Non-linear regression of chemical source terms using Deep Neural Networks

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Combustion modelling using Principal Components

Modelling the turbulent combustion phenomena is a challenging task due to **high dimensionality** of the problem. Even for a simple fuel such as methane the chemical mechanism involves 53 species and 325 reactions [1]. Recently, techniques from data science community were applied to combustion data sets to reduce their dimensionality to only few, most significant modes. One of them is Principal Component Analysis (PCA) which finds the directions of the largest variance in the data. PCA proved to identify the optimal low-dimensional combustion manifolds [2].

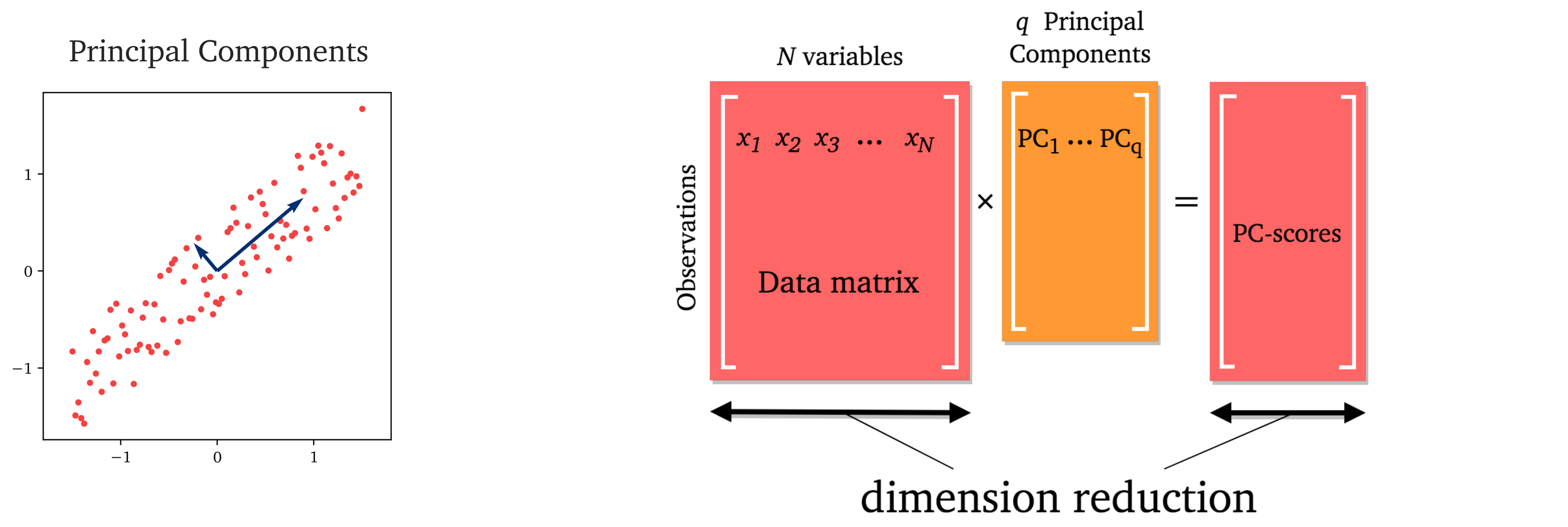

Fig. 1. Identification of Principal Components and dimensionality reduction.

PC-transport approach

In a simulation, instead of transporting large number of variables such as species mass fractions, temperature and pressure, one may transport the identified Principal Components, which are a linear combination of the original variables.

$$\rho \frac{\partial \boldsymbol{\Phi}}{\partial t} + \rho \vec{\boldsymbol{V}} \cdot \nabla \boldsymbol{\Phi} = \nabla \rho \mathbb{D}_{\Phi} \nabla \boldsymbol{\Phi} + \boldsymbol{S}_{\Phi}$$

Linear transformation $\quad \mathbf{z} = \boldsymbol{\Phi} \mathbf{A_q}$

$$\rho \frac{\partial \mathbf{z}}{\partial t} + \rho \vec{\boldsymbol{V}} \cdot \nabla \mathbf{z} = \nabla \rho \mathbb{D}_{z} \nabla \mathbf{z} + \boldsymbol{S}_{z}$$

Much fewer equations are solved on the simulation grid, since only the first few Principal Components carry most of the information in a data set. This is known as the PC-transport approach [3].

