Deep Learning Dynamical Latencies for the Parameterization of Complex Chemical Kinetics

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Objective

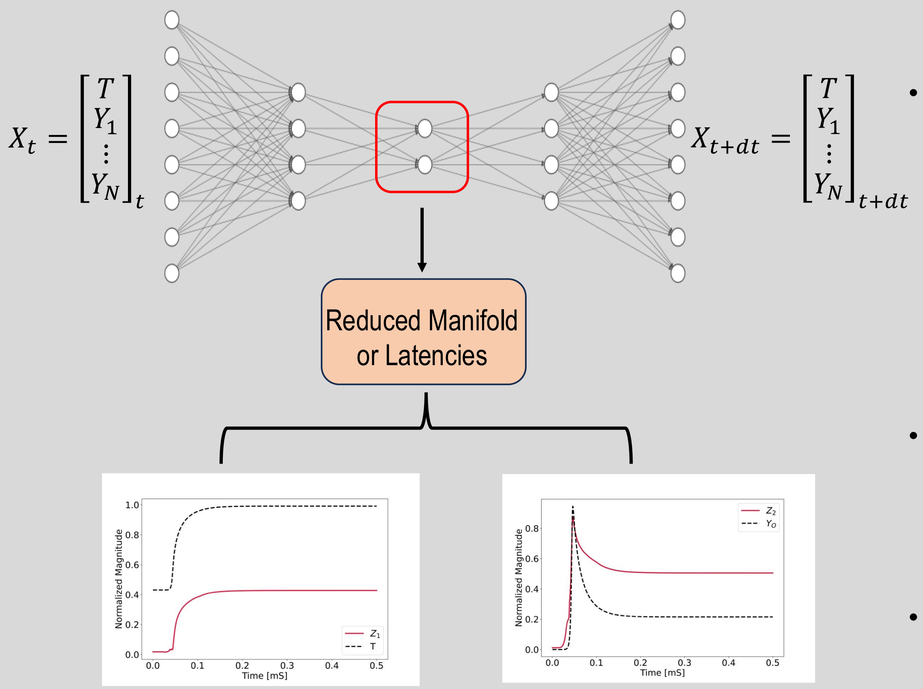
Evaluate the application of **Time-lag Autoencoders (TAE)** for the **analysis** and **reduction** of **complex mechanisms**.

Introduction

- Modelling combustion chemical kinetics is computationally costly, especially as more chemical species are considered. Combustion Machine Learning [1] helps by using techniques to predict thermochemical states more efficiently or reduce the number of variables.
- One such method, **TAE** (a time-shifted modification of an Autoencoder), **simplifies the thermochemical states** into a set of **latent variables**, which are **correlated** to specific chemical species called **chemical carriers** [2].
- The goal is to better understand the TAE methodology and apply it to complex scenarios.

Methodology

- Neural networks are challenging to train with multidimensional inputs and diverse data. To tackle this, a subspace is sampled with different **mixture compositions**, so **different reactive pathways** are represented**.**
- Separate networks are trained for different ignition cases with varying mixture compositions.
- **Chemical carriers** are then identified and **analyzed** using a **permutation importance test** [3] to evaluate how well they describe other chemical species.



TAE schematic with reduction results the hydrogen mechanism of the University of San Diego, reduction to manifold size 2 [2].

- The permutation importance test uses a **hypothesis** relating inputs and outputs, and the **error is measured**.
- Afterward, the **input variables** are **scrambled individually**, and the error is measured again. If the **error increases**, the **scrambled variable** is of **importance** for the output. A permutation importance index is allocated in agreement to the error's behavior:

