Machine Learning Framework for Chemistry Tabulation and Lookup

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Abstract

Modeling of combustion system requires modeling the underlying chemistry and the flow. Solving both systems simultaneously is computationally prohibitive. In most cases the two sub-systems have different scales and can be (re)solved separately.

Chemistry model describes the governing reaction kinetics of a large number of reacting species and the resulting source terms and other dependent variables. This higher dimensional thermochemical state is often parametrized using combination a reduced number of reaction variables. These reduced number of variables are then used in the transport equations when solving the flow system.

Two main challenges with this approach are the creation of the reduced basis that is spanned by reduced number of variables and learning and representation of a unique mapping function of the thermochemical state in this reduced basis.

A lot of research has focused on the problem of selection of a reduced basis and techniques like Flamelet Generated Manifold focusing on selection of basis that are interpretable have been favored over pure numerical techniques like Principal Component Analysis (PCA). However this choice often sacrifices a lot of accuracy when describing the thermochemical state in this reduced basis: standard interpolation and extrapolation techniques on the fine grain tabulation make several simplifying assumptions which may violate the actual governing reaction kinetics.

The parameterization of the thermochemical state using purely numerical techniques like PCA in conjunction with Gaussian Process Regression have show promise but this framework has several limitations: lack of interpretability, inheritance of noise as signal due to PCA's need to maximize variance capture and most importantly we cannot jointly optimize the reduction basis creation and function learning to overcome the aforementioned limitations.

In this paper we present two Machine Learning based Frameworks, compare the performance of these ML Frameworks to the existing non-ML Framework. The first ML Framework we construct using the state of the art components for the reduced basis construction and regression function learning. The second ML Framework we present a unified deep neural network model inspired by the Physics Guided Neural Network framework that learns a reduced basis using the Physics Constraints and a regression model that learns the unique mapping function of the thermochemical state in this reduced basis.

The proposed deep neural network which we call Physics Constrained Deep Neural Network (PCDNN) shows quantitatively accurate predictions for source energy terms and is comparable in performance to the PCA and GP Framework.

This is a significant first step in creation of a broader framework that helps jointly optimize reduced basis learning and unique mapping function learning.

Keywords. Deep learning, Combustion modeling, 1D Flamelet, Tabulated chemistry, Physics Constrained Neural Network

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1 Introduction

Detailed kinetic mechanisms for combustion can comprise thousands of chemical reactions amongst hundreds of molecular species. Despite significant advances in the power and availability of computational resources, numerical simulations of realistic combustion problems remain prohibitively expensive due to the large number of species and the disparate range of important chemical and flow scales present.

To overcome this challenge, several methods have been developed which project the high-dimensional thermochemical state-space onto a low-dimensional manifold.

In this approach, the entire state-space is pre-computed and parameterized in terms of a reduced set of scalar variables that are conveniently computed in a combustion simulation, thus providing efficient access to detailed thermochemistry at a greatly reduced computational expense. These thermochemical manifolds are typically parameterized using a combination of conserved and reactive scalars[3].

Generally speaking, the chemical composition of the fully-reacted mixture is determined from conserved quantities such as mixture fraction Z or equivalence ratio, while the progress of combustion between unburned and burned states is described by reactive scalars, which are also referred to as reaction progress variables.

The chemistry system and the corresponding thermochemical state space described by the species is often parameterized by preset dimensions into a reduced order manifold. Reverse lookups from the The dimensionality of the reduced order manifold is directly proportional to the computational efficiency of the flow simulation.

Chemistry systems that are based on Flamelet paradigm are parameterized using a combination of mixture fraction that has a physical interpretation and a reaction progress variable. Experts agree that this two dimensional parameterization produce reduced order/lower dimensional manifolds that are highly non-linear, discontinuous, irregular and convoluted and do not guarantee bijection. Many simplifying assumptions about properties of the reduced order/lower dimensional manifolds are made to assist in efficient tabulations of the manifold.

Run time lookups on these tabulations are done using lagrange polynomial interpolation and many non-linear machine learning methods have been tried instead of tabulation lookup.

Purely numerical techniques like Principal Component Analysis for Reduced Basis Learning and non-linear regression techniques like Gaussian Process Regression for Reverse Lookup Learning have been applied with some success. However,the prameterization lack interpretability and may also not be generalizable enough due to variation capture maximization that may overlearn the numerical errors. And fundamentally these sub-problems are solved independently there's a lack of ability to jointly optimize the two together [2, 5–7].

Deep Neural Networks for the problem of Reverse Lookup Learning has been suggested, however it wasn't very accurate [1].