However, PCA is a linear technique and the combustion manifolds can be **highly non-linear**. One of such non-linear terms is the source **S**, which after the linear transformation becomes the source of the corresponding Principal Component (PC-source).

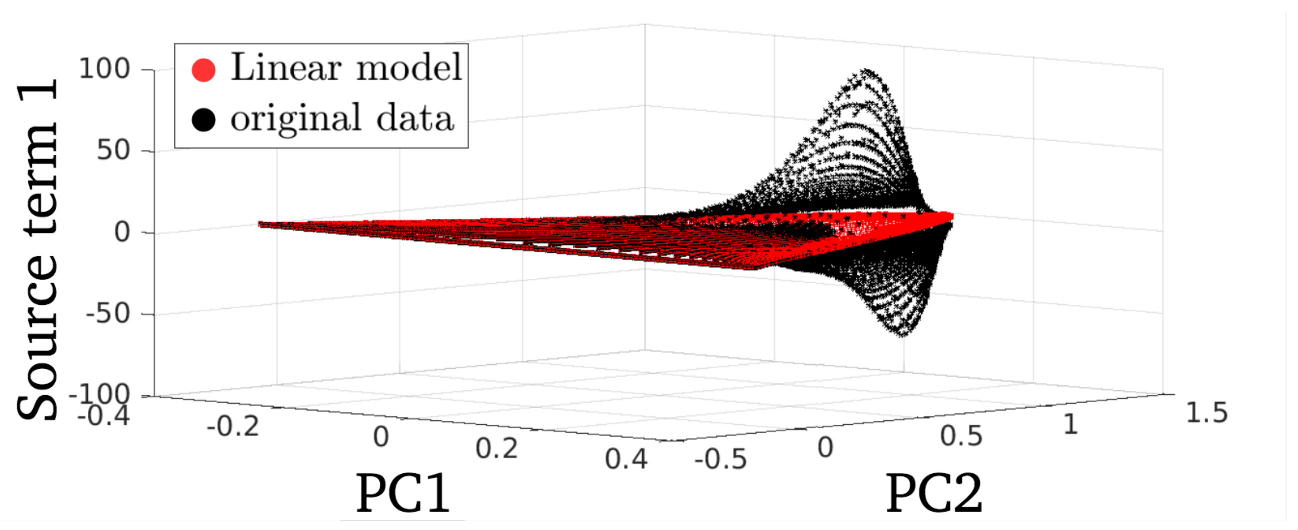

Fig. 2. Using a linear model (such as PCA) to approximate source terms can lead to significant errors. Figure: M. R. Malik.

Preliminary results

Non-linear regression techniques can be used in conjunction with a dimensionality reduction method for a more accurate parameterization of the low-dimensional manifold [4, 5].

In the present work, a Deep Neural Network (DNN) was implemented in Python language using TensorFlow library to regress the PC-source terms from the Sandia flame D.

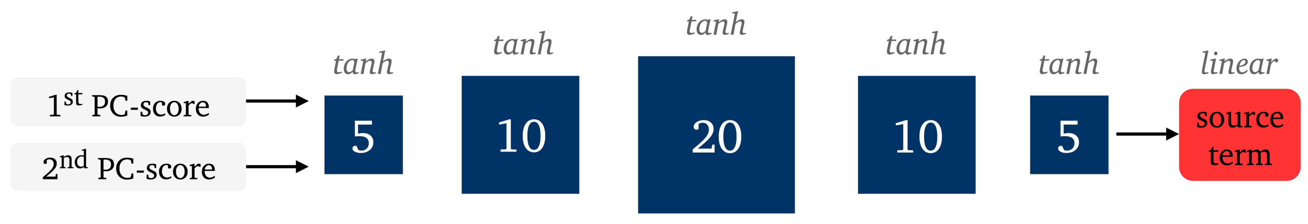

Fig. 3. Architecture of the neural network. Using Adam optimizer and MSR loss.

