Combustion Reduced-Order Modeling with Nonlinear Projections

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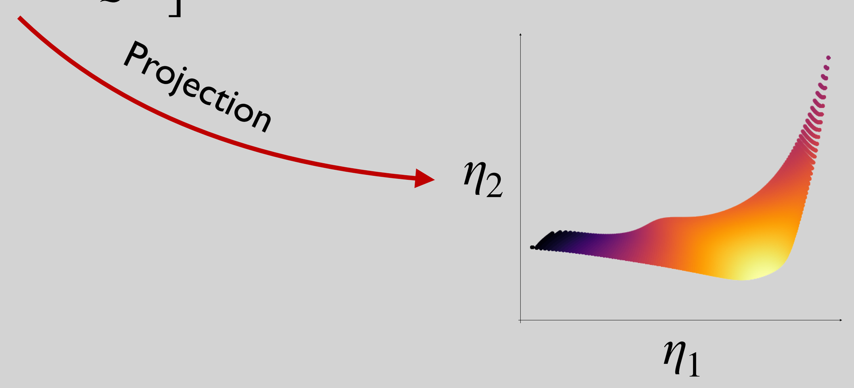
Idea

Reduce the number of variables (equations) needed to describe a system.

Thermo-Chemical State

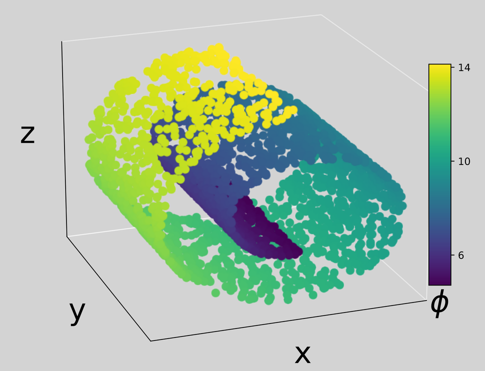
$\boldsymbol{\phi} = \left[T, Y_1, \ldots, Y_{Q-1}\right]$

$n_\eta < n_\phi$



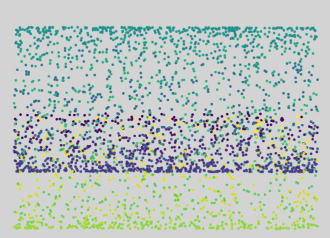
Methods

Combustion data is highly nonlinear. Linear methods project data onto a fixed basis. Nonlinear projections create a new representation of the data.