In the following sections we describe the current framework based on the Flamelet Generated Manifold Technique then compare this with the purely numerical/machine learning approach suggested and then finally present a Physics Constrained Deep Neural Network based on the principles outlined in the work of [4].

2 Existing Framework

The current framework solves the two sub-problems of Reduced Basis Learning and Reverse Lookup learning separately.

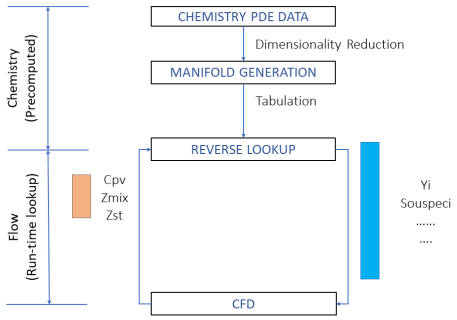

Figure 1. Combustion system simulation workflow.

Reduced Basis learning problem is solved by using Flamelet Generated Manifold technique. The manifold is then tabulated into a library on which a lookup is performed at runtime during the flow simulation.

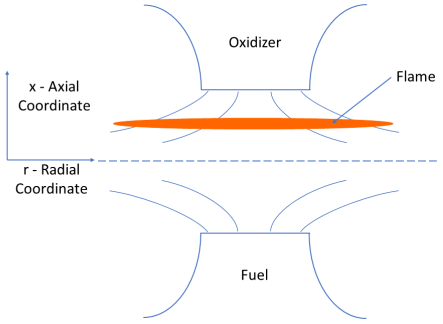

Figure 2. Axial Coordinate.

Instead of solving transport equations for all of the numerous species in a typical chemical mechanism and modeling the unclosed chemical source terms, the present study adopts an indirect mapping approach, whereby all of the detailed chemical processes are mapped to a reduced system of tracking scalars. Presently, only two such scalars are considered: a mixture fraction variable (Zmix), which tracks the mixing of fuel and oxidizer, and a progress variable (Cpv), which tracks the global extent-of-reaction of the local mixture.

The mapping functions, which describe all of the detailed chemical processes with respect to the tracking variables, are

determined by solving quasi-steady diffusion-reaction equations with complex chemical kinetics and multicomponent mass diffusion.

The performance of the new model is compared to fast chemistry and steady flamelet models for predicting velocity, species concentration, and temperature fields in a methane-fueled coaxial jet combustor for which experimental data are available.

The progress-variable approach is able to capture the unsteady, lifted flame dynamics observed in the experiment, and to obtain good agreement with the experimental data and significantly outperform the fast chemistry and steady flamelet models, which both predict an attached flame.

The flamelet based chemistry resolution the system is described by Eq. (1). These set of equations capture the physical phenomenon.

Conservation equations for mass, species, momentum and energy for the one-dimensional, fully compressible and viscous flame is given by:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_x)}{\partial x} = 0 \tag{1a}$$

$$\frac{\partial (\rho Y_i)}{\partial t} + \frac{\partial \rho u_x Y_i}{\partial x} = \frac{\partial}{\partial x}\left(\rho \mathcal{D}_i \frac{\partial Y_i}{\partial x}\right) + \dot{w}_i \tag{1b}$$

$$\frac{\partial (\rho u_x)}{\partial t} + \frac{\partial \left(\rho u_x^2\right)}{\partial x} = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x}\left(\mu \frac{\partial u_x}{\partial x}\right) \tag{1c}$$

$$\begin{aligned}&\frac{\partial (\rho e_t)}{\partial t} + \frac{\partial}{\partial x}\left(\rho u_x H_t\right) \\ &= \frac{\partial}{\partial x}\left(u_x \mu \frac{\partial u_x}{\partial x}\right) + \mu \frac{c_p}{Pr}\left(1 - \frac{1}{Le}\right)\frac{dT}{dx} + \frac{1}{Sc}\frac{dh}{dx} - \sum \dot{w}_i h^o_{f,i}\end{aligned} \tag{1d}$$

where, $\dot{w}_i$ is the mass consumption or production rate of the i^{th} species, e_t $(= e + u_x^2/2)$ is the total sensible energy, H_t $(= e_t + p/\rho)$ is the total enthalpy, and $h^o_{f,i}$ is the heat of formation of the i^{th} species. Diffusivity is assumed to be constant, Pr is the Prandtl number, Sc is the Schmidt number, Le is the Lewis number, and h is the sensible enthalpy. Prandtl (Pr) and Schmidt (Sc) numbers are both set equal to 0.707, resulting in a unity Lewis number assumption. Viscosities μ are determined from the Sutherland viscosity model, while thermal and molecular diffusivities are calculated using the definitions of Pr and Sc, respectively. Now, in 1D cartesian coordinates, the steady state solution to 1 is obtained only when the total mass flux is zero, i.e., velocity field is zero $(u_x = 0)$ and 1 reduces to,