The performance of the network was summarized by the normalized Root Mean Squared error (NRMSE) when reconstructing the original source term.

$$\text{NRMSE} = \sqrt{\frac{\overline{(\mathbf{X} - \mathbf{f})^2}}{\overline{\mathbf{X}^2}}}$$

where **X** is the original data and **f** is the model fit

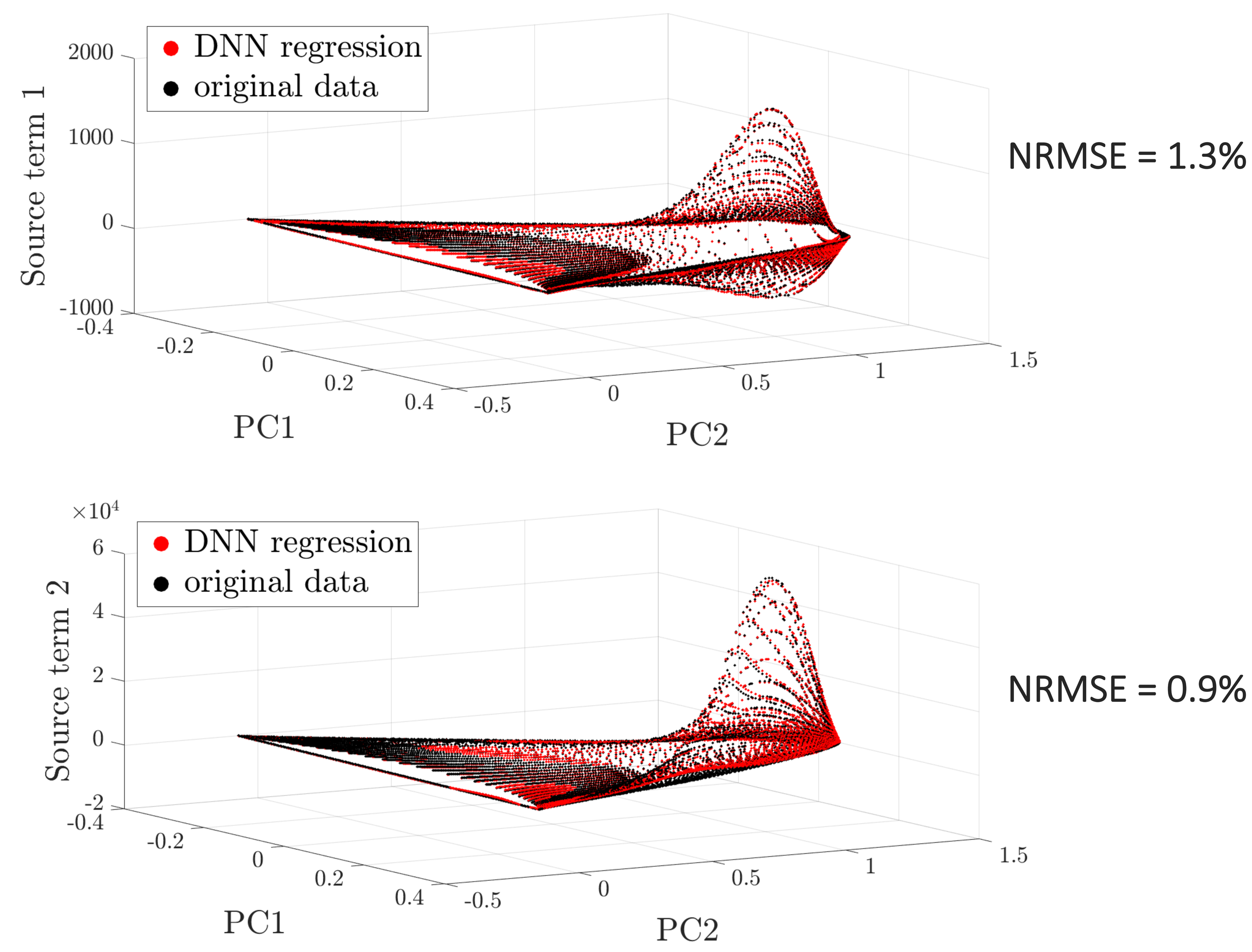

Fig. 4. Regression of the first two PC-source terms using a non-linear technique is capable of **following the curvature of the manifold**.