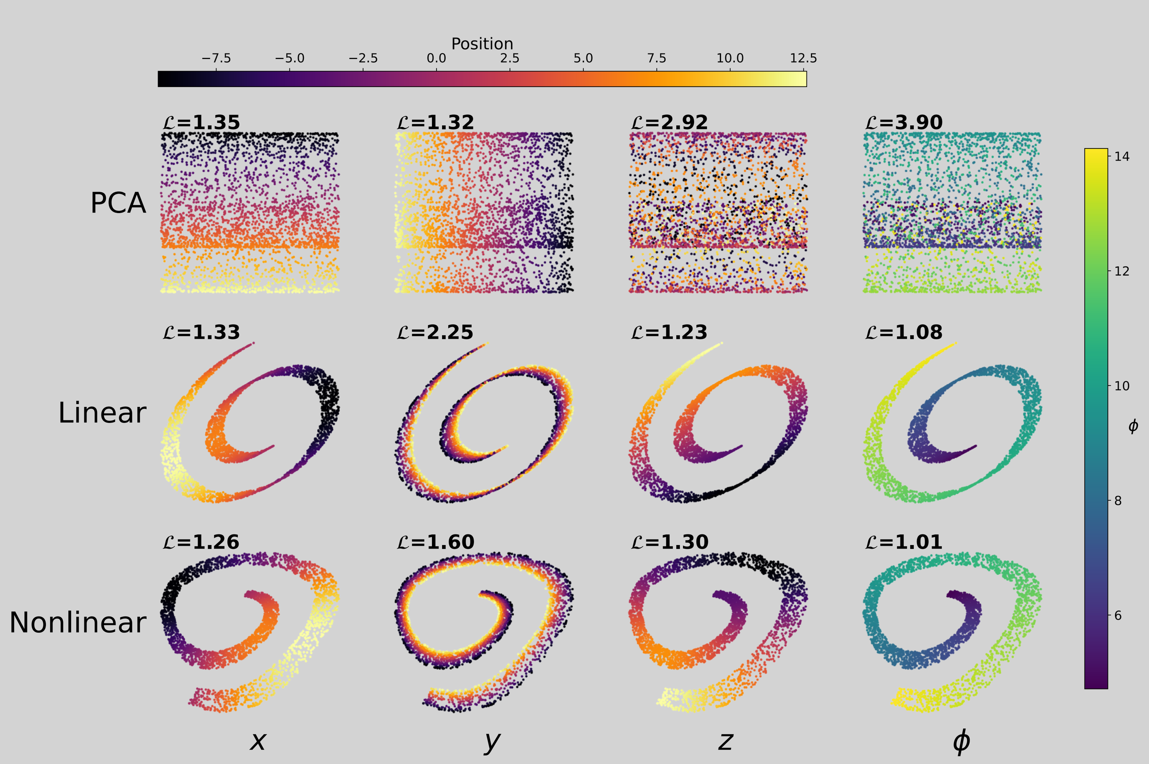


Swiss Roll Dataset Example

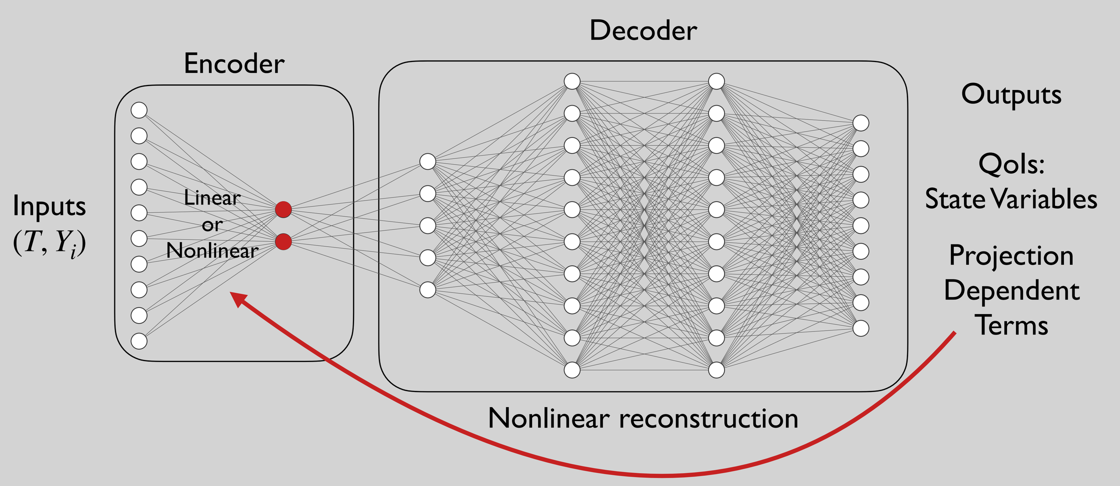
PCA only informed by original coordinates



