Using Matrix and Tensor Factorization for Analyzing Radiation Transport Data

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Abstract

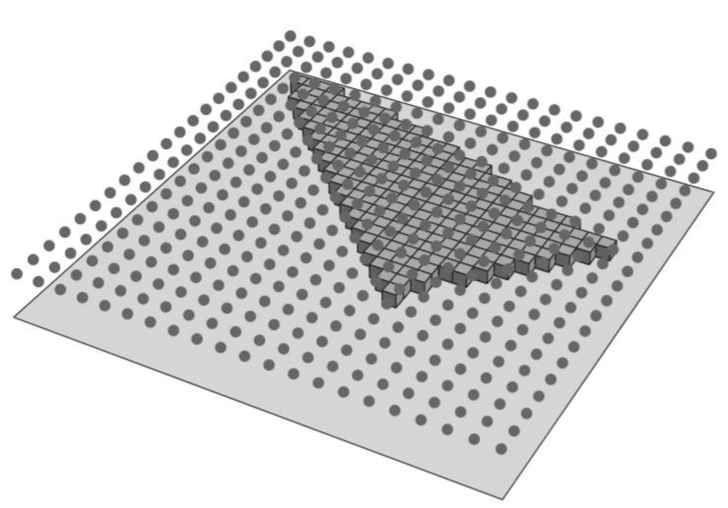
Understanding how radiation particles are transported throughout a system and interact with shielding is extremely computationally expensive. Reduced order models (ROMs) can be used to significantly increase the speed of these calculations [1]. This project focuses on analysis of the simulated radiation transport for Cobalt-60, Cesium-137, and Technetium-99. A ROM may be developed from several formalisms and then analyzing the feature vectors of each. The methods considered here include principal component analysis (PCA), non-negative matrix factorization (NNMF), and CP tensor decomposition (CPT). By comparing the signal from fitted Lorentzian profiles to spectral features, we evaluate whether each ROM is capable of accurately displaying the radiation signal traces in the data. This model will be able to locate possible sources of radiation from real world data and quickly identify them without the need to reconstruct a computationally expensive ROM.

Introduction

Much of the science at Pacific Northwest National Laboratory (PNNL) involves radiation in some aspect. Understanding how radiative particles interact with shielding and how particles are emitted by machines, X-ray sources and radioactive materials is critical for detection and remediation of the radioactive sources. In order to study radiation, it must be measured, which is typically done by analyzing radiation spectra. Historically, the developed reduced order models (ROM) serve to generate basis functions that can compactly represent the radiation spectra. These ROMs are generated by several different numerical methods: principal component analysis (PCA), nonnegative matrix factorization (NNMF), and CP tensor decomposition (CPT).

Our aim is to test these procedures with the given simulated data and develop methods for qualitatively comparing the results and generate the best ROM that may be used to model larger data sets. This will provide us with a model that best describes real-world data, where we are able to extract information about the radiation, among the most important being the identification and location of the source. In this work, we analyze three different simulated radiation sources,cobalt-60, cesium-137, and technetium-99, and their spectra. The spectra have an energy range 70 keV to 2 MeV and are taken over a 21x21 grid of detectors, with a triangular steel shield laying across the top half of the of the detector grid, see the figure below.

(a)



(b)

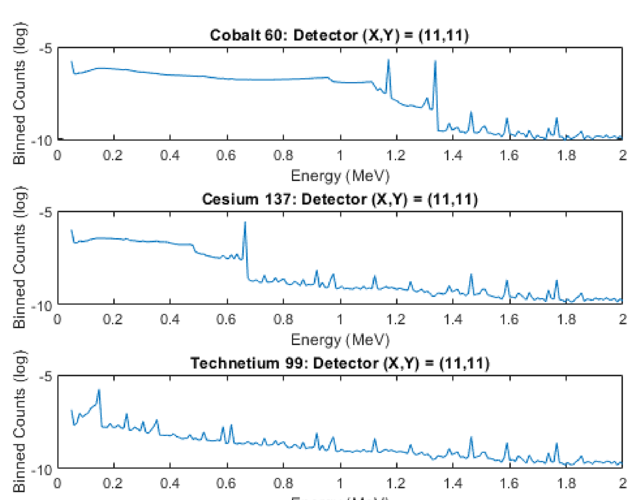


Figure 1: (a): The grid points of the simulation. The dark grey is concrete shielding and the light grey is open air. (b): Energy spectrums of Co60, Cs137 and Tc99 respectively. The data contains three sets of spectrum for each element (Co60, Cs137, Tc99) overlaid on the grid in (a) at each gridpoint.

