Combustion and Flame 162 (2015) 1650–1652

Contents lists available at ScienceDirect

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

The reconstruction of thermo-chemical scalars in combustion from a reduced set of their principal components

Hessam Mirgolbabaei, Tarek Echekki *

Department of Mechanical and Aerospace Engineering, North Carolina State University, Raleigh, NC, USA

ARTICLE INFO

Article history:
Received 15 August 2014
Received in revised form 18 November 2014
Accepted 19 November 2014
Available online 11 December 2014

Keywords:
Principal component analysis
Turbulent combustion

ABSTRACT

We compare two reconstruction approaches for thermo-chemical scalars (TCSs) in turbulent combustion using principal component analysis. The first approach is based on the inversion of the linear relation between the TCSs and their principal components (PCs). The second is based on a regression of TCSs with a reduced set of the PCs using artificial neural networks. The study is based on one-dimensional turbulence simulation data of Sandia Flame F. We find that regression potentially offers superior reconstruction to the inversion expression when a truncated set of the original PCs is used.

1. Introduction

Principal component analysis (PCA) has been proposed recently as a method to reduce the computational cost of turbulent combustion simulations where thermo-chemical scalars (TCSs) can be represented by a smaller number of principal components (PCs) using principal component analysis (PCA) [1–14]. This approach, among other approaches (see for example Ref. [15] and references cited therein), aims at reducing the complexity of combustion chemistry and accelerate its integration. Reconstruction methods to map a reduced set of PCs to the TCSs include (1) the inversion of the expressions relating the PCs to the TCSs [3,9–11] or (2) the regression of the TCSs and transport terms for the PCs in terms of the PCs as adopted in recent work by the authors using artificial neural networks (ANN) [10,12,13]. In this paper, we compare the two reconstruction methods using one-dimensional turbulence (ODT) simulation data of the Sandia Flame F.

2. Thermo-chemical scalars' reconstruction

PCA relates a vector $\boldsymbol{\phi}$ of N TCSs (e.g. temperature, pressure and species composition), and a vector $\boldsymbol{\Psi}$ of N corresponding principal components through a linear relation:

$$\boldsymbol{\psi} = \mathbf{Q}^T \boldsymbol{\phi} \text{ or } \boldsymbol{\phi} = \mathbf{Q}\,\boldsymbol{\Psi} \tag{1}$$

where $\mathbf{Q}$ is the $N \times N$ matrix of orthonormal eigenvectors of the correlation matrix for the TCSs. The superscript "T" refers to the transpose of the matrix. The eigenvectors are ordered such that the largest contributions come from the corresponding leading eigenvalues. Therefore, it is desired to select a subset of the PCs such that:

$$\boldsymbol{\Psi}_{\text{red}} = \mathbf{A}^T\ \boldsymbol{\phi}. \tag{2}$$

where $\mathbf{A}^{\mathrm{T}}$ is an $M \times N$ matrix, which corresponds to the first M eigenvectors of $\mathbf{Q}$. The subscript "red" in Eq. (2) refers to the reduced subset of M eigenvalues where $M \leq N$. With this set, a reconstruction of the TCSs may be implemented through different approaches. One approach adopted in previous studies (see for example Refs. [3–9]) is based on the inversion of Eq. (2):

$$\boldsymbol{\phi} \approx \mathbf{A}\boldsymbol{\Psi}_{\text{red}} \tag{3}$$

where $\mathbf{A}$ also represents the left-inverse of $\mathbf{A}^{\mathbf{T}}$. The "inversion relation" uses only information retained in the leading M eigenvectors.

Recently [10,12,13], we have used regression based on ANN instead of inversion (Eq. (3)). The regression exploits the concurrent information available between PCs and TCSs. In this paper, we argue that regression (based on ANN or other methods) should yield better reconstruction than the inversion relation. Although regression has been used within the context of PCA (see for example Refs. [3,5,6,11]), this study represents the first direct comparison between inversion and regression.

To illustrate our argument, we use ANN for regression. Figure 1 shows a schematic of the ANN layout: (1) an input layer with M PCs neurons as well as a bias neuron (black circles), (2) $n-1$ hidden layers containing a number of neurons, and (3) an output layer, which contains the N TCSs neurons. The strength of the connection between the neurons of adjacent layers is quantified with weights.