$$\frac{\partial}{\partial x}\left(\rho \mathcal{D} \frac{\partial Y_i}{\partial x}\right) + \dot{w}_i = 0 \tag{2a}$$

$$\frac{\partial}{\partial x}\left(\mu \frac{c_p}{Pr}\left(1 - \frac{1}{Le}\right)\frac{\partial T}{\partial x} + \frac{1}{Sc}\frac{\partial h}{\partial x}\right) - \sum \dot{w}_i h^o_{f,i} = 0 \tag{2b}$$

where, pressure work and viscous dissipation are neglected. The resulting system of non-linear equations are solved on discrete domain lengths (L) using a time marching technique until steady-state is reached. Dirichlet boundary conditions are used for the fuel and air side.

In 2b, the final term in the energy equation is represented by the total sum of the product of all the source species and their respective heat of formation and is collectively called the source energy.

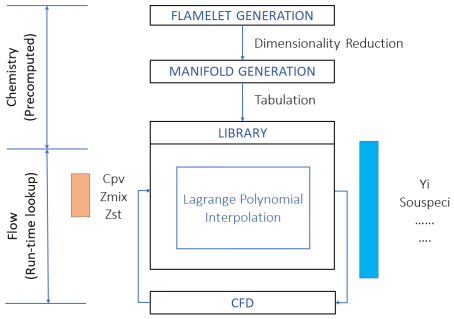

Figure 3. Current Framework.

The accuracy of the combustion simulation is governed by the accurate description of the chemistry and the flow. This essentially translates into the resolution, tabulation and lookup accuracy of the chemistry system and the resolution of the flow system.

The grid resolution of the turbulent flow system is usually decided based on the Reynolds number of the flow. However, there is no such guiding measure in the chemistry system that governs the required resolution on the tabulation i.e. the lower dimensional manifold tabulation.

Due to the curse of dimensionality of the tabulation and the run time inefficiency of large tabulations, practitioners often resolve the Chemistry in manner that the the run time lookup performed on the the tabulated chemistry by the Flow system solver is highly responsive. This practice has an implicit risk of missing out tabulation of highly discontinuous phenomenon. In most cases lookups on non nodal values is approximated using some numerical interpolation. Many subject matter experts agree that this interpolation done on tabulation to arrive at higher dimensional data is completely ignorant of the underlying Physics and the values approximated may completely violate the underlying governing equations.

This is what we noticed when dealing with the current FGM based Manifold creation and Tabulation. The original manifold generated when fitted with all the flame data was highly convoluted and secondly for storage efficiency the generated tabulation of the Manifold was coarse.

3 Machine Learning Framework I

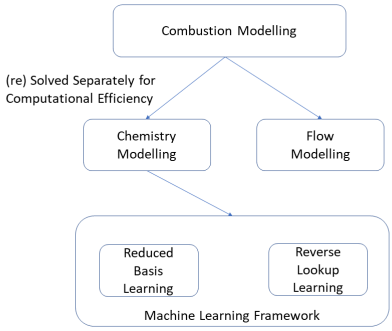

Figure 4. ML Problems in focus

In the Machine Learning Framework I we modified the approach used by [5]. For the reduced basis learning instead of using only two such scalars: a mixture fraction variable (Zmix), which tracks the mixing of fuel and oxidizer, and a orthogonal progress variable (Cpv), which tracks the global extent-of-reaction of the local mixture, we used multiple orthogonal progress variables. The optimal number of the progress variables was found using PCA analysis.

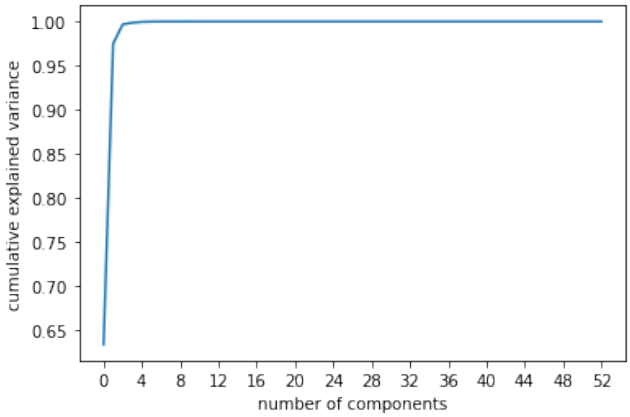

Figure 5. PCDNN Framework.

