Proper Orthogonal Decomposition Based Reduced Order Modeling for Monte Carlo Simulations in Radiation Transport

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Outline

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Objectives

- Develop a reduced order model (ROM) for a class of Monte Carlo (MC) simulations
- Use proper orthogonal decomposition (POD) to generate modes for representing photon number distribution
- Once modes are known, project MC simulations to have more accurate / faster predictions (use smaller number of particle histories for future calculations)
- Perform probabilistic PCA / POD to radiation transport
- Estimate noise in training data
Physical Problem

- Terrestrial radiation detection scenario
- Three different source materials are simulated: a Cobalt-60 source, a Cesium-137 source, and a Technetium-99 source.
- Ground radiation
- Simulation with MCNP6, a Monte Carlo-based radiation transport code (Los Alamos National Laboratory (U.S.))

Figure: Schematic of the particle simulations
Energy Spectrum

Spectra with $10^{10}$ particle histories

Figure: center point
Normalized Particle Counts

(a) Background

(b) Co60

(c) Cs137

(d) Tc99
Effect of Particle History Count

Co60 spectra with different numbers of particle histories

Figure: Co60 spectra at center point
Simulations are slow ...

Can we make some training data with more particles and use that for fast simulations with small numbers of particle histories?

Can we use reduced order model (ROM) approach to speed up the simulations?
Reduced Order Modeling

- Generate an accurate low-dimensional model for a full-scale, high-dimensional RT, MC simulation
- Use that model for further simulations with few particle histories

Idea
Create a compact representation of the normalized photon number distribution, \( n(\vec{x}, e) \), such that a small number of particle histories is needed for MC simulations to predict the distribution.

\[
n(\vec{x}, e)_M = \sum_{j=1}^{M} a_j(\vec{x}) \varphi_j(e) \tag{1}
\]

where, \( \vec{x} \) is the detector location, \( e \) is the photon energy, \( a_j(\vec{x}) \) are weighting coefficients, \( \varphi_1, \varphi_2, \ldots, \varphi_M \) are basis functions
Generate basis functions (POD modes) using data obtained from the Monte Carlo simulations

Mathematically, the dominant POD basis function $\varphi_1$ is a solution to the optimization problem

$$\varphi_1 = \arg\max_{\tilde{\varphi} \in L^2(\Omega)} \left\langle \left( \int_{\Omega} \tilde{\varphi}(e)n(\vec{x}, e)\,de \right)^2 \right\rangle,$$

subject to $\int_{\Omega} \varphi_1(e)^2\,de = 1$

Can generate a hierarchy of basis functions
A solution to the maximization problem (2) is also the solution to the Fredholm integral equation

$$\int_{\Omega} R(e, e') \varphi_1(e') de' = \lambda \varphi_1(e),$$

(3)

the two-point correlation tensor $R(e, e')$ is given by

$$R(e, e') = \langle n(\vec{x}, e)n(\vec{x}, e') \rangle$$

(4)

$\lambda$ is an eigenvalue associated with (3).

Eigenvalues are given by

$$\lambda_j = \left\langle \left( \int_{\Omega} \varphi_j(e)n(\vec{x}, e) de \right)^2 \right\rangle$$

(5)

$\lambda$'s determine importance of a given mode.
Create modes from simulations of pure radiation sources with \(10^{10}\) particle histories

- 200\(\times\)1764 data matrix - 200 energy bins and 21 \(\times\) 21 array from 4 simulations

- Averaging data over sources and space

- Obtain the eigenvalue spectrum
Eigenvalue Spectrum

![Eigenvalue Spectrum Graph]

- Eigenvalues are decaying
- Four order of magnitude decay by first 6 modes

**Figure:** Eigenvalue spectrum of the ROM
First 4 POD Modes

(a) mode 1

(b) mode 2

(c) mode 3

(d) mode 4
Accelerating Future MC Simulations

Use the constructed ROM to complete the remaining simulations with few particle histories

- Simulate a mixed source composed with Co60, Cs137, Tc99 and background

- Use generated POD modes from the ROM model to represent
  \[
  n(\vec{x}, e)_{M,N} = \sum_{j=1}^{M} a_j(\vec{x}) \varphi_j(e)
  \]

- Use projection of MC simulations with fewer particle histories to determine the weighting coefficients
  \[
  a_j(\vec{x}) = \int_{\Omega} n(\vec{x}, e)_{N} \phi_j(e) \, de. \quad (6)
  \]
Completing the mixed spectra simulations with $10^6$ particle histories using ROM

**Figure:** 6 mode $-10^6$ projection
The error in the representation

\[ E^2 = \int_{\Omega} (n(\vec{x}, e)_{M,N} - n(\vec{x}, e))^2 \, de \]  

(7)

Compare POD projections with $10^{10}$ MC simulation data

Figure: Error in the POD reconstruction with different number of modes

- Increasing number of modes may not result in a better prediction of the $10^{10}$ data
- As number of modes in the representation increases, projection converges to the MC simulation data with few particle histories
Projection with 2 modes gives the best reconstruction of the $10^{10}$ with $10^6$ MC simulations.
Consider the following scenario:

