Deep learning for presumed probability density function models

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Abstract

In this work, we use machine learning (ML) techniques to develop presumed probability density function (PDF) models for large eddy simulations of reacting flows. The joint sub-filter PDF of mixture fraction and progress variable is modeled using various ML algorithms and commonly used analytical models. The ML algorithms evaluated in the work are representative of three major classes of ML techniques: traditional ensemble methods (random forests), deep learning (deep neural networks), and generative learning (conditional variational autoencoder (CVAE)). The first two algorithms are supervised learning algorithms, and the third is an unsupervised learning algorithm. Data from direct numerical simulation of the low-swirl burner are used to develop training data for sub-filter PDF models. Models are evaluated on predictions of the sub-filter PDFs as well as predictions of the filtered reaction rate of the progress variable, computed through a convolution of the sub-filter PDF and the conditional means of the reaction rate. This a-priori modeling study demonstrates that deep learning models for presumed PDF modeling are three times more...
accurate than analytical \(\beta-\beta\) PDF models. These models are as accurate as random forest models while using five times fewer trainable parameters and being 25 times faster for inference. We illustrate how models generalize to other regions of the flow and develop criteria based on the Jensen-Shannon divergence to quantify the performance of a model on new data.

**Keywords:** large eddy simulation, presumed probability density function, low-swirl burner, machine learning, \(\beta-\beta\) PDF

1. Introduction

Simulation has the potential to accelerate the development of cost-effective combustion technologies. Even with modern high-performance computing hardware however, the computational cost of fully resolving the reacting flows in these devices can be prohibitive. Large eddy simulations (LES) reduce the computational burden of simulating turbulent reacting flows. LES work with spatially filtered state variables, which exhibit considerably less temporal and spatial structure and thus require much less numerical resolution. However, physical processes occurring at scales smaller than the filter width must then be approximated with “closure models,” which of course then determine the accuracy of the approach. LES closure models for nonreacting flows have received a great deal of recent attention, and they are now in standard use for a wide range of engineering applications. For reacting flows, considerable complexity arises from the necessity to incorporate additional fine scales because of chemical processes and chemistry-turbulence interactions. One approach to constructing sub-filter LES models for reacting flows is to express modeled quantities as convolutions between the physical state and a probability density function (PDF). A presumed PDF approach posits a class of parameterized functional shapes for such PDFs, and thus it defines a parameterized model based on the resulting convolution integrals. In some of the earliest work in this area, Cook and Riley [2] proposed the use of \(\beta\) functions for the PDF shape; much of the work in the field since then has followed this basic strategy. Jiménez et al. [3] provided
further analysis to justify the appropriateness of the $\beta$ PDF for passive scalar mixing. Ihme and Pitsch [4, 5] determined that the “statistically most likely distribution” was most appropriate for a reacting scalar case.

The objective of the work presented here is to expand on the presumed $\beta$ approach, with specific focus on the case of reacting scalars. We incorporate a variety of machine learning (ML) algorithms to explore the accuracy of a number of PDF shape functionals for their use with an LES model, and we judge them by their ability to reproduce a large-scale, direct numerical simulation (DNS) data set for a specific reacting flow configuration. We explore three major classes of ML algorithms for use in this context: traditional ensemble methods (random forests); deep learning (deep neutral network); and deep, generative, unsupervised learning (conditional variable autoencoder). More broadly, traditional ML methods include techniques such as linear and polynomial regression, k-nearest neighbors, support vector machines, Gaussian processes, and random forests. Of these, we focus only on the latter because they have demonstrated widespread success for complex modeling applications [6, 7]. Random forests are based on an ensemble of decision trees, where decisions are based on the model parameters to provide estimates of the target. Deep neural networks (DNNs) are universal function approximators [8, 9] based on a sequence of learnable linear operators and activation functions that are tuned using a gradient-descent optimizer. DNNs have received much attention in recent years, in large part because of the availability of large public training data sets and powerful computing platforms such as graphics processing units (GPUs) [10]. Additional advances in deep learning, particularly in the types of neural network architectures, have led to breakthroughs in generative and unsupervised learning, where new data are generated using the models with unlabeled data and then by identifying trends and commonalities in the generated data. Variational auto-encoders (VAEs) leverage neural networks to encode information from input data into a latent space, which can then be sampled through a decoder to generate new distributions that are similar to the original data set.

