# Stochastic Subspace via Bootstrap for Characterizing Model-form Uncertainty

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## Abstract

We propose a probabilistic model of subspaces based on the Bootstrap method. It is applicable to projection-based reduced-order modeling methods, such as proper orthogonal decomposition. The stochastic subspace thus constructed can be used, for example, to characterize model-form uncertainty in computational mechanics and digital twinning. The proposed method has multiple desirable properties: (1) it uses the empirical distribution of the data; (2) it satisfies linear constraints, such as boundary conditions of all kinds, by default; (3) it has only one hyper-parameter, which greatly simplifies training; and (4) its algorithm is very easy to implement. We compare the proposed method with existing approaches in characterizing the uncertainty of a dynamics model of a space structure.

## 1 Introduction

Model error is ubiquitous in computational engineering, but its probabilistic analysis has been a notoriously difficult challenge. Unlike parametric uncertainties that are associated with model parameters, model-form uncertainties concern the variability of the model itself, which are inherently nonparametric (Morrison et al., 2018). A recent seminal work in model-form uncertainty merges ideas from projection-based reduced-order modeling and random matrix theory (Soize and Farhat, 2016). The key observation is that since a reduced-order basis (ROB) determines a reduced-order model (ROM), randomizing the ROB also randomizes the ROM, which can be used for efficient probabilistic analysis of model-form error. In this context, a few probabilistic models and estimation procedures have been proposed to construct a stochastic ROB (Soize and Farhat, 2016; Zhang and Guilleminot, 2023). However, the existing methods have limitations in terms of practical application due to high numbers of hyper-parameters, complex implementation, and poor uncertainty quantification (UQ). This study aims to develop an efficient way to construct a stochastic subspace that is free from the aforementioned limitations. The proposed method can be used to build surrogate models and digital twins. We showcase its use in the characterization of model-form error.

## 2 Stochastic reduced-order modeling

**High-dimensional model:** In general, we consider a parametric nonlinear system given by a set of ordinary differential equations (ODEs): $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, t; \boldsymbol{\mu})$, with $\mathbf{x} \in \mathbb{R}^n$ and $t \in [0, \infty)$, and is subject to initial conditions $\mathbf{x}(0) = \mathbf{x}_0$ and linear constraints $\mathbf{B}^\intercal \mathbf{x} = \mathbf{0}$, where $\mathbf{B} \in \mathbb{R}^{n \times n_{CD}}$. These equations often come from a spatial discretization of a set of partial differential equations that govern a given physical system, with dimension $n \gg 1$. We call this the *high-dimensional model* (HDM).

**Reduced-order model:** The Galerkin projection of the HDM onto a $k$-dim subspace $\mathscr{V}$ of the state space $\mathbb{R}^n$ gives a reduced-order model (ROM). Let $\mathbf{V} \in St(n, k)$ be an orthonormal basis of the

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subspace $\mathscr{V}$, the ROM can be written as: $\dot{\mathbf{q}} = \mathbf{V}^\intercal \mathbf{f}(\mathbf{V}\mathbf{q}, t; \boldsymbol{\mu})$, with $\mathbf{q} \in \mathbb{R}^k$, $\mathbf{x} = \mathbf{V}\mathbf{q}$, and initial conditions $\mathbf{q}(0) = \mathbf{V}^\intercal \mathbf{x}_0$. To satisfy the linear constraints, we must have $\mathbf{B}^\intercal \mathbf{V} = \mathbf{0}$. A common way to find a reduced-order basis (ROB) $\mathbf{V}$ and the associated subspace $\mathscr{V}$ is *proper orthogonal decomposition* (POD).