Future work

So far, the technique has been tested on **0D reactors** (such as PSR) [4]. The next step would be to implement the regression for gradually more complex systems, such as simulation of **1D** or **2D flames**.

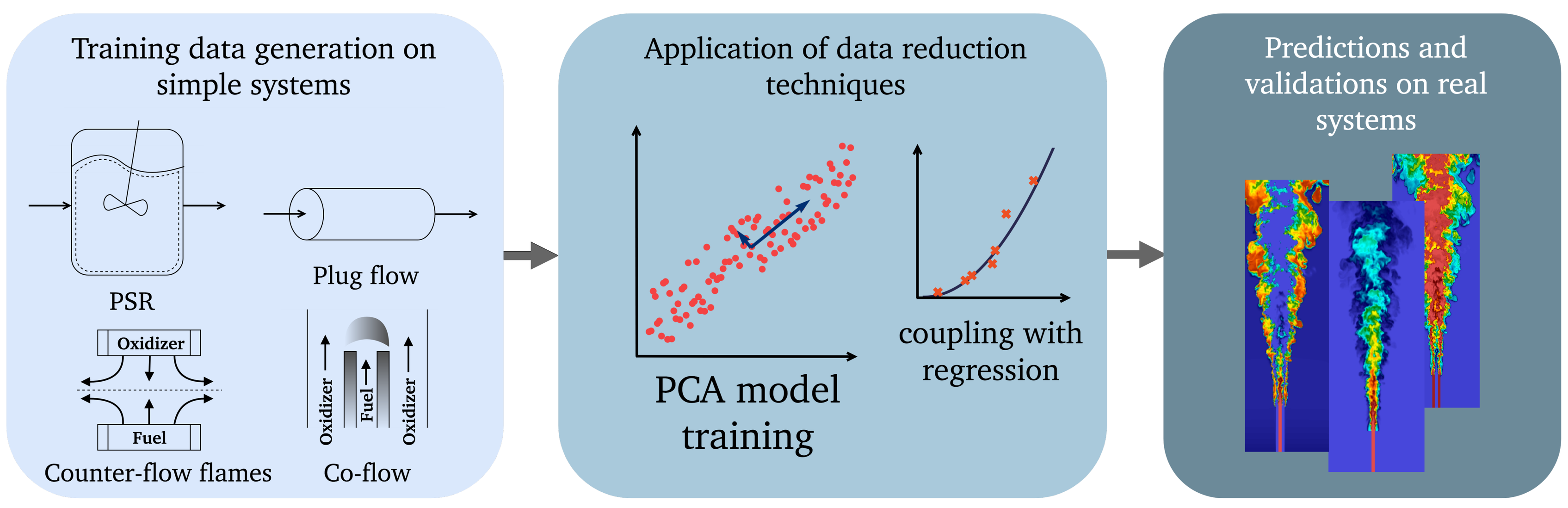

Fig. 5. Workflow for future work.

[1] G.P. Smith, D.M. Golden, M. Frenklach, N.W. Moriarty, B. Eiteneer, M. Golden- berg, C.T. Bowman, R.K. Hanson, S. Song, W.C.G. Jr., V.V. Lissianski, Z. Qin, GRI- Mech 3.0, The Gas Research Institute, http://www.me.berkeley.edu/gri_mech/, 1999. **[2]** A. Parente, J.C. Sutherland, L. Tognotti, P.J. Smith, Identification of low-dimensional manifolds in turbulent flames, Proc. of the Comb. Institute 32 (2009) 1579-1586. **[3]** J.C. Sutherland, A. Parente, Combustion modelling using principal component analysis, Proc. of the Comb. Institute 32 (2009) 1563-1570. **[4]** M.R. Malik, B.J. Isaac, A. Coussement, P.J. Smith, A. Parente, Principal component analysis coupled with nonlinear regression for chemistry reduction, Combust. Flame 187 (2018) 30-41. **[5]** B. Isaac, J. Thornock, J. Sutherland, P. Smith, A. Parente, Advanced regression methods for combustion modelling using principal components, Combust. Flame 162 (6) (2015) 2592–2601.