In this work, we use the three ML approaches discussed here to construct pre-
sumed PDF models for a DNS data set that is a snapshot of a quasi-stationary simulation of a low-swirl, premixed methane-air burner [1]. We then evaluate the suitability of the different classes of ML algorithms, and of the presumed PDF model itself, both for data from a subregion of the DNS and for the entire simulation domain. In Section 2, we formulate the target problem and methods, including the details of the presumed PDF approach, the DNS target data, and the ML algorithms and network architectures explored. In Section 3, we compare the ML-based constructions to simple analytic models.

2. Formulation

2.1. Presumed probability density function modeling for combustion

In LES of reacting flows using presumed forms of PDFs, an important unclosed term in the equations is the filtered reaction rates, appearing as a source term in the transport equation for species mass fractions or progress variables [11, 12]. A common approach to modeling the filtered reaction rates is to express it as a convolution of a reaction rate derived from a physical model and a PDF. The conditioning variables are typically chosen to correlate strongly with mixing (mixture fraction) and flame propagation (progress variable) space, accounting for much of the subgrid variation about the mean. The conditional rate can then be modeled through a variety of approaches to identify the manifold, such as canonical calculations and tabulation (e.g., flamelet-generated manifolds [13], flame prolongation of intrinsic low dimensional manifold [14]), solving conditional transport equations (e.g., conditional moment closure [15]), or estimated on the fly using conditional source term estimation [16]. Once the conditional rate is obtained, through whatever means, the unconditional mean that appears in the source term for the transport equations can be recovered by weighting with the distribution and integrating over the conditioning space:

\[
\tilde{\omega} = \int \langle \dot{\omega} | Z, c \rangle P(Z, c | \tilde{Z}, \tilde{Z}', \tilde{c}, \tilde{c}') dZ dc. \tag{1}
\]

Here, \(\langle \cdot \rangle\) denotes the volumetric mean of a quantity; \(\tilde{\cdot} = \tau_{\tilde{\cdot}}/\tau\) denotes the Favre filter; \(\tau\) denotes the LES filter; \(Z\) is the mixture fraction, capturing the mixing
of fuel and oxidizer; \( c \) is the progress variable, capturing the overall reaction progress; \( \dot{\omega} \) is the reaction rate of the progress variable (units of \( 1/s \), omitted for brevity); \( \tilde{Z}'' = (Z - \bar{Z})^2 \) is the mixture fraction variance; \( \tilde{c}'' = (c - \bar{c})^2 \) is the progress variable variance; and \( P(Z, c; \bar{Z}, \bar{Z}'', \bar{c}, \bar{c}'') \) is the density-weighted PDF of \( Z \) and \( c \), conditioned on \( \bar{Z}, \bar{Z}'', \bar{c}, \bar{c}'' \). The objective of this work is to develop accurate models of this PDF using ML techniques. Current analytical models often rely on using a \( \beta \) PDF \[2\], defined as:

\[
\beta(x; a, b) = \frac{\Gamma(a + b)}{\Gamma(a)\Gamma(b)} x^{a-1}(1-x)^{b-1},
\]

where \( \Gamma(\cdot) \) is the gamma function; \( a \) and \( b \) are the \( \beta \) PDF parameters, which can be related to the mean, \( \mu \), and variance, \( \sigma^2 \), as

\[
a = \mu \left( \frac{(1-\mu)}{\sigma^2} - 1 \right), \quad b = (1 - \mu) \left( \frac{(1-\mu)}{\sigma^2} - 1 \right).
\]

In this work, \( \bar{Z} \) and \( \bar{Z}'' \) are used as the mean and variance for a \( \beta \) PDF in the mixture fraction space, and \( \bar{c} \) and \( \bar{c}'' \) form the \( \beta \) PDF in the progress variable space, such that \( P(Z, c) = \beta(Z; a_{\bar{Z}}, b_{\bar{Z}})\beta(c; a_{\bar{c}}, b_{\bar{c}}) \).

This model will be used for comparisons with data-driven models using different ML techniques.