ANN relates the input and the output through the weight connections linking all layers:

* Corresponding author.

http://dx.doi.org/10.1016/j.combustflame.2014.11.027
0010-2180/

$$\boldsymbol{\phi} = f_n(\mathbf{W}_n f_{n-1}(\mathbf{W}_{n-1} f_{n-2}(\mathbf{W}_{n-2}(\ldots f_1(\mathbf{W}_1 \boldsymbol{\Psi}_{\text{red}} + \mathbf{b}_1)\ldots) + \mathbf{b}_{n-2}) + \mathbf{b}_{n-1}) + \mathbf{b}_n) \tag{4}$$

where f_i is the transfer function of the neurons in the ith layer (starting from the first hidden layer). $\mathbf{W}_i$ and $\mathbf{b}_i$ are the $p_i \times p_{i-1}$ weight connection matrices relating neurons at the $(i-1)$th layer and the ith layer, and the p_i bias connection vector of the ith layer, respectively. Both $\mathbf{W}_i$ and $\mathbf{b}_i$have constant coefficients.

If the transfer functions are linear, Eq. (4) can be simplified to a form, which can be directly compared to Eq. (3):

$$\boldsymbol{\phi} \approx \mathbf{W}\,\boldsymbol{\Psi}_{\text{red}} + \boldsymbol{\phi}_0 \tag{5}$$

In this expression, $\mathbf{W}$ is the $M \times N$ product of the weight connection matrices:

$$\mathbf{W} = \mathbf{W}_{n+1}\ldots\mathbf{W}_1 \tag{6}$$

Matrix $\mathbf{W}$ is similar to matrix $\mathbf{A}$ in Eq. (3). The additional vector $\boldsymbol{\phi}_0$ is an $M \times 1$ vector expressed as:

$$\boldsymbol{\phi}_0 = (\mathbf{W}_{n+1}\ldots\mathbf{W}_2\mathbf{b}_1 + \mathbf{W}_{n+1}\ldots\mathbf{W}_3\mathbf{b}_2 + \ldots + \mathbf{b}_{n+1}) \tag{7}$$

and helps to fine-tune the ANN regression. An optimum regression with ANN using all N eigenvectors results in $\mathbf{W}$ being equal to $\mathbf{Q}$ and zero $\boldsymbol{\phi}_0$. However, by retaining the first M leading eigenvalues, we expect ANN to provide an optimum reconstruction of the TCSs by adjusting the weights of $\mathbf{W}$ relative to $\mathbf{A}$ or the coefficients of $\boldsymbol{\phi}_0$.

Finally, based on the above discussion, it is important to emphasize the following two points:

- The Levenberg–Marquardt back-propagation algorithm used in the ANN regression attempts to minimize the mean squared error (MSE) difference between the predictions based on the current weights and the desired output. In contrast, the inversion relation incurs a truncation error associated with the missing PCs. There are different measures of errors that need to be tracked for optimum reconstruction of the TCSs. However, the same ANN procedure divides the data into training, testing and validation subsets, which enables these different measures to be evaluated.
- Our choice of linear transfer functions with ANN is implemented only to enable a direct comparison with the inversion relation of Eq. (3). Based on our previous work with PCA-ANN [10,12,13], we have found that the use of non-linear transfer functions enables better ANN regression and improvements in minimizing the MSE.
- The use of a regression approach enables some additional advantages over the inversion relation to reproduce TCSs from a truncated set of PCs. First, if there is sufficient variance in the data reproduced by the first PCs, this will enable adequate regression between TCSs and the truncated set of PCs. In the inversion relation, the error resulting from the truncation of the original matrix $\mathbf{Q}$ cannot be recovered. Second, the regression relations can be developed for each TCS separately enabling further optimization of the regression relations. Finally, regression can be established even if the TCSs are not part of the reduced set used for PCA analysis. With the inversion relation, only TCSs that are represented in the PCA analysis can be reconstructed from a set of PCs.