Theory and Methods

a. Principal Component Analysis

When PCA is applied to large data sets, it calculates eigenvectors (called the principle components) [2]. This is accomplished by the PCA algorithm which:

- Iterates the data to minimize least-squares-error between eigenvectors and the data
- **Maximizes variance with each iteration to best span the data**
- Reduces the number of dimensions (eigenfunctions) used to describe the data

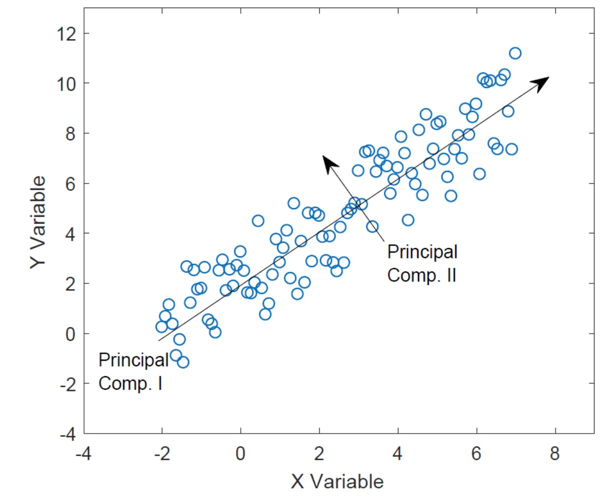


Figure 2 (PCA): This figure demonstrates constraining to eigenvectors which best cover the space while minimizing the variance

b. Nonnegative Matrix Factorization

In NNMF, a given data matrix, A, is approximated by taking the low-rank product of two or more generated matrices, W and H, with the constraint that the matrix elements are nonnegative [3]:

- Extracts sparse features from the data matrix A
- Is easily interpretable (following logical or physical patterns)
- **Reduces dimensionality of data into linear combination of bases**
- Learns part-based representations by combining parts to form a whole

To the right shows the decomposition of a large matrix A into spatial information in W and Source information (energy) contained in the H matrix.

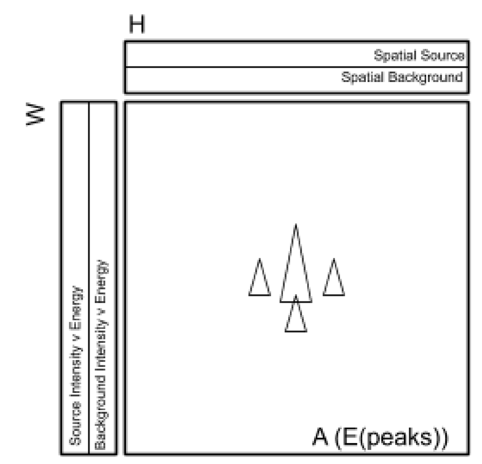


Figure 3 (NNMF): Visualization of the matrices of NNMF. A is the data matrix, and W, and H are the decomposed matrices.

c. CP Tensor Decomposition

Similar to NNMF in decomposition and PCA in the developed vectors, CPT gives a low-rank approximation. However, the approximated tensor is unique and provides useful information from [4]:

- **Separated mixtures of sources/ signals**
- Measured concentrations of sources and signals
- Approximated spectral profiles

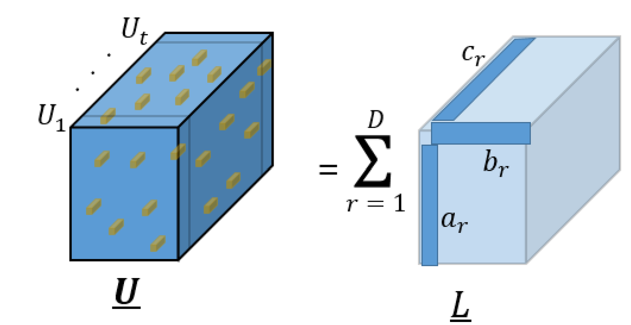


Figure 4 (CPT) : Tensor decomposition visualization into arrays a, b, c, reproduced from: ref. [5].

d. Qualitative Method Comparison

Comparison
Comparing metrics gives us a better idea of which method is the best before developing our own analysis

Notice
- Highlighted most desirable traits from each method

We conclude
PCA has the most qualitatively favorable attributes.