**Stochastic reduced-order model:** In this work, we use the stochastic subspace model in 3 to derive a stochastic reduced-order model (SROM) from the HDM. As with POD, the stochastic basis $\mathbf{W}$ satisfies the linear constraints $\mathbf{B}^\intercal \mathbf{W} = \mathbf{0}$ automatically. To find an optimal hyper-parameter $p \in [k, \infty)$, we minimize $\mathbb{E}[|d_o(u_E) - d_o(u_L)|^2]$, where $u_E$ is the experimental or ground-truth observation of the output, $u_L$ is the low-fidelity prediction of the SROM, and $d_o(u) := \|u - u_L^o\|_{L^2}$ is the $L^2$ distance to the low-fidelity prediction $u_L^o$ of a reference model. This objective function aims to improve the consistency of the SROM in characterizing the error of the reference model, and it can be optimized efficiently using any 1-D optimization scheme and point estimates using Monte Carlo.

## 3 Bootstrap: distribution-free modeling

The bootstrap (Efron, 1979) is a non-parametric sampling-based approach to estimate the sampling distribution of a statistic. The stochastic subspace model is derived by resampling the data with replacement from the empirical distribution and performing POD. In this work, we introduce a new class of stochastic subspace models based on the bootstrap method, incorporating a hyper-parameter $p$ to control the number of data points sampled. Algorithm 1 gives a procedure for sampling stochastic reduced order basis from the SS-Bootstrap model.

**Algorithm 1** `SS-Bootstrap`: Stochastic subspace via bootstrap.

**Input:** $\widetilde{\mathbf{V}}$; $\widetilde{\boldsymbol{\Sigma}}$; $\widetilde{\mathbf{W}}$; subspace dimension $k \in \{1, \cdots, n\}$; resample size $p \in \{k, k+1, \cdots\}$; number of snapshot is m.

1: Generate vector $\mathbf{b} = (b_i)_{i=1}^p$ with $b_i \overset{\text{iid}}{\sim} U(\{1, \cdots, m\})$

2: $\mathbf{M} \leftarrow \widetilde{\boldsymbol{\Sigma}} \widetilde{\mathbf{W}}(\mathbf{b}, :)^\intercal$

3: Truncated SVD: $[\mathbf{U}_k, \sim, \sim] \leftarrow \text{svds}(\mathbf{M}, k)$

**Output:** $\mathbf{W} = \widetilde{\mathbf{V}}\mathbf{U}_k$, an orthonormal basis of a random subspace sampled from the bootstrap model.

## 4 Numerical experiment: dynamics problem of a space structure

We consider a major component of a space structure given an impulse load in the $z$-direction, see **Fig. 1**. We take the quantity of interest (QoI) to be the $x$-velocity of a critical point at one of the essential components. The HDM is solved using the Newmark-$\beta$ time integration scheme with a time step of $5 \times 10^{-2}$ ms. We construct a ROM with dimension $k = 10$ via POD, and characterize its model error. From **Fig. 2** and **Fig. 3** we see that the 95% PI of the Bootstrap method is consistent and much sharper than that of the NPM. While both methods are mostly consistent, Bootstrap is at least a few times sharper than NPM, depending on the QoI being displacement, velocity, or acceleration.

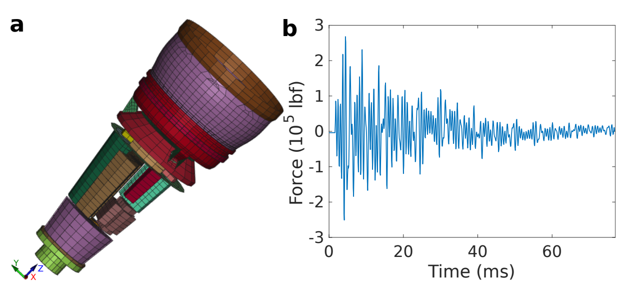


Figure 1: (a) space structure; (b) loading.

## 5 Conclusion

We introduced a stochastic subspace model which is used to characterize model-form error. It is simple, consistent, and very easy to train. Via numerical example, we reveal the characteristics of this model, establish its consistency, and quantify its remarkable improvement in sharpness over current methods. It opens up a promising path to the challenging problem of model-form uncertainty. Furthermore, the developed surrogate model, i.e., the stochastic subspace model via bootstrap, can be used in different applications like digital twins and design and optimization under uncertainty.