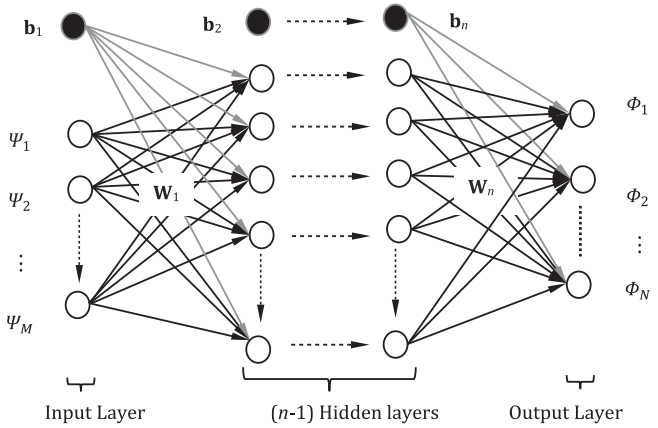

Fig. 1. Schematic of the artificial neural network.

3. Results

In this section, we present a quantitative comparison of the "inversion relation" and the ANN "regression" based on linear transfer functions using data from stand-alone ODT simulations of Sandia's Flame F [16], which exhibits important non-equilibrium effects, including extinction and reignition [16].

The simulation, described in Ref. [10], is based on a chemical scheme involving 17 TCSs of which only 7 are retained for PCA analysis (i.e. $N = 7$); they include: temperature and H_2, O_2, H_2O, CH_4, CO, and CO_2 mass fractions. The original set also included the H, HO_2, H_2O_2, CH_2O, C_2H_2, C_2H_4, C_2H_6 and N_2 mass fractions. The 7 retained TSCs are normalized using their minimum and maximum values prior to the PCA analysis. The selection of the retained TCSs is based on maintaining only temperature and the major species; such a selection was found to be a good choice for the different datasets we have used in the past [10,12,13]. Other more systematic approaches for selecting the retained TCSs may be adopted, including the methods proposed in Refs. [9,11].

Although not shown here, the choice of $M = N = 7$ yields $\mathbf{Q} = \mathbf{W}$ and zero $\boldsymbol{\phi}_0$. With $M = 3$:

$$\mathbf{A} = \begin{bmatrix} 0.4273 & 0.2235 & 0.1683 \\ 0.3484 & -0.3952 & -0.4951 \\ -0.4373 & -0.0843 & -0.1775 \\ 0.4357 & 0.1721 & 0.1033 \\ 0.0863 & -0.7515 & 0.6459 \\ 0.3680 & -0.3339 & -0.4653 \\ 0.4148 & 0.2845 & 0.2252 \end{bmatrix}, \mathbf{W} = \begin{bmatrix} 0.4363 & 0.2509 & 0.1913 \\ 0.2858 & -0.3119 & -0.3919 \\ -0.5010 & -0.0194 & -0.1309 \\ 0.4690 & 0.1091 & 0.0157 \\ 0.0797 & -0.7454 & 0.6495 \\ 0.4128 & -0.3975 & -0.5475 \\ 0.3175 & 0.3761 & 0.3284 \end{bmatrix},$$

$$\boldsymbol{\phi}_0 = \begin{bmatrix} -0.0115 \\ -0.1980 \\ -0.2945 \\ 0.1081 \\ -0.0318 \\ 0.1270 \\ 0.3519 \end{bmatrix}$$

Now, the coefficients of $\mathbf{W}$ are different from those of $\mathbf{A}$; however, there is similarity between their magnitudes and signs. Moreover, the bias connections are no longer negligible. Although not shown here, a lower M results in further deviations of $\mathbf{W}$ from $\mathbf{A}$ and higher contributions from $\boldsymbol{\phi}_0$.

Table 1 summarizes the root mean squared (RMS) errors for reconstruction of the TCSs for different numbers of PCs based on regression and inversion. The RMS error is based on 50 ODT realizations at 4 different downstream distances corresponding to (1) pilot-stabilized ($x/d = 3$ and 7.5, where d is the fuel jet diameter and x is the downstream distance from the jet inlet), (2) extinction ($x/d = 15$), and (3) self-stabilized non-premixed flame modes ($x/d = 30$). For all species in the selected subset and temperature, at least one extra PC is required for the inversion relation to get a similar accuracy based on regression. The advantages of regression are more pronounced for O_2, H_2O and CO_2.

Table 1
The RMS error for the TCSs regression based on ANN (first entry) and inversion (second entry) or different numbers of PCs.