We computed the progress variables orthogonal to Zmix using an Constrained PCA formulation. We solve for a unit vector, $\mathbf{v}$, which maximizes the variance of the given data set, and is orthogonal to Zmix.

$$\underbrace{\arg\max}_{\mathbf{v}} \quad \mathbf{v}^\top \mathbf{A}\mathbf{v} \tag{3}$$

$$\text{subject to:} \quad \mathbf{v}^\top \mathbf{w} = 0 \tag{4}$$

$$\mathbf{v}^\top \mathbf{v} = 1 \tag{5}$$

The solution to this constrained optimization problem is given by the first eigenvector for the following equation:

$$A - \mathbf{w}\mathbf{w}^\top A$$

Using this Constrained PCA reduced basis we then moved on to solving for Reduced Lookup Learning.

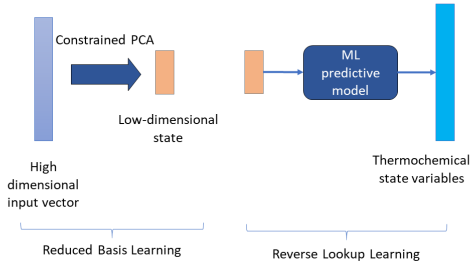

Figure 6. ML Framework I.

The Reduced Lookup Learning problem is posed to solve for the following Objective function.

$$min \quad MAE = (\frac{1}{n}) \sum_{i=1}^{n} |y_i - \phi(x_i)|$$

where,

y_i is the actual target value

$\phi(x_i)$ is the predicted value

n is the number of training samples

We trained several non-linear ML models ($\phi(x)$) and found out that the top 2 performant models were Gaussian Process Regression and Deep Neural Networks.

We tried several different Kernels for Gaussian Process Regression and found that the top 3 kernels were: Matern, Rational Quadratic and Custom Kernel with 50% Matern and 50% Rational Quadratic. Through several experiments we chose the Matern Kernel.

Similarly we experimented with several Network Architectures and found out that for the current data set the following fully connected 7 layered architecture with Relu Activation function worked the best:

Architecture

Layer	Nodes
Normalized Input	Reduced Basis Size
Fully Connected	512
Fully Connected	512
Fully Connected	128
Fully Connected	128
Fully Connected	512
Fully Connected	512
Fully Connected	Number of Output Parameters

We also conducted several ablation studies and found out that plain vanilla architecture without any regularization gave the best results.

4 ML Framework II: Physics Constrained Deep Neural Network (PCDNN)

In the Machine Learning Framework II we jointly solved for reduced basis learning and reverse lookup learning. We use a Deep Neural Network inspired by the work of [4].

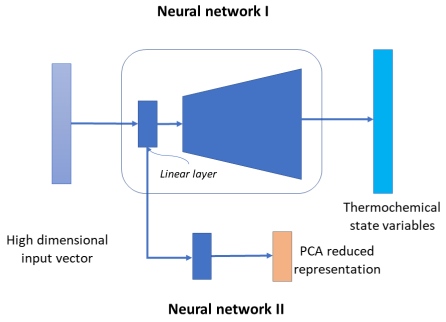

Figure 7. PCDNN Framework.

We set up the DNN Architecture to consists of two Networks each representing a subproblem.:

4.1 Model Formulation

$$\begin{aligned} & min \quad \text{Prediction Loss} \\ s.t. \quad & \text{Physics Inconsistency} \quad \leq 0 \end{aligned} \tag{6}$$

We set up our prediction problem as a minimization problem. Minimize the Prediction Loss such that there is no Physics Inconsistency. In this case the Prediction Loss is essentially the same as ML Framework I where we predict the Thermochemical State Variables using the reduced basis. The Physics Inconsistency in this case is the prediction error as compared to the mixture fraction variable (Zmix), and the multiple orthogonal progress variables that we derived using a constrained raleigh PCA formulation.

4.1.1 Neural Network Formulation.

$$MAE = \lambda_{reg} * MAE_{reg} + \lambda_{phy} * MAE_{phy} \tag{7}$$

4.2 Architecture

Prediction Network

Layer	Nodes
Fully Connected	Normalized Input
Fully Connected	Reduced Basis Size
Fully Connected	32
Fully Connected	64
Fully Connected	128
Fully Connected	512
Fully Connected	128
Fully Connected	64
Fully Connected	32
Fully Connected	Number of Output Parameters

Physics Inconsistency Network

Layer	Nodes
Fully Connected	Normalized Input
Fully Connected	Reduced Basis Size (Linear Activation)

For the joint formulation to be effective we had to not only scale the Input data but also the Target Variable. We used a MinMax scaler for all the scaling and found out that the optimal weight ratio of λ_{phy} to λ_{reg} was 10:1.