$$i_j = s - \frac{1}{Q}\sum_{n=1}^{Q} s_{q,j}$$

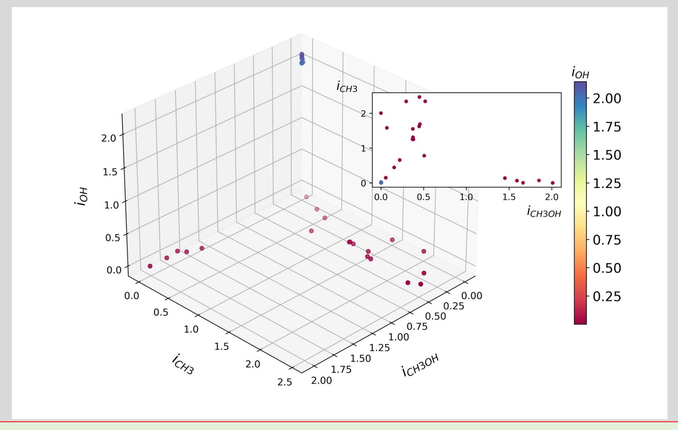
- Where i_j is the coefficient of importance of the $j\text{-}th$ variable, s is the model's R^2 score without scrambling, and $s_{q,j}$ is the R^2 score when a single variable is scrambled. Q refers to the number of times the input variable is scrambled.
- **Methane combustion** is studied; ignition cases have initial temperature $T_0 = 1418\text{K}, \text{P} = 4.33\ \text{atm}$, and $\phi \in [0.45, 1.25]$ with $\Delta\phi = 0.2$.
- **Two mechanisms** (GRI-Mech 2.11 [4] and Aramco 2.0 [5]) are considered to **analyze** the method's behavior with **different complexities**. The manifold size reduction is to 3 latent variables.

$$\Delta t = 2.5ns$$

Results

GRI-Mech 2.11

ϕ	Chemical Carriers
0.45	$\dot{\omega}_{02}$, O2, $\dot{\omega}_{02}$
0.65	HO2, CO, OH
0.85	H, CH2OH,CH4
1.05	H, CH2OH, H
1.25	OH, CH3OH, CH3



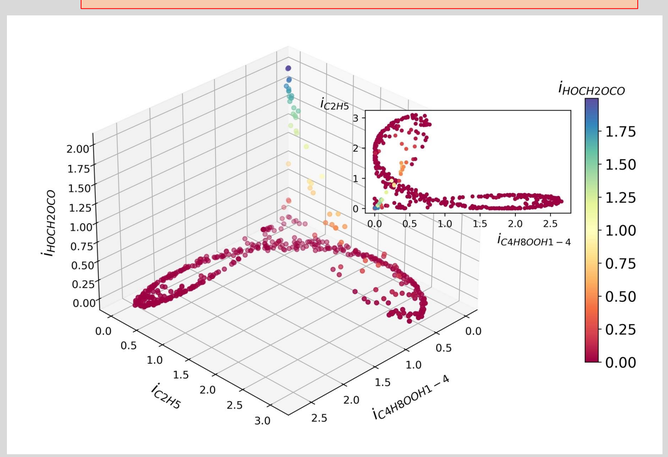
Permutation importance indexes for ignition case $\phi = 1.25$, observe how most of the thermochemical variable show sensitivity to at least one of the chemical carriers. Top view in x,y plot.

31 species, 277 reactions

- CH2OH interacts with H, O, OH, O2, H2, HO2, etc
- CH3O interacts with O, H, OH, etc.
- H, OH, and HO2 react with CH4, promoting oxidation.
- The chemical carriers track throught the reactions the most species as possible.

Aramco 2.0

ϕ	Chemical Carriers
0.45	C2H, IC4H8O2H-I, C2H4O2H
0.65	CH3OH, C2H4, CH3O2H
0.85	C2H5, $\dot{\omega}_{HO2CHO}$, SC4H9
1.05	O2CCHOOJ, $\dot{\omega}_{02}$, C4H7O1-4
1.25	C4H8OOH1-4, C2H5, HOCH2OCO



Permutation importance indexes for ignition case $\phi = 1.25$, observe how most of the thermochemical variable show sensitivity to at least one of the chemical carriers. Top view in x,y plot.

491 species, 2716 reactions

- C2H5 is related to many key species (HO2, OH, H2, H2O, CH4, CH3, CH2, etc.).
- HOCH2OC is related to the CO2 and CO production.
- C4H8OOH1-4 specie allows the description of other C4 species and to key species through the PC4H9O2 specie.
- Note that C4 species appear only in rich fuel conditions.

Conclusions

- **TAE** provides information that help identify thermochemical variables (**chemical carriers**) that **track most** of the **species' concentrations** through their **chemical reactions**.
- Since the **chemical carriers** are strongly **based** in the **chemical reactions present** in the mechanism, it is possible to use the **same** set of **variables** to **parametrize another subspace** with similar chemistry.
- TAE tends to chose **chemical species** that **characterizes** the **chemical pathways visible** for the network, **without relying** on the **chemical species concentration**, but only in how this specie interacts with others.

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