### 2.2. Description of the direct numerical simulation of the low-swirl burner

The DNS of an experimental lean premixed turbulent low-swirl methane flame provide the data for model development \[1\,\,\[17\]. In this configuration, a nozzle imposes a low swirl (geometric swirl number of 0.55) to a CH\(_4\) and air mixture with a fuel-air equivalence ratio of 0.7 at the inflow. A co-flow of cold air surrounds the nozzle region with an upward velocity of 0.25 m/s. The inflow velocity of the fuel-air mixture at the nozzle is 15 m/s. The laminar flame thickness is 600 \( \mu \)m. The simulation was performed using LMC, a low Mach number Navier-Stokes solver for turbulent reacting flows that leverages adaptive mesh refinement to resolve finer scales \[18\]. Three levels of refinement were used, leading to effective resolution of 100 \( \mu \)m in the flame region. The computational domain was 0.25 m in each dimension. The DRM 19 chemical mechanism was used to model the finite rate kinetics \[19\]. The domain pressure is 1 atm. The mixture fraction, \( Z \), is computed through a linear combination of the nitrogen
mass fraction in the burner exit stream and the co-flow and it is normalized such that it varies between 0 in the co-flow stream and 1 in the burner exit stream. The progress variable is computed as \( c = Y_{CO_2} + Y_{CO} + Y_{H_2} + Y_{H_2O} \) and varies between 0 and 0.21, where \( Y_i \) is the mass fraction of species \( i \), \( \sum_{i=1}^{N_s} Y_i = 1 \), and \( N_s \) is the number of species.

2.3. Generation of the modeling data

A data set of sample moments and associated sub-filter PDFs was generated from a statistically stationary single time snapshot at \( t = 0.0626 \) s from this DNS by considering different sub-volumes of the domain that span the flame, from the region of premixed burning of the fuel-air mixture from the nozzle to the non-premixed burning of the products from the primary premixed flame zone. These volumes — denoted by \( \mathcal{V}_i \), where \( i = 1, \ldots, n_v \) and \( n_v = 9 \) is the number of sub-volumes — are centered at \( z_i = 0.0525 \) m + \((i - 1)0.0125 \) m, with height 0.00625 m and width 0.14 m, composed of 1146 × 1146 × 51 cells. The locations of several of these subregions and planar slices of \( \tilde{\omega} \) are presented in Figure 1. The premixed burning from the nozzle is evident around \( z = 0.05 \) m, with high values of \( \tilde{\omega} \) and steep gradients. Farther downstream of the nozzle, the non-premixed burning of the products is evidenced in lower and more diffuse values of \( \tilde{\omega} \). Representative slices of the filtered DNS data in \( \mathcal{V}_3 \) are presented in Figure 2. From these slices, it is clear that high values of \( \tilde{Z}'' \) and \( \tilde{c}' \) correlated with high values of \( \tilde{\omega} \). The core of the flame is fully burned, and the reactions take place in a thin region at the interface of the fuel-air mixture from the nozzle and co-flow air.

Throughout this work, samples refer to a pointwise sampling of the filtered fields, each with an associated collection of moments and sub-filter PDFs; volumes refer to a subset of the samples divided according to regions of the domain; and the sub-filter PDF for each sample is described by the four sample moments, \( [\tilde{Z}, \tilde{Z}'', \tilde{c}, \tilde{c}''] \). In each volume, sample moments and associated sub-filter PDFs
(a) $x = 0 \text{ m.}$

(b) $z = 0.0525 \text{ m (center height of } V_1).$

(c) $z = 0.0775 \text{ m (center height of } V_3).$

(d) $z = 0.1025 \text{ m (center height of } V_5).$

(e) $z = 0.1275 \text{ m (center height of } V_7).$

(f) $z = 0.14 \text{ m (center height of } V_9).$

Figure 1: Slices of $\dot{\omega}$ in DNS. White dashed lines: $z$ locations of slices shown in (b)–(f).
Figure 2: Slices of filtered DNS data at $z = 0.0775$ m (center height of $\mathcal{V}_3$).
were generated by using a discrete box filter:

\[
\phi(x, y, z) = \frac{1}{n_f^3} \sum_{i=-n_f/2}^{n_f/2} \sum_{j=-n_f/2}^{n_f/2} \sum_{k=-n_f/2}^{n_f/2} \phi(x + i \Delta x, y + j \Delta x, z + k \Delta x) \tag{3}
\]

where \( \phi \) is the variable to be filtered, \( n_f = \Delta / \Delta x \) is the number of points in the discrete box filter, \( \Delta = 32 \Delta x \) is the filter length scale, and \( \Delta_x = 100 \mu m \) is the smallest spatial discretization in the DNS (six times smaller than the laminar flame thickness). The filter length scale was chosen to be representative of typical LES filter scales \[12\] and to ensure an adequate sampling of the PDF at the filter scale. These filters were equidistantly spaced at \( 8 \Delta x \), leading to 58800 sub-filter PDFs for each volume. The computed conditional sub-filter PDFs are the density-weighted PDFs of \( Z \) and \( c \), discretized with 64 bins in \( Z \) and 32 bins in \( c \). For notational convenience, \( P(Z, c) = P(Z = Z^*, c = c^*) \) will be used in this work, and the discrete PDFs will be referred to as PDFs instead of probability mass functions. The conditional means of the reaction rate, \( \langle \dot{\omega} | Z, c \rangle \), are also computed for each sample with an identical discretization.