We also conducted several ablation studies and found out that plain vanilla architecture without any regularization gave the best results.

5 Training Data

We trained several ML Frameworks on data generated by solving 1-D Steady State Flamelets using the GRI-Mech 3.0 which has 53 species and 325 reactions.

The Flamelet solver generated the dataset using a finite volume based PDE solver. The solver discretizes the domain into 200 grid points (200 observations on the axial coordinate) in between the fuel and the air boundary and 1000 flame are solved to steady-state. Once the solution reaches steady-state the solver completes one iteration. For the next iteration flame solution is strained by reducing the domain by 0.99 and the process is continued until the flame extinguishes. Each flame is then tagged with the corresponding strain rate that is called a flame-key. To model the chemical kinetics reaction rates, a variety of mechanisms are adopted in the combustion community. Depending on the hydrocarbon fuel different mechanisms are chosen which closely describe the chemistry associated with the fuel of simulation. Methane is the basic hydrocarbon and one of the major products of many higher order hydrocarbons. GRI-Mech 3.0 is one of the widely used Methane mechanism to model the reaction kinetics. This mechanism consists of 53 chemical species and 325 reactions. However, in this work, Methane - CSM2 reduced mechanism is used which consists of 7 species and 4 reactions to further simplify the problem. To train the model 200,000 data points (1000 flames and 200 grid points) for a single pressure setting are used. The data is generated using

an in-house solver which creates the flame solutions and stores the required data.

6 Results

We conducted several experiments to learn the sufficiency of the number of basis vectors needed. We conducted a PCA analysis to learn the number of components needed to capture the maximum variance.

Our first experiment focused on trying to learn a Reverse Function using the basis vectors (Zmix, Cpv) generated using the current framework that leverages regularized Flamelet Generated Manifold Technique.

Training using Untrimmed Flames & Testing using Trimmed Flames 2 Parameters (Zmix, Cpv)

Method	Total Abs Error	MAE
Non-ML Framework	3.68E+13	5.02E+09
ML Framework I (GP)	7.70E+13	5.99E+09
ML Framework I (DNN)	1.10E+14	8.53E+09

For this experiment the training data was the data from (untrimmed) flames; the flames that are used by the current framework for the manifold generation. The test data was the flames that were trimmed by the current framework. The Gaussian Process and DNN were trained and tested on these data sets.

The current framework performed the best, however there were two things that we uncovered.

The analysis of the prediction residuals on the ML models shows a high degree of correlation.

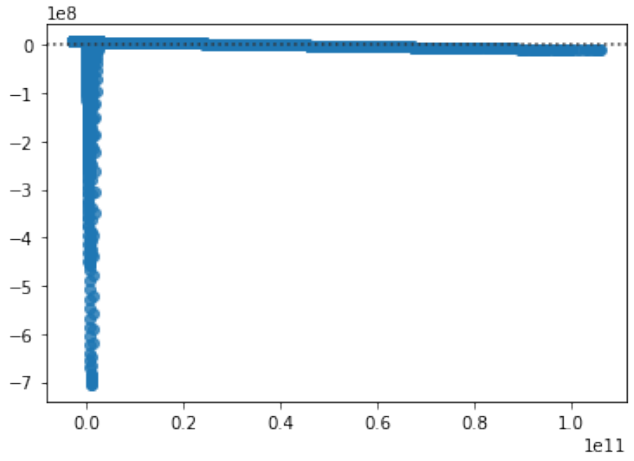

Figure 8. Gaussian Process correlated errors (Zmix, Cpv).

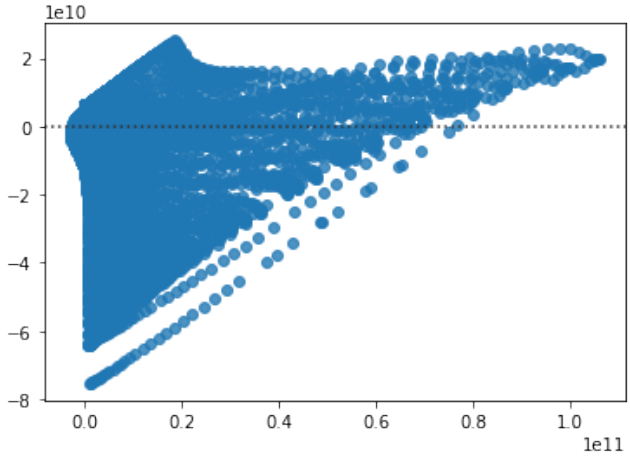

Figure 9. DNN correlated errors (Zmix, Cpv).