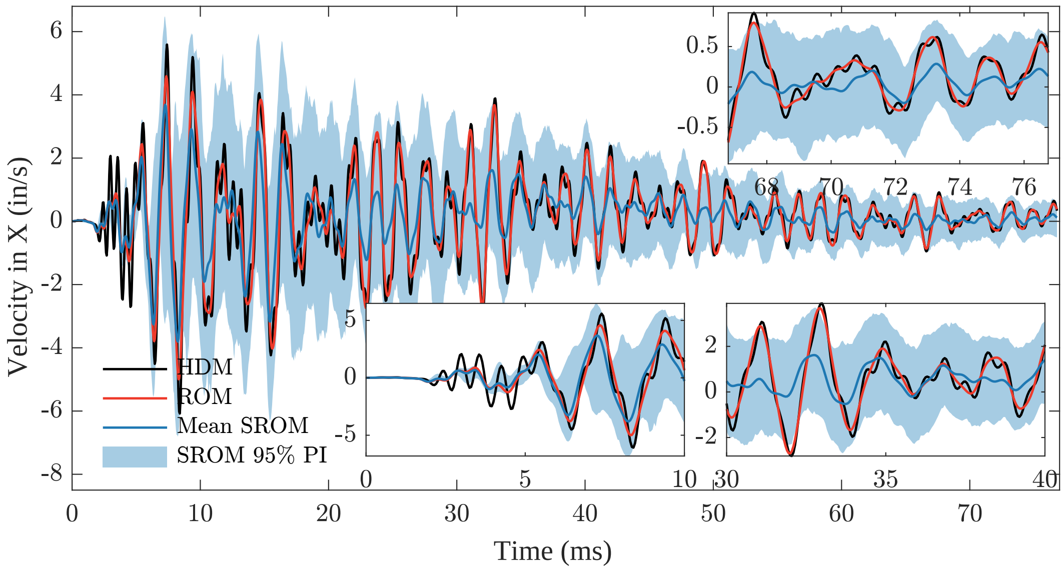

Figure 2: Dynamic prediction of the NPM model

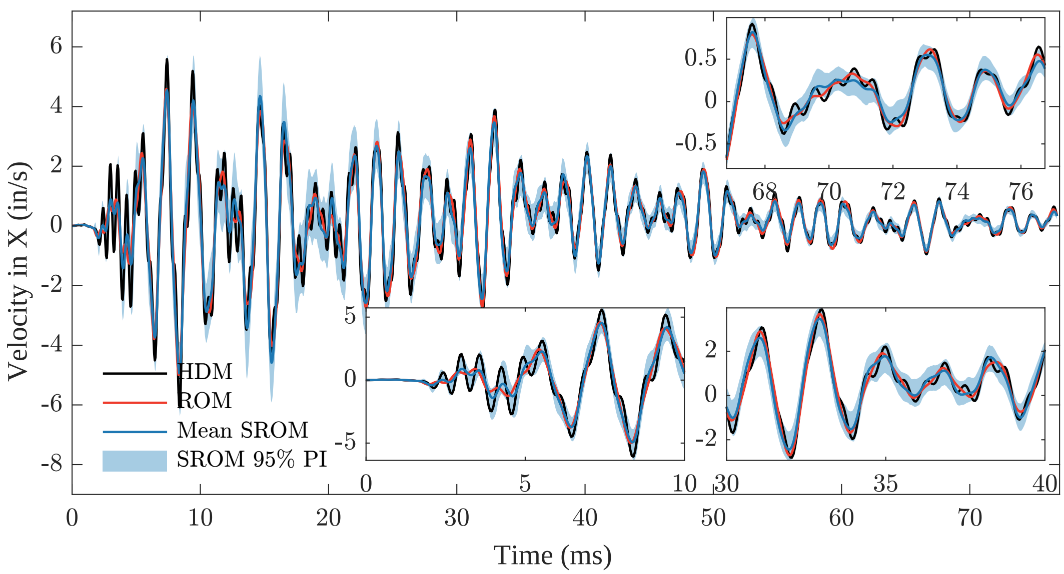

Figure 3: Dynamic prediction of the Bootstrap model

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