Examples of \( P(Z, c) \) and \( \langle \dot{\omega} | Z, c \rangle \) in \( V_3 \) for increasing \( \tilde{\omega} \) illustrate the wide range of observed shapes, Figure 3. For high \( \tilde{\omega} \), the conditional means of \( \dot{\omega} \) peak at \( c = 0.16 \) and exhibit a bimodal distribution at high \( Z \) because of the burning of the fuel stream from the nozzle (\( Z = 1 \)) and the burning of the products mixing with the co-flow. For intermediate \( \tilde{\omega} \), the conditional means of \( \dot{\omega} \) are largest at \( Z = 0.7 \) and \( c = 0.14 \), which is also attributed to the burning of the mixed products. As \( \tilde{\omega} \) increases, the location of the peak of \( P(Z, c) \) increases in the \( Z \) and \( c \) space because reactions happen at higher \( Z \) and \( c \).

Figure 4 illustrates the distribution of moments, \( \left[ \tilde{Z}, \tilde{Z}^\prime, \tilde{c}, \tilde{c}^\prime \right] \), across the samples in \( V_3 \). Most sub-filter PDFs are associated with fully burned states originating from the premixed burning of the fuel-air mixture from the nozzle or the nonreacting unburned states and are double \( \delta \) PDFs centered at \( (\tilde{Z}, \tilde{c}) = (1, 0.2) \) and \( (0, 0) \) with small \( \tilde{Z}^\text{nr} \) and \( \tilde{c}^\text{nr} \). A significant number of sub-filter PDFs, however, are associated with intermediate states spanning the full range of \( \tilde{Z} \) and \( \tilde{c} \) with larger \( \tilde{Z}^\text{nr} \) and \( \tilde{c}^\text{nr} \) because of the non-premixed burning of the products.
Figure 3: Examples of $P(Z, c)$ and $\langle \dot{\omega} | Z, c \rangle$ for increasing $\tilde{\omega}$. Red solid: $\tilde{\omega} = 0$ ($\tilde{Z} = 0$, $\tilde{Z}' = 0$, $\tilde{c} = 0$, $\tilde{c}' = 0$); green dashed: $\tilde{\omega} = 0.03$ ($\tilde{Z} = 0.4$, $\tilde{Z}' = 0.006$, $\tilde{c} = 0.03$, $\tilde{c}' = 0.0006$); blue dash-dotted: $\tilde{\omega} = 7.4$ ($\tilde{Z} = 0.7$, $\tilde{Z}' = 0.01$, $\tilde{c} = 0.08$, $\tilde{c}' = 0.003$); orange short dashed: $\tilde{\omega} = 42.2$ ($\tilde{Z} = 0.9$, $\tilde{Z}' = 0.003$, $\tilde{c} = 0.12$, $\tilde{c}' = 0.005$).
Figure 4: Scatter plots of moments $\tilde{Z}$ and $\tilde{c}$ for samples in $\mathcal{V}_3$ (centered at $z = 0.0775 \text{ m}$) colored by $\tilde{Z}''$ (left) and $\tilde{c}''$ (right) with associated marginal distributions.

from the primary premixed flame zone. It is clear from these data that $\mathcal{V}_3$ contains characteristics of both types of burning in the flame.

2.4. Machine learning algorithms

In this work, we evaluate the performance and suitability of three different types of ML algorithms, each representative of a prevalent class in ML: (i) random forest for traditional ML, (ii) feed-forward DNN for deep learning, and (iii) conditional variational autoencoder (CVAE) for generative and unsupervised learning.