	PCA	NNMF	CPT
Non-negativity	No	Yes	No
Residuals	Machine Precision	Normal	Normal
Feature Type	Eigenvector	Feature Vector	Feature Vector
Characterization of breakdown	By highest variance	By high/low energy component	Both high/low energy comp./var.
Fixed Features	Yes	No	No
Run time	0-1s	15-60s	~1000s
Linearity	Linear	**Non-linear**	**Non-linear**
Total	4	3	3

Analysis

(1) Test of the similarity between the eigenvectors:
We normalize the eigenvectors generated by PCA, NNMF, and CPT in order to determine the coefficient of sameness, S, given by

$$S_{ij} = \langle \psi_{\mathrm{Method},i} | \psi_{\mathrm{Method},j} \rangle^2 \qquad \langle \psi_{\mathrm{Method},i} | \psi_{\mathrm{Method},i} \rangle = 1$$

This quantity provides a comparison between eigenvectors, both within and between each method.

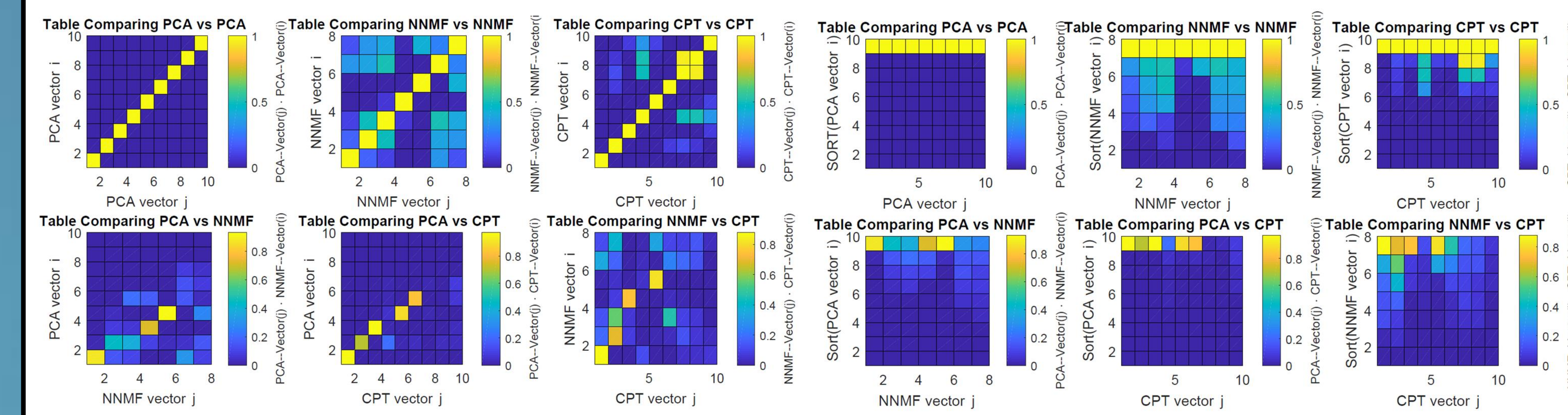
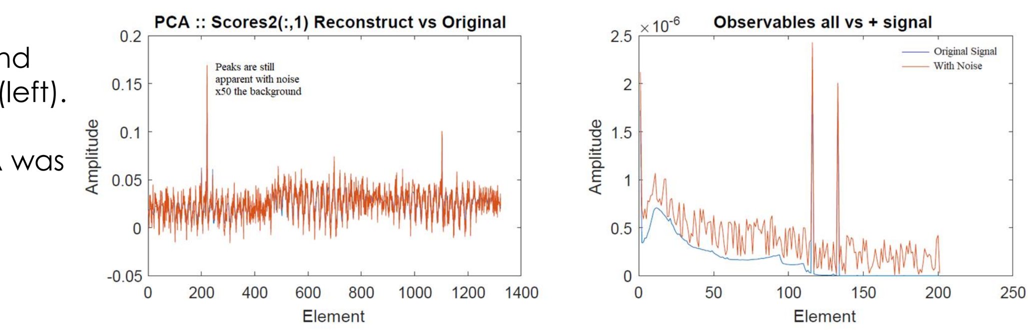