This confirms that the data is trimmed by the current framework to guarantee bijection is the cause for error correlation. And secondly the number of basis vectors may alleviate this issue. This was the second experiment we conducted.

Training using Untrimmed Flames & Testing using Trimmed Flames 5 Parameters (Zmix, 4 Orthogonal PCAs)

Method	Total Abs Error	MAE
ML Framework I (GP)	3.41E+13	2.65E+09
ML Framework I (DNN)	3.47E+13	2.70E+09

Including more basis vectors reduced the error however the prediction residuals were still correlated.

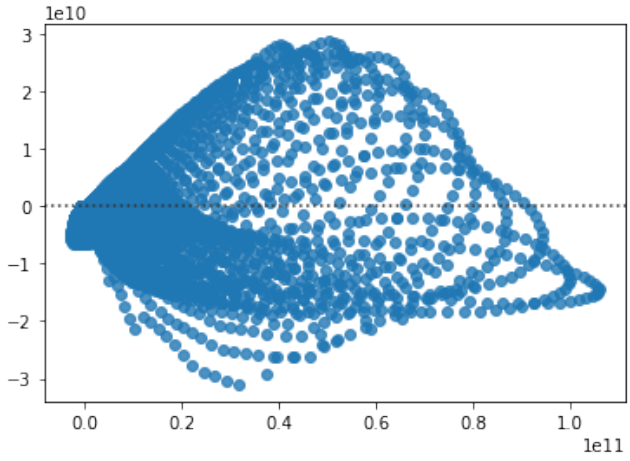

Figure 10. Gaussian Process correlated errors (Zmix, 4 PCA).

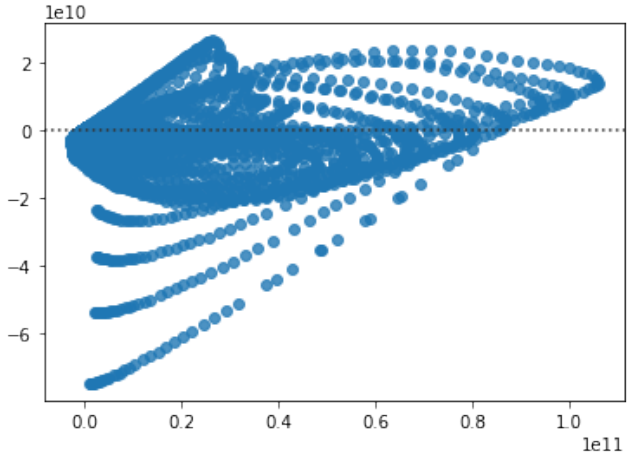

Figure 11. DNN correlated errors (Zmix, 4 PCA).

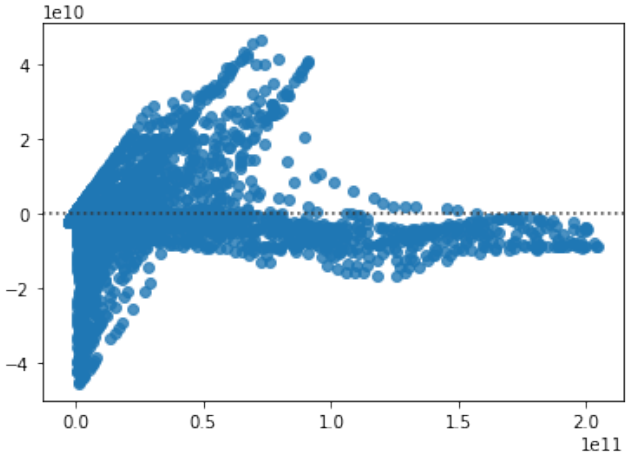

Figure 13. DNN uncorrelated errors (Zmix, Cpv).

We thus concluded that the training data set construction for the ML Models had to be done differently

In this experiment we randomly split the entire dataset equally and used 50% of the data for training and the other 50% for testing.

Training using 50% random Flames 2 Parameters (Zmix, Cpv)

Method	Total Abs Error	MAE
ML Framework I (GP)	8.00E+13	9.74E+09
ML Framework I (DNN)	2.44E+13	2.97E+09

Splitting the data randomly increased the performance of the ML Models.

Just 2 basis vectors were not sufficient and there was still some correlation among the prediction residuals.

And so the last experiment was using 5 basis vectors and 50% of data for training.

Training using
50% random Flames 5 Parameters (Zmix, 4 Orthogonal PCAs)

Method	Total Abs Error	MAE
ML Framework I (GP)	3.97E+12	4.83E+08
ML Framework I (DNN)	3.36E+12	4.09E+08
ML Framework II (PCDNN)	4.08E+12	4.95E+08
Unconstrained DNN	4.14E+12	5.04E+08

The performance was much improved and the prediction residuals were uncorrelated.

