoI)

$$\mathcal{W} = \left\{ \begin{array}{ccccccc} u(\mathbf{x}_1, t_1; y_1) & \dots & u(\mathbf{x}_1, t_{N_3}; y_1) & \dots & u(\mathbf{x}_1, t_1; y_{N_1}) & \dots & u(\mathbf{x}_1, t_{N_3}; y_{N_1}) \\ u(\mathbf{x}_2, t_1; y_1) & \dots & u(\mathbf{x}_2, t_{N_3}; y_1) & \dots & u(\mathbf{x}_1, t_1; y_{N_1}) & \dots & u(\mathbf{x}_2, t_{N_3}; y_{N_1}) \\ \vdots & \ddots & \vdots & \dots & \vdots & \ddots & \vdots \\ u(\mathbf{x}_{N_2}, t_1; y_1) & \dots & u(\mathbf{x}_{N_2}, t_{N_3}; y_1) & \dots & u(\mathbf{x}_{N_2}, t_1; y_{N_1}) & \dots & u(\mathbf{x}_{N_2}, t_{N_3}; y_{N_1}) \end{array} \right\}$$

where random discretization $\{y_{n_1}\}_{n_1=1}^{N_1}$, spatial discretization $\{\mathbf{x}_{n_2}\}_{n_2=1}^{N_2}$, and temporal discretization $\{t_{n_3}\}_{n_3=1}^{N_3}$.

Owing to the high computational requirements, the classical Monte Carlo method is not an appropriate option. Reduced-order models (ROMs) have attracted much interest for lessening the computational cost of simulations for nonlinear, stochastic, time-dependent PDEs, such savings can be effective due to the relatively low dimensionality of the approximations that ROMs can provide.

POD and CVT

Proper Orthogonal Decomposition

- Given modified snapshot set $\mathcal{W} = \{\mathbf{u}_1, ..., \mathbf{u}_N\}$ and an integer $M \ll N$.
- Find a reduced set of orthonormal functions $\{\mathbf{\Phi}_m\}_{m=1}^M$ that minimizes the error measure

$$\mathcal{J}(\mathbf{\Phi}_1, \mathbf{\Phi}_2, ..., \mathbf{\Phi}_M) = \frac{1}{N}\sum_{n=1}^{N} ||\mathbf{u}_n - \sum_{m=1}^{M} (\mathbf{u}_n, \mathbf{\Phi}_m)\mathbf{\Phi}_m||^2$$

where the orthonormal function has form $\mathbf{\Phi}_m = \sum_{n=1}^{N} \phi_n^{(m)} \mathbf{u}_n$ for $m = 1, ..., M$.

Centroidal Voronoi Tessellation

- Given modified snapshot set $\mathcal{W} = \{\mathbf{u}_1, ..., \mathbf{u}_N\}$, an integer $M \ll N$ and a (discrete) density function ρ defined for $\mathbf{u}_i$ $(i = 1, ..., N)$ in $\mathcal{W}$.
- Find a reduced set of points $\{\mathbf{z}_i \in \bar{\mathcal{W}}\}_{i=1}^M$ and a tessellation of $\bar{\mathcal{W}} = \cup_{i=1}^N \bar{V}_i$ satisfying $V_i \cap V_j = \emptyset$ such that simultaneously for each i :

  V_i is the Voronoi region for $\mathbf{z}_i$ and $\mathbf{z}_i$ is the mass centroid of V_i , i.e.

$$\bar{V}_i = \{\mathbf{u} \in \mathcal{W} \mid |\mathbf{u} - \mathbf{z}_i| \le |\mathbf{u} - \mathbf{z}_j| \text{ for } i \neq j\} \text{ and } \mathbf{z}_i = \frac{\sum_{\mathbf{u}_j \in V_i} \rho(\mathbf{u}_j)\mathbf{u}_j}{\sum_{\mathbf{u}_j \in V_i} \rho(\mathbf{u}_j)}.$$

Reduced-order Models

Originally we seek a solution $\mathbf{u} \in \mathcal{W} = span\{\mathbf{u}_1, ..., \mathbf{u}_N\}$, now we seek a reduced-order solution $\mathbf{u}_{POD} \in \mathcal{W}_{POD} = span\{\mathbf{\Phi}_1, ..., \mathbf{\Phi}_M\}$ or $\mathbf{u}_{CVT} \in \mathcal{W}_{CVT} = span\{\mathbf{z}_1, ..., \mathbf{z}_M\}$. The cost of a reduced-order solution would be much smaller if $M \ll N$ ignoring the cost of the off-line determination of reduced basis.