The model inputs are the four sample moments, $[\tilde{Z}, \tilde{Z}'', \tilde{c}, \tilde{c}'']$, and the outputs are the 2048 discrete points representing the joint sub-filter PDF (64 in $Z$, 32 in $c$). The samples from a volume, $\mathcal{V}_i$ ($i = 1, \ldots, n_v$), are randomly distributed among two distinct data sets: a training data set, $\mathcal{D}_t^i$, used to train the algorithms; and a validation data set, $\mathcal{D}_v^i$, used to validate the algorithms and comprising 5% of the samples, i.e., $|\mathcal{D}_v^i| = 2940$, where $|\cdot|$ denotes the cardinality of the data set. Figure 5 illustrates this process for $\mathcal{V}_3$. In this work, we evaluate different models using different training strategies:

1. Models trained using $\mathcal{D}_t^i$ and evaluated on $\mathcal{D}_v^i$ ($i = 1, \ldots, n_v$);
2. Models trained using $\mathcal{D}_i^t$ and evaluated on $\mathcal{D}_i^v$ ($i = 1, \ldots, n_v$);
3. Models trained using $\mathcal{D}^t = \bigcup_{i=1,3,5,7,9} \mathcal{D}_i^t$ and evaluated on $\mathcal{D}_i^v$ ($i = 1, \ldots, n_v$).

The first two strategies involve training and validating on different physical regions of the flame. The third strategy uses training data from the entire flame and the validation data from the training regions and intermediate regions. Prior to training, the sample moments were independently scaled by subtracting the median and dividing the data by the range between the 25th and 75th quantiles. This scaling is robust to outliers [20]. A separate scaling was computed for each training data set and applied to the associated validation data set. The evaluation of a model $m$ on a data set $\mathcal{D}$ is denoted $m(\mathcal{D})$.

The first of the investigated models, random forests (RF), is an ensemble model that creates ensembles of low-bias/high-variance individual decision trees and uses the average of the individual model predictions to provide the prediction for the overall forest [21]. A decision tree is a model that uses a treelike structure to represent nodes that encode conditions based on the input variables, branches that split from each node, and termination points, i.e., leaves, which provide the target value predictions, Figure 6a. The main parameter for
a decision tree model is the maximum tree depth, which is the length of the longest path from the root of the tree to a leaf.

Two key insights have driven the effectiveness of random forests models for complex tasks while avoiding overfitting [6, 7], a problem arising when a model is overly accurate on the training data while failing to predict non-training data. The first is that it leverages bootstrap aggregating or bagging, a method that improves model stability, accuracy, and overfitting problems by dividing the training set into several smaller training sets, called bootstraps, populated through random uniform sampling with replacement. In random forests, each decision tree is built using a different bootstrap of the training data. The second is that, instead of splitting each node in the tree according to the best split of all the variables, the split is done using the best split among a random subset of the variables. The two key parameters of the random forests algorithm are the number of decision trees and the depth of the decision trees. For this work, the random forests model contains 100 decision trees and a maximum tree depth of 30 nodes, beyond which results were insensitive to the model size, and the model size grew larger than can be effectively trained on what we consider a typical analysis workstation with 256 GB of memory. The total model degrees of freedom (DoFs), measured as the sum of nodes in each tree, is 5.2 million.

The field of deep learning has exhibited success in developing models for tasks ranging from image processing [22, 23, 24, 25, 26, 27, 28] to text generation [29, 30, 31] and games [32]. Several reviews of the field give a summary of recent breakthroughs and developments [33, 34, 35, 10, 36]. As a first example of deep learning, we develop a feed-forward, fully connected DNN for modeling PDFs. Similar to the decoder network presented below, this network consists of two hidden layers and an output layer. The hidden layers comprise, respectively, 256, and 512 fully connected nodes, a leaky rectified linear unit activation function:

\[
y = R(x) = \begin{cases} 
  x, & \text{if } x \geq 0, \\
  \alpha x, & \text{otherwise,}
\end{cases}
\]

where \( x \) is the layer input vector, \( y \) is the layer output vector, and \( \alpha = 10^{-2} \) is
a small slope; and a batch normalization layer [37]:

\[ y = B(x) = \gamma \frac{x - \mu_x}{\sqrt{\sigma_x^2 + \epsilon}} + \delta, \]  

(5)

where \( x \) is the layer input vector of size \( n \), \( y \) is the layer output vector of size \( n \), 
\( \mu_x = \frac{1}{n} \sum_{i=1}^{n} x_i \), 
\( \sigma_x^2 = \frac{1}{n} \sum_{i=1}^{n} (x_i - \mu_x)^2 \), 
\( \epsilon = 10^{-5} \), and \( \gamma \) and \( \delta \) are learnable parameter vectors of the same size as \( x \). For inference, i.e., prediction on new data, the batch normalization layer uses a moving average of \( \mu_x \) and \( \sigma_x \) with a decay of 0.1 computed during training. Because we are interested in predicting PDFs, we apply a softmax activation function:

\[ y = S(x) = \frac{\exp(x)}{\sum_{i=1}^{n} \exp(x_i)}, \]  