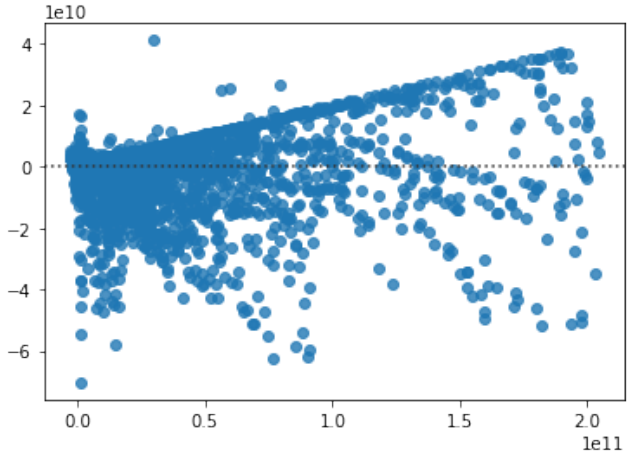

Figure 12. Gaussian Process uncorrelated errors (Zmix, Cpv).

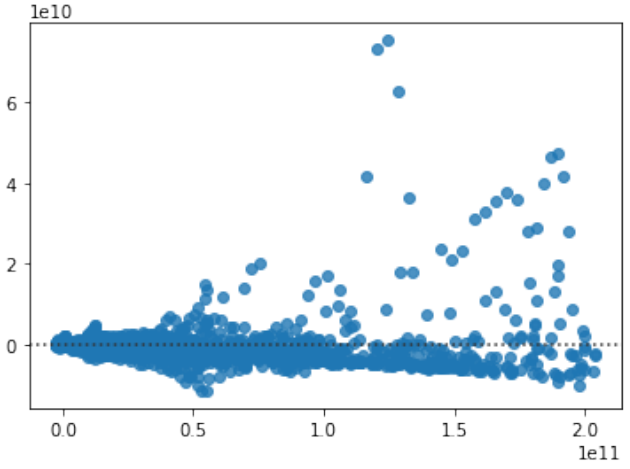

Figure 14. Gaussian Process uncorrelated errors (Zmix, 4 PCA).

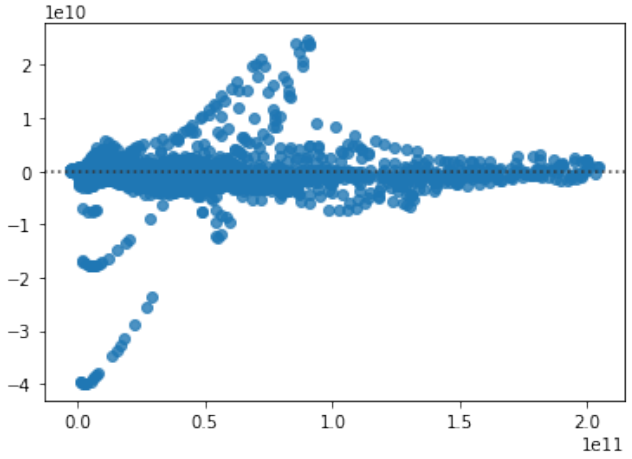

Figure 15. DNN uncorrelated errors (Zmix, 4 PCA).

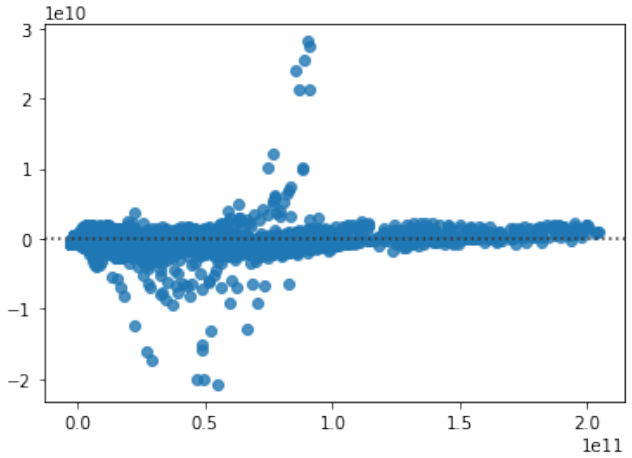

Figure 16. PCDNN un-correlated errors.