CVOD

CVT combined with POD

- POD basis $\{\mathbf{\Phi}_m\}_{m=1}^M$ is optimal in the sense of minimizing cumulative energy

$$\mathcal{J}(\mathbf{\Phi}_1, \mathbf{\Phi}_2, ..., \mathbf{\Phi}_M) = \frac{1}{N}\sum_{n=1}^{N} ||\mathbf{u}_n - \sum_{m=1}^{M} (\mathbf{u}_n, \mathbf{\Phi}_m)\mathbf{\Phi}_m||^2 = \sum_{n=M+1}^{N} \lambda_n$$

  where $\{\lambda_n, \mathbf{\Phi}_n\}_{n=1}^N$ are singular-pairs of snapshot set $\mathcal{W}$.
- CVT basis $\{\mathbf{z}_i\}_{i=1}^M$ is optimal in the sense of minimizing clustering energy

$$\mathcal{F}((\mathbf{z}_i, V_i), i = 1, ..., M) = \sum_{i=1}^{M} \sum_{\mathbf{u}_j \in V_i} \rho(\mathbf{u}_j) |\mathbf{u}_j - \mathbf{z}_i|^2$$

Comparing POD and CVT we find

- CVT is cheaper than POD since
  - it avoids solving an $N \times N$ eigenvalue problem;
  - it can handle many more snapshots;
  - it adaptively changing reduced basis is cheaper.
- CVT avoids the over-crowding or reduced basis into a few dominant modes.
- CVT naturally introduces the concept of clustering into construction of reduced basis.
- POD basis contain more global information than CVT under same number of basis since it doesn't cut off the connections between different Voronoi regions.

How about combine POD and CVT to take advantage of both approaches

- The basic idea is to replace the generators $\{\mathbf{z}_i\}_{i=1}^M$ with M sets of orthonormal basis $\{\mathcal{Z}_{i=1}^M\}$ where $\mathcal{V}_i = span\{\mathcal{Z}_i\}$ in CVT, with a new distant measure from $\mathbf{u}_j \in \mathcal{V}_i$ to $\mathcal{Z}_i$ which minimize POD energy in every $\mathcal{V}_i$.
- One can deduce that CVOD basis $\{\mathcal{Z}_{i=1}^M\}$ minimize the clustering-cumulative energy

$$\mathcal{G}((\mathcal{Z}_i, \mathcal{V}_i), i = 1, ..., M) = \sum_{i=1}^{M} \sum_{\mathbf{u}_j \in \mathcal{V}_i} \rho(\mathbf{u}_j) \delta^2(\mathbf{u}_j, \mathcal{Z}_i) = \sum_{i=1}^{M} |\mathcal{V}_i| \sum_{j=dim(\mathcal{V}_i)+1}^{|\mathcal{V}_i|} \lambda_{i_j}$$

CVOD Algorithms

CVOD Algorithms (Generalized Lloyd's Method)

To CVT with generalized notions of distance and centroid, we need to define the square of distance from a vector $\mathbf{u}_j$ to a subspace $\mathcal{V}_i = span\{\mathcal{Z}_i\} = span\{\theta_i^{(1)}, ..., \theta_i^{(dim(\mathcal{V}_i))}\}$ by

$$\delta^2(\mathbf{u}_j, \mathcal{V}_i) = \delta^2(\mathbf{u}_j, \mathcal{Z}_i) = 1 - \frac{1}{||\mathbf{u}_j||^2} \sum_{k=1}^{dim(\mathcal{V}_i)} |\mathbf{u}_j^T \theta_i^{(k)}|^2$$

- Given modified snapshot set $\mathcal{W} = \{\mathbf{u}_1, ..., \mathbf{u}_N\}$, an integer M , a (discrete) density function ρ .

(0) Choose an initial set of M subspaces $\{\mathcal{V}_i\}_{i=1}^M$ and corresponding orthonormal basis $\{\mathcal{Z}_i\}_{i=1}^M = \{\{\theta_i^{(k)}\}_{k=1}^{dim(\mathcal{V}_i)}\}_{i=1}^M$;

(1) Determine the new generalized Voronoi tessellation

$$\mathcal{V}_i^* = \{\mathbf{u}_j \in \mathcal{W} \mid \delta^2(\mathbf{u}_j, \mathcal{Z}_i) \le \delta^2(\mathbf{u}_j, \mathcal{Z}_l) \; \forall \; l \neq i\}$$

and corresponding orthonormal basis

$$\{\mathcal{Z}_i^*\}_{i=1}^M = \{\{\theta_i^{*(k)}\}_{k=1}^{dim(\mathcal{V}_i^*)}\}_{i=1}^M$$

for $i = 1, ..., M$;

(2) Set $\{\mathcal{V}_i = \mathcal{V}_i^*\}_{i=1}^M$ and $\{\mathcal{Z}_i = \mathcal{Z}_i^*\}_{i=1}^M$

(3) If the new tessellation and corresponding basis meet some convergence criterion, terminate; otherwise, return to step 1.

Comparing CVOD with POD and CVT

- CVOD is cheaper than POD since it requires the solution of several smaller eigenproblems instead of one large one.
- CVOD basis contain more global information than CVT but less than POD under same number of basis since piecewise optimal doesn't give global optimal.
- CVOD = POD if one takes $M = 1$ and CVOD = CVT if one takes $\{dim(\mathcal{V}_i) = 1\}_{i=1}^M$.

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