Reduced Order Modeling using Shallow ReLU Networks with Grassmann Layers

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Problem Statement

Approximate:

$$f : \Omega \subseteq \mathbb{R}^m \to \mathbb{R}^n \text{ where } m \gg 1 \text{ , given } \{(x_\ell, f(x_\ell), Df(x_\ell))\}_{\ell=1}^{M}$$

Application Examples

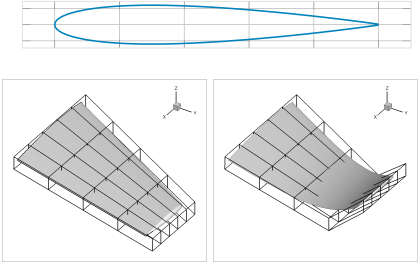

Figure 1: Top: **NACA0012 airfoil**, $m = 18$ (Hicks-Henne shape parameters); Bottom: **ONERA-M6 wing**, $m = 50$ (free-form deformation parameters) (image source: Lukaczyk et al. 2014); $f =$ lift/drag coefficients

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Overview

Reduced Order Modeling (ROM)

ROMs: approximate high-dimensional complex systems by simpler low-dimensional systems

Examples:

- proper orthogonal decomposition (POD), e.g. Berkooz, Holmes, and Lumley 1993; Holmes et al. 2012
- global sensitivity analysis, e.g. Saltelli et al. 2008
- sliced inverse regression, e.g. Li 1991
- compressed sensing, e.g. Fornasier, Schnass, and Vybiral 2012
- *active subspace*, e.g. Russi 2010; Constantine, Dow, and Wang 2014

Illustrative Function for Active Subspace

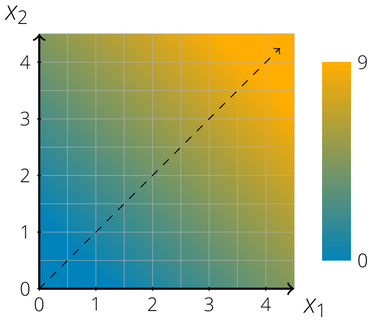


Figure 2: $f(x_1, x_2) = x_1 + x_2$

Active Subspace

Consider:

$$f \in C^1(\Omega; \mathbb{R}^n), \quad \Omega \subseteq \mathbb{R}^m \quad ; \quad C \in \mathbb{R}^{m\times m} \text{ defined by } C := \mathbb{E}\left[Df^T Df\right] = W\Lambda W^T$$

$$W = \Big[\overbrace{W_1}^{m\times k} \quad \underbrace{W_2}_{m\times(m-k)}\Big], \quad \Lambda = \begin{bmatrix} \overbrace{\Lambda_1}^{k\times k} & \\ & \underbrace{\Lambda_2}_{(m-k)\times(m-k)} \end{bmatrix}, \quad (\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_m)$$

Lemma (based on Lemma 2.2[1])

Under the rotated coordinates $y = W_1^T x \in \mathbb{R}^k$ and $z = W_2^T x \in \mathbb{R}^{m-k}$:

$$\sum_{i=1}^{n} \mathbb{E}[\nabla_y(f_i)^T \nabla_y(f_i)] = \lambda_1 + \cdots + \lambda_k$$

$$\sum_{i=1}^{n} \mathbb{E}[\nabla_z(f_i)^T \nabla_z(f_i)] = \lambda_{k+1} + \cdots + \lambda_m$$

[1] Constantine, Dow, and Wang 2014

Methodology

Surrogate Model

Given:

$$f : \Omega \subseteq \mathbb{R}^m \to \mathbb{R}^n, \text{ with } m \gg 1$$

Surrogate Model:

$$f \approx g_\theta \circ U^T$$

where

- $U \in \mathbb{R}^{m \times k}$; maps input space to k-dimensional subspace
  - construction inspired by the *active subspace* method, i.e. utilizing the dominate left singular vectors of the matrix

$$\left[Df(x_1)^T \ldots Df(x_M)^T \right]$$

- $g_\theta : \mathbb{R}^k \to \mathbb{R}^n$; approximates f with respect to k- dimensional inputs
  - represented by a *shallow ReLU network* with hidden dimension h and trainable parameters $\theta \in \mathbb{R}^d$ ($d = h(k + n + 1) + n$)

$$g_{\theta(y)} = A_2(\text{ReLU}(A_1 y + b_1)) + b_2$$

Alternating Minimization

$$\min_{\theta \in \mathbb{R}^d,\ \mathrm{Range}\, U \in Gr(k,m)} \frac{1}{M} \sum_{\ell=1}^{M} \| f(x_\ell) - g_\theta(U^T x_\ell) \|_2^2 + \lambda \|\theta\|_2^2.$$

Algorithm 1 (alternating minimization scheme)

Initialize: U via active subspace method, θ for ReLU network g, learning rate τ.