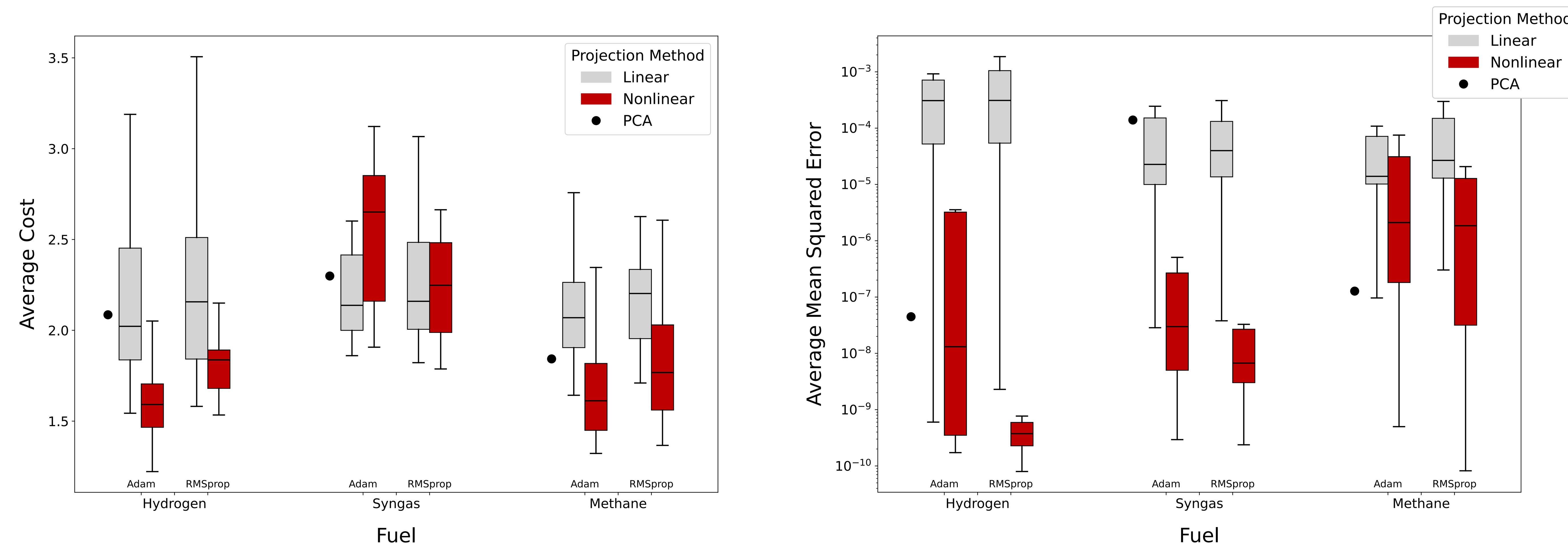
Linear and Nonlinear Encoder-Decoders informed by scalar ϕ