Φ	Number of PCs					
	1	2	3	4	5	6
T (K)	50.386/122.360	29.943/80.085	8.590/24.2	8.115/23.370	6.260/34.176	0.087/6.863
$H_2 \times 10^4$	2.118/6.338	1.766/4.655	0.392/0.936	0.051/0.205	0.003/0.012	0.0003/0.026
$O_2 \times 10^3$	2.628/16.509	2.581/10.302	0.614/13.561	0.411/13.350	0.346/14.031	0.155/12.254
$H_2O \times 10^3$	1.685/7.424	0.748/2.057	0.725/1.395	0.685/1.503	0.264/1.864	0.041/3.209
$CH_4 \times 10^2$	1.850/6.164	0.821/1.980	0.0029/0.1053	0.0028/0.1073	0.0025/0.1107	0.0012/0.9808
$CO \times 10^3$	4.069/7.460	3.503/7.010	0.618/0.909	0.025/0.660	0.023/0.615	0.006/0.488
$CO_2 \times 10^3$	5.650/7.314	3.689/11.193	0.857/6.770	0.852/6.768	0.057/3.412	0.046/3.611

4. Concluding remarks

We have compared the reconstruction of TCSs based on the inversion and a regression scheme that relates the TCSs and PCs. We have adopted here ANN regression; although, other regression methods can be equally predictive.

Although linear regression is used, we have found that it still yields a better reconstruction of the TCSs based on a reduced set of PCs. This regression provides additional adjustable parameters (the coefficients of matrix $\mathbf{W}$ and ϕ_0) that can provide an improved correlation between PCs and TCSs. Nonlinear regression as implemented in [10,12,13] potentially yields better reconstruction of the TSCs based on a limited set of PCs.

The ability of the PCA-ANN approach to achieve an effective reconstruction of the original TCSs is constrained by whether the training data adequately span the targeted composition space and the number of retained PCs needed to maintain the error of reconstruction at a minimum.

Acknowledgments

The work was supported by the National Science Foundation Computational Mathematics Program under grant DMS-1217200.

References

[1] C.E. Frouzakis, Y.G. Kevrekidis, J. Lee, K. Boulouchos, A.A. Alonso, Proc. Combust. Inst. 28 (2000) 75–81.
[2] S.J. Danby, T. Echekki, Combust. Flame 144 (2006) 126–138.
[3] J.C. Sutherland, A. Parente, Proc. Combust. Inst. 32 (2009) 1563–1570.
[4] A. Parente, J.C. Sutherland, L. Tognotti, P.J. Smith, Proc. Combust. Inst. 32 (2009) 1579–1586.
[5] A. Parente, J.C. Sutherland, B.B. Dally, L. Tognotti, P.J. Smith, Proc. Combust. Inst. 33 (2011) 3333–3341.
[6] A. Bilgari, J.C. Sutherland, Combust. Flame 159 (2012) 1960–1970.
[7] A. Coussement, O. Gicquel, A. Parente, Combust. Flame 159 (2012) 2844–2855.
[8] A. Parente, J.C. Sutherland, Combust. Flame 160 (2013) 340–350.
[9] A. Coussement, O. Gicquel, A. Parente, Proc. Combust. Inst. 34 (2013) 117–1123.
[10] H. Mirgolbabaei, T. Echekki, Combust. Flame 160 (2013) 898–908.
[11] Y. Yang, S.B. Pope, J.H. Chen, Combust. Flame 160 (2014) 1967–1980.
[12] H. Mirgolbabaei, T. Echekki, Int. J. Hydrogen Energy 39 (2014) 4622–4633.
[13] H. Mirgolbabaei, T. Echekki, Combust. Flame 161 (2014) 118–126.
[14] E. Chiavazzo, C.W. Gear, C.J. Dsilva, N. Rabin, I.G. Kevrekidis, Processes 2 (2014) 112–140.
[15] U. Maas, D.A. Goussis, Model reduction for combustion chemistry, in: T. Echekki, E. Mastorakos (Eds.), Turbulent Combustion Modeling, Springer, NY, 2010, pp. 193–220.
[16] R.S. Barlow, J.H. Frank, Proc. Combust. Inst. 27 (1998) 1087–1095.