- A radioactive source composed of a mixture of various radioactive materials
- The composition of sources is chosen from a joint distribution function for the probability of having various amounts of mass of the different materials
- For each choice of source mixture, photon distribution $\vec{n}$ at a location $x$ can be measured
Forward model for the energy spectrum for any given realization of source materials,

\[
\vec{n} = \sum_{j=1}^{M} w_j \vec{\phi}_j + \vec{\mu} + \vec{\epsilon} = \Phi \vec{w} + \vec{\mu} + \vec{\epsilon}
\]  \hspace{1cm} (8)

\(\vec{n}\) - \(D\)-dimensional vector describing energy spectrum
\(\vec{w}\) - \(M\)-dimensional latent variable representing the choice of source and location (assume Gaussian random variable)
\(\Phi\) - \(D \times M\) matrix of basis functions
\(\vec{\epsilon}\) - noise associated with the measurements \(\left( \vec{\epsilon} \sim \mathcal{N} \left( 0, \sigma_{\epsilon}^2 I \right) \right)\)
\(\vec{\mu}\) - mean energy distribution for distribution of sources

Probability distribution of \(\vec{n}\) conditioned on \(\vec{w}\), \(\Phi\) and \(\sigma_{\epsilon}^2\) is

\[p \left( \vec{n} | \vec{w}, \Phi, \sigma_{\epsilon}^2 \right) = \mathcal{N} \left( \Phi \vec{w} + \vec{\mu}, \sigma_{\epsilon}^2 I \right)\]
Define a Gaussian distribution, \( p(\vec{w}) \) over the latent variable

Assume Probability distribution of \( \vec{w} \) is given by zero mean unit covariance Gaussian

\[
p(\vec{w}) = \mathcal{N}(0, I), \tag{9}\]

Marginalize over \( \vec{w} \) to get the probability distribution of \( \vec{n}|\Phi, \sigma^2_\epsilon \)

\[
p\left(\vec{n}|\Phi, \sigma^2_\epsilon\right) = \int p\left(\vec{n}|\vec{w}, \Phi, \sigma_\epsilon\right) p(\vec{w}) \, d\vec{w} \tag{10}\]

Evaluating mean and covariance of predictive distribution,

\[
p\left(\vec{n}|\Phi, \sigma^2_\epsilon\right) = \mathcal{N}(\vec{\mu}, C), \tag{11}\]

where \( C = \Phi \Phi^T + \sigma^2_\epsilon I \).

Assuming \( \vec{n}_k \)'s are independent identically distributed variables, Bayes' formula for the above probabilistic model with \( N = \{\vec{n}_k\}, k=1, \ldots, K \)

\[
p\left(\Phi, \sigma^2_\epsilon|N\right) = p\left(N|\Phi, \sigma^2_\epsilon\right) \times p\left(\Phi, \sigma^2_\epsilon\right), \tag{12}\]
Assuming uniform prior, posterior distribution is

\[
p\left(\Phi, \sigma^2_\epsilon | N\right) \propto 2\pi^{-DK/2} |C|^{-K/2} \exp \left(-\frac{1}{2} \sum_{k=1}^{K} (\vec{n}_k - \vec{\mu})^T C^{-1} (\vec{n}_k - \vec{\mu})\right)
\]

Negative log posterior is

\[
L = - \log p\left(\Phi, \sigma^2_\epsilon | N\right) = C_1 + \frac{K}{2} \log |C| + \frac{1}{2} \sum_{k=1}^{K} (\vec{n}_k - \vec{\mu})^T C^{-1} (\vec{n}_k - \vec{\mu})
\]

\[
= C_1 + \frac{K}{2} \left( \log |C| + Tr \left( C^{-1}S \right) \right),
\]

where \(S\) is the covariance matrix and \(C_1\) is a constant.
Maximum posterior solution for $\Phi$ is given by

$$\Phi_{MAP} = U_M \left( L_M - \sigma^2 I \right)^{\frac{1}{2}} R,$$  

(16)

where $U_M = D \times M$ matrix whose columns are given by any subset of eigenvectors of the data covariance matrix $S$, $L_M$ is $M \times M$ diagonal matrix of eigenvalues, and $R$ is an arbitrary $M \times M$ orthogonal matrix.$^1$

Maximum posterior solution for $\sigma^2_\epsilon$ is given by

$$\sigma^2_{\epsilon MAP} = \frac{1}{D - M} \sum_{i=M+1}^{D} \lambda_i,$$  

(17)

where $M \leq D$, $D$ - dimension of $\vec{n}_k$'s $M$ - dimension of $\vec{w}$

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Modes with $M=4$

- Identical modes can be obtained using PPCA
Noise in the training data

\[
\sigma_\varepsilon^2 = \frac{1}{D - M} \sum_{i=M+1}^{D} \lambda_i
\]

\[
\sigma_\varepsilon^2 = 4.6125 \times 10^{-11} \text{MeV}^{-1}
\]

Average variance associated with the discarded dimensions

Figure: Eigenvalue spectrum of the ROM
Conclusions

- Radioactive sources composed of mixtures of pure sources can be accurately simulated with ROM
- 4 orders of magnitude reduction in computational time
- Probabilistic PCA / POD can be performed to generate modes and identify the noise in the training data
Future Work

- Choose appropriate value for M using Bayesian PCA
- Estimate weighting coefficients using Bayesian approach
- Use model selection to determine most likely weighting coefficients
- Quantify the uncertainty associated with the ROM