Improved Probabilistic Principal Component Analysis for Application to Reduced Order Modeling.

A fundamental application of classical PCA is reduced order modeling (ROM), where the principal components are computed from a training data (TD) set and used as a reduced basis for the data space. In our previous work, we made a ROM for stochastic systems by projecting rapidly calculated (but noisy) data onto the basis vectors to obtain rapid, accurate predictions. All of these steps were done using techniques that do not account for noise in the data and $L_2$ projection to create the reduced representations of the noisy data. In this work, stochastic approaches are used. The PPCA is used to generate the basis, which then allows estimating the noise in the TD. The standard PPCA has also been improved so that the variance of the basis expansion coefficients when representing the TD can be estimated. Another benefit of PPCA is to use model selection (MS) criteria to automatically truncate the basis used for the ROM. A new statistical approach for the projection step is used. The holistic approach gives a fully stochastic method for computing a ROM from noisy TD, determining the ideal MS, and projecting noisy test data onto the ROM. We demonstrate our framework on synthetic data and on an application to computing radiation transport with MC simulations. (Received September 20, 2016)