repeat

(1) Update weights θ via ADAM method applied to:

$$\min_{\theta \in \mathbb{R}^d} \frac{1}{M} \sum_{\ell=1}^{M} \| f(x_\ell) - g_\theta(U^T x_\ell) \|_2^2 + \lambda \|\theta\|_2^2$$

(2) Update U via the Grassmann manifold-constrained least squares problem:

$$\min_{\mathrm{Range}\, U \in Gr(k,m)} \frac{1}{M} \sum_{\ell=1}^{M} \| f(x_\ell) - g_\theta(U^T x_\ell) \|_2^2$$

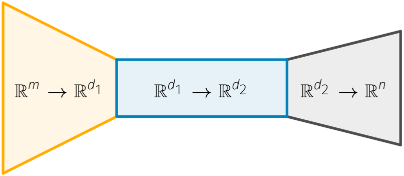
(3) Update: $\tau = 0.9\tau$

until converged

Other Neural Network (NN) based ROMs

- POD method with NN applied to fluid flows, Hesthaven and Ubbiali 2018; Lui and Wolf 2019
- PCA-based approach with NN applied to PDEs, Bhattacharya et al. 2020
- NN used to pick models from a dictionary of local ROMs, Daniel et al. 2020
- manifold learning using deep NN, Shaham, Cloninger, and Coifman 2018; Chui and Mhaskar 2018; Zhu et al. 2018
- encoder/decoder structured NN, Hinton and Salakhutdinov 2006; Ravi 2017
- *active subspace for input reduction and POD for output reduction with NN nonlinear fit in-between*, O'Leary-Roseberry et al. 2020

Example Encoder/Decoder Structure



Experimental Results

Strength in Data Scarce Setting

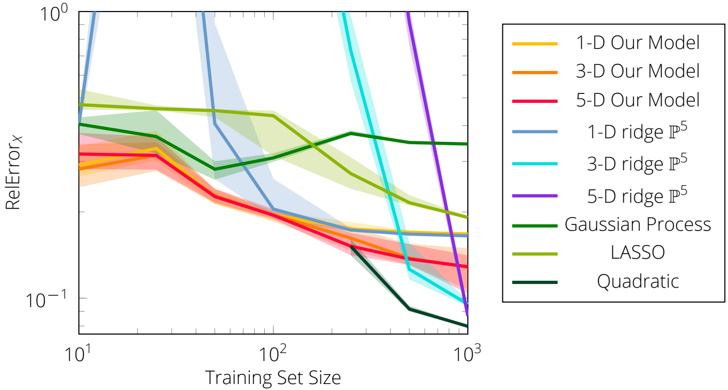
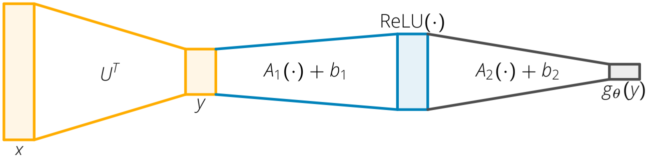


Figure 3: NACA0012 drag coefficient data; $\text{RelError}_X = \left(\frac{\sum_{x \in X} \|f(x) - \tilde{f}(x)\|_2^2}{\sum_{x \in X} \|f(x)\|_2^2} \right)^{\frac{1}{2}}$, $\tilde{f}$ represents the trained model for a given approach.

Benefits of Additional Structure/Interpretability



Our Model

	h=8	h=64	h=256
k=1	0.41	0.41	0.48
k=2	0.41	0.37	0.37
k=3	0.40	0.37	0.33

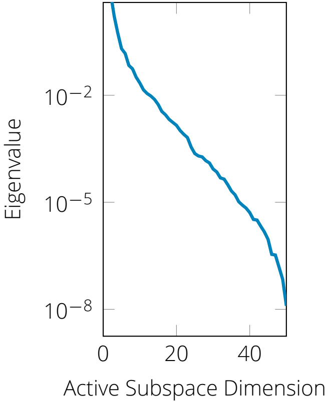
Bowtie Model

	h=8	h=64	h=256
k=1	0.47	0.47	0.47
k=2	0.50	0.48	0.52
k=3	0.49	0.51	0.51

Table 1: Relative validation error $\left(\frac{\frac{1}{|X_{Val}|} \sum_{x \in X_{Val}} \|f(x) - \tilde{f}(x)\|_2^2}{\frac{1}{|X|} \sum_{x \in X} \|f(x)\|_2^2} \right)^{\frac{1}{2}}$ of models applied to NACA0012 drag coefficient data; training/validation set size of 50.

Application to ONERA-M6 Wing

Eigenvalues (Λ) Show Potential
for Accuracy in Low Dimensions



	h=8	h=64	h=256
k=1	0.12	0.12	0.15
k=2	0.11	0.09	0.10
k=3	0.11	0.08	0.08

Table 2: Relative validation error of *our model* applied to **ONERA-M6 drag** coefficient data; training/validation set size of 50.

Acknowledgements

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(Virtual) Questions?

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Code: https://github.com/kaylabollinger/ROM_AS-NN.git