Figure 5 (left): The top row of panels evaluate the inner product of the normalized eigenvector (below denotes with psi). Methods are either: PCA, NNMF, or CPT. By normalizing the eigenvectors, we could then calculate a coefficient called "sameness" which ranged from 0 (no similarity) to one which means they are identical.
Figure 6 (right): Sorting the last figure (in y) in order to see the spread of the data. For NNMF dotted with NNMF, we see the vectors are not all orthogonal like they are in PCA or like they are close to in CPT.

(1) Test Ambient Noise:
Testing our reconstruction (see below) by introducing gaussian noise to the signal, we looked to see which method could best isolate the signal.

Figure 7 (right): Demonstration of noise addition (right) and our ability to identify the features even in this noisy data (left).

Running this on PCA, NNMF, and CPT we found that PCA was typically able to best at retrieving the features in the reconstruction.



(3) Reconstruction of the original Matrix
From our reduced order model, we can rebuild our original matrices by simple matrix products. This is useful for calculating the frobenius norm: $f_{norm} = ||A - A_{Rebuild}||$. These are calculated by

$$A_{\mathrm{reconstructed,PCA}} = M_{\mathrm{scores}} N_{\mathrm{coeff.}}^{T} \qquad A_{\mathrm{reconstructed,NNMF}} = WH \qquad A_{\mathrm{reconstructed,CPT}} = (A_{\mathrm{CPT}} \cdot C)B^{T}$$

(4) Determination of Locations & Determination of Radiation Types
Using our eigenvectors PCA, and feature vectors, NNMF and CPT, from our reduced order models (ROMs) we can solve the system of equations to determine the types and locations of the radiation types.

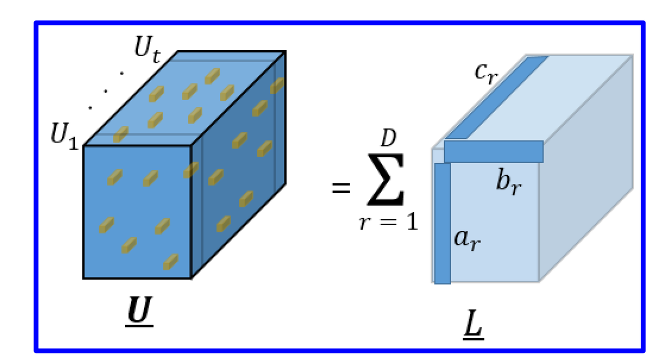
$$N_{\mathrm{reconstructed,coeff.}} = [\ A^{T} \vdots M_{\mathrm{scores}}^{T}\ ] \qquad H_{\mathrm{reconstructed}} = [\ A^{T} \vdots W^{T}\ ] \qquad B_{\mathrm{reconstructed}} = [\ A^{T} \vdots (A_{\mathrm{CPT}} \cdot C)^{T}\ ]$$

(5) Conclusions and Future Work

CPT is the best for describing radiation data

Pros (of CPT):
- Non-linear method, which can extrapolate non-linear features
- CPT and NNMF require less dimension to describe the data
- Sameness test verifies the near-uniqueness of the CPT vectors (efficiently describing data)

Cons (of CPT):
- Missing the positivity enforced by NNMF
- Qualitative comparison indicates PCA had the most overall-positive attributes
- Reconstruction error is low, and identifies features which have significant noise



Future work:
We have only begun to scratch the surface. Quantitative analysis between PCA, NNMF, and CPT will be lastingly important because of their relativity to machine learning.

Future Results…

Acknowledgement :
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[3] Gillis, Nicolas. The why and how of nonnegative matrix factorization. Regularization, optimization, kernels, and support vector machines 12.257 (2014): 257-291.
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