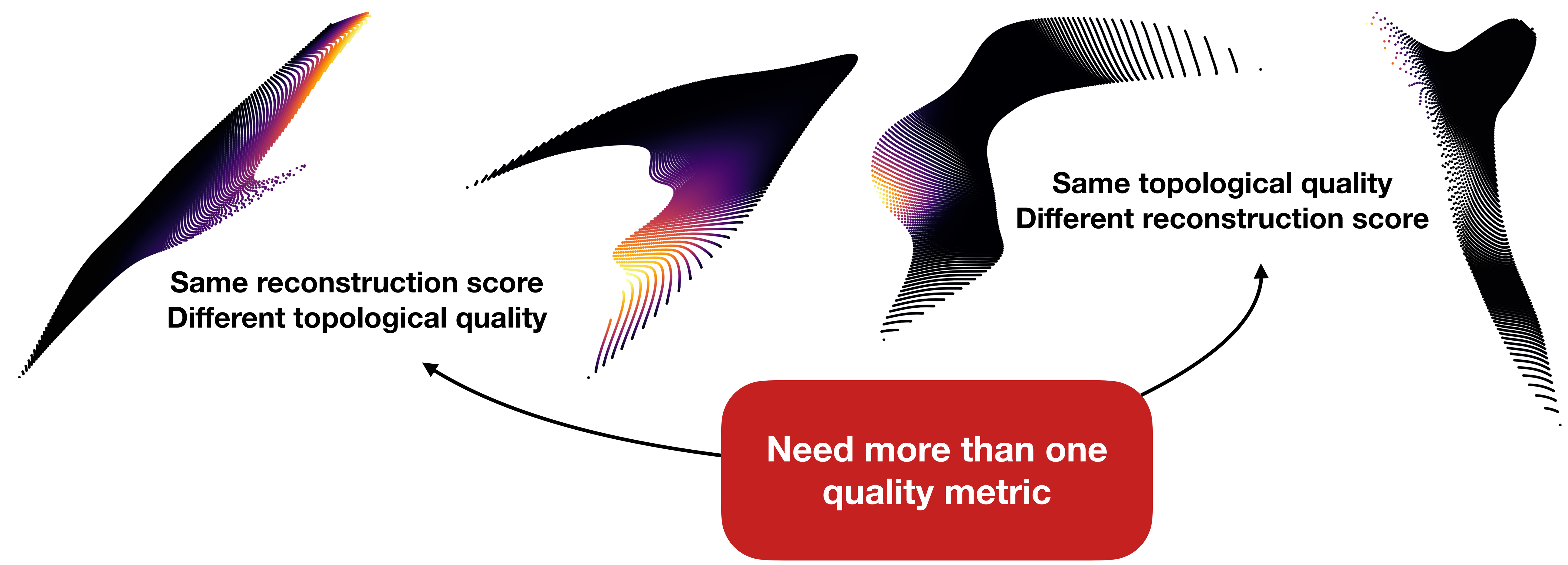


Inform projection training with reconstruction errors of quantities of interest that are functions of the projection



Nonlinear projections can achieve better quality manifolds than linear projections





Low-dimensional transport equations for nonlinear projections have additional terms

Ex: Flamelet equations

Linear:

$$\frac{\partial \eta_i}{\partial t} = \frac{\chi}{2}\frac{\partial^2 \eta_i}{\partial f^2} + S_{\eta_i}$$

Nonlinear:

$$\frac{\partial \eta_i}{\partial t} = \frac{\chi}{2}\frac{\partial^2 \eta_i}{\partial f^2} - \frac{\chi}{2}\frac{\partial F_j}{\partial \eta_\ell}\frac{\partial \eta_\ell}{\partial f}\frac{\partial F_k}{\partial \eta_m}\frac{\partial \eta_m}{\partial f}\frac{\partial^2 G_i}{\partial \phi_j \partial \phi_k} + S_{\eta_i}$$

Diffusion

Sources

Nonlinear term

Nonlinear term describes how the definition of the projection changes

Nonlinear term utilizes reconstruction: $\boldsymbol{\phi} = \boldsymbol{F}(\boldsymbol{\eta})$

Data

Training data generated with adiabatic flamelet equations

$$\frac{\partial \phi_j}{\partial t} = \frac{\chi}{2}\frac{\partial^2 \phi_j}{\partial f^2} + S_{\phi_j}$$

Training Data Generation		
Fuel	**Dissipation Rate Range (s^{-1})**	**Number of State Variables**
H_2	0.1-400	9
Syngas	1-1400	11
CH_4	0.1-200	31

Encoder-Decoder Specs		
Hidden Layer Architecture	**Activation Functions**	**Retained State Variables**
22,22,9	T,T,L,L	T, H, H_2, OH, H_2O, O_2, H_2O_2
26,26,11	T,T,L,L	T, H_2, O_2, OH, H_2O, CO, CO_2, HCO
66,66,31	T,T,L,L	T, H_2, O_2, OH, H_2O, CH_2, CH_3, CH_4, CO, CO_2, CH_2O, C_2H, C_2H_2

T - hyperbolic tangent, L - linear

Definitions

$\boldsymbol{\phi}$ - state variables

$\boldsymbol{\eta}$ - parameterizing variable

S_ϕ - source terms

S_η - projected source terms

Linear Projections

A - matrix of weights $\left(n_\eta \times n_\phi\right)$

$$\boldsymbol{\eta} = A \cdot \boldsymbol{\phi} \qquad \mathbf{S}_\eta = A \cdot \mathbf{S}_\phi$$

Nonlinear Projections

$\boldsymbol{G}$ - C_2 continuous nonlinear function

Inputs: n_ϕ Outputs: n_η

Encoding layer of neural network

$$\boldsymbol{\eta} = \boldsymbol{G}(\boldsymbol{\phi}) \qquad S_{\eta_i} = \frac{\partial G_i}{\partial \phi_j} S_{\phi_j}$$

$\frac{\partial G_i}{\partial \phi_j}$ - encoder sensitivities $\left(n_\eta \times n_\phi\right)$

Neural networks allow encoder sensitivities to be easily obtained.

Local PCA obtains better projections than global PCA by clustering the state space, but low-dimensional transport equations cannot be derived since sensitivities aren't defined between the state space discontinuities.

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