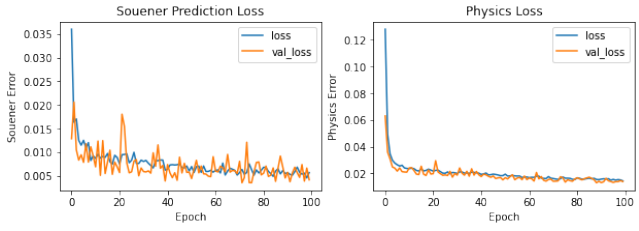

Figure 17. PCDNN Training Losses by Epoch.

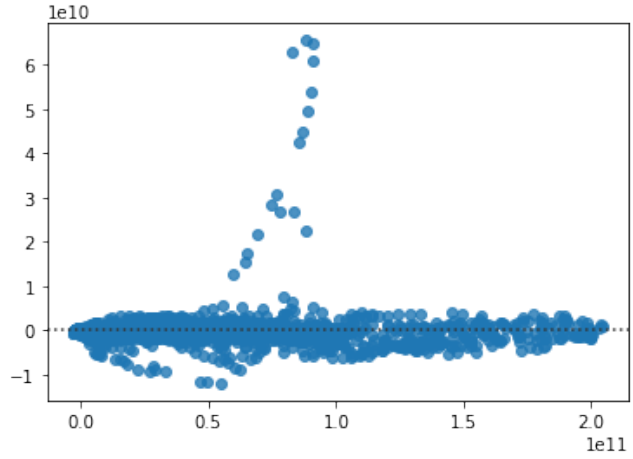

Figure 18. Unconstrained DNN un-correlated errors.

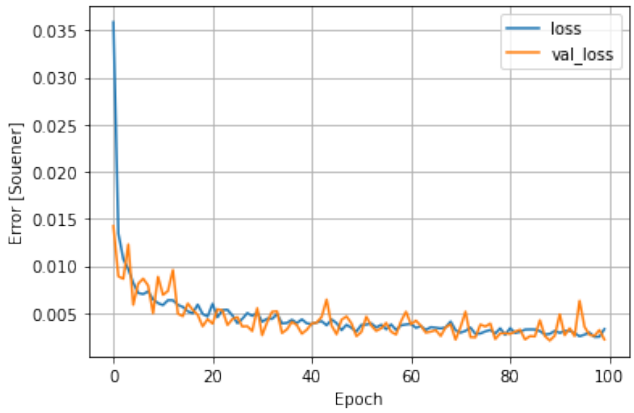

Figure 19. Unconstrained DNN on all species Training Losses by Epoch.

Both ML Frameworks perform better than the current non-ML Framework. ML Framework I with a reduced basis using mixture fraction and constrained orthogonal PCA with Deep Neural Network regression based lookup currently performs the best.

The ML Framework that currently performs the best is the Physics Constrained PCA based lower order manifold generation and Gaussian Process based lookup. The ML Framework with Physics Constrained PCA and Deep Neural Regressor based lookup gives fairly similar performance.

7 Conclusion

The better performing ML Frameworks use more than 2 dimensions and as a result the flow simulation will run slower however will yield more accuracy in the flow simulation.

One problem we identified with the current non-ML Framework is that of high bias: in the creation of a manifold in

the reduced basis the non-ML Framework throws away a significant amount of data. When we used only the data that was used by by the non-ML Framework as the training data for the non-linear regression methods used in the ML Frameworks we noticed that the errors were highly correlated.

When we randomly used 50% of the data in training the non-linear regression methods used in the ML Frameworks the errors were random.

The ML Framework with Deep Neural Regressor based lookup is faster at predictions and can be easily extended to predict multiple output variables at a time.

Although the Physics Constrained Deep Neural Network did yield the same level of performance as that of ML Framework I based on Constrained PCA and DNN we believe that it will generalize better and is the right direction forward: in part it will be robust as it will not (over)learn some of the numerical error generated variances that are captured by PCA. And secondly we will also be able to constrain/regularize the linear embedding to guarantee certain manifold properties like continuity & smoothness.

8 Future Work

We are going to focus on improving the accuracy of the the ML Framework II Physics Constrained Deep Neural Network to get the same level of performance. The impact of including of some of the local/neighborhood features on the accuracy will be explored.

In the same PCDNN setup we would like to implement some of the physics regularization on the linear embedding layer (reduced basis) rather than just using PCA based variance capture maximization. In addition we would like to explore the possibility of adding uncertaininty estimated to the predictions to provide some uncertainty quantification.

Although the DNN provides more accurate estimates we want to explore Deep Gaussian Process to come up with a framework like PCDNN that can be used for joint optimization of the reduced basis generation and regression function learning.

The inherent uncertainty measure around the prediction provided by Deep Gaussian Process can assist in the overall uncertainty quantification.

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