(6)

where \( x \) is the layer input vector of size \( n \), and \( y \) is the layer output vector of size \( n \), on the output layer to ensure that \( \sum_{i=1}^{n} y_i = 1 \) and \( y_i \in [0, 1] \) \( \forall i = 1, \ldots, n \). Additionally, the loss function for the network is the binary cross entropy between the target, \( t \), and the output, \( y \):

\[ l(y, t) = \frac{1}{n} \sum_{i=1}^{n} (t_i \log(y_i) + (1 - t_i) \log(1 - y_i)), \]  

(7)

and is a good metric for measuring differences between PDFs. The total DNN DoFs, measured as the number of trainable parameters, is 1.1 million. The training occurs during 500 epochs, where an epoch implies one training cycle through the entire training data, after which the loss on the training data is converged. For each epoch, the training data is fully shuffled and divided into batches with 64 training samples per batch. The specific gradient descent algorithm for this work is the Adam optimizer [38] with an initial learning rate of \( 10^{-4} \). The learning rate is a dimensionless parameter that determines the step size of the stochastic gradient descent used to adjust the model weights of the neural network. The Adam optimizer presents many more advantages than traditional stochastic gradient descent by maintaining a per-parameter learning rate, which is adapted during training based on exponential moving averages of the first and second moments of the gradients. The network was implemented in Pytorch [39] and trained on a single NVIDIA Tesla K80 GPU.
Recently, deep generative algorithms, in the form of VAEs [40,41] and generative adversarial networks (GANs) [22], have illustrated how encoding features into a latent space can provide an accurate framework for generating samples from a learned data distribution. Interpolation and other operations in the latent space have shown success in generating samples that usefully combine features of the data set. Though supervision can be built into the network by adding labels to the input and latent spaces, these algorithms are unsupervised learning algorithms. The VAE relies on an encoder, decoder, and loss function. The encoder transforms the input data into a latent space. Unlike encoders for standard autoencoders, the encoder outputs two vectors: a vector of means and a vector of standard deviations. These form the parameters of the random normal variable to be sampled in the latent space. This implies that, given the same data, the encoding in the latent space will differ slightly on different passes. The decoder transforms the resulting encoding in the latent space into outputs that are designed, through the definition of the loss function, to be generated samples from the same distribution as the input data. The loss function is a negative log-likelihood combined with a regularizer. The negative log-likelihood measures the reconstruction loss by the decoder. The regularizer is the Kullback-Leibler divergence between the encoder distribution and the distribution in the latent space, thereby enforcing a continuous latent space. The VAE used in this work follows an hourglass-type architecture, Figure 6b. The encoder network comprises an input layer with 2048 nodes, a hidden layer with 512 nodes, and the last hidden layer with 256 nodes. The decoder network is a mirror image of the encoder (256, 512, and 2048 nodes in each layer). The activation functions in the encoder and decoder are rectified linear units. The final activation function in the decoder is a softmax function, similar to the DNN. The total DNN DoFs, measured as the number of trainable parameters, is 2.3 million. The batch size for each epoch is 64, and the network was trained for 500 epochs. The Adam optimizer was used with an initial learning rate of $10^{-3}$. The latent space dimension is 10. We use a minor variation of the VAE called the CVAE, allowing for the conditioning of the input on a set of labels. The labels
are passed both to the encoder with the input data and to the decoder with the latent space sample data. Therefore, unlike the two previous models, the CVAE model input is the discrete exact sub-filter PDFs and the four sample moments, \( \tilde{Z}, \tilde{Z}^\prime, \tilde{c}, \tilde{c}^\prime \) (the sample moments are also inputs for the latent space); and the CVAE model output is the discrete modeled sub-filter PDF. For the sub-filter PDF inference, the sample moments are combined with a latent space sampling of a standard normal distribution and passed through the decoder part of the CVAE. The network was implemented in Pytorch [39] and trained on a single NVIDIA Tesla K80 GPU.

Although a conditional GAN using the infoGAN network architecture [42] was evaluated for this work, it did not perform as well as the CVAE because of difficulties related to the stability of training a multi-agent model, and results from this model are omitted for brevity.

3. Results

In this section, we present results of using the ML techniques to model the sub-filter PDF, \( P(Z, c|\tilde{Z}, \tilde{Z}^\prime, \tilde{c}, \tilde{c}^\prime) \), from Equation (1). We first focus on using data from the volume centered at \( z = 0.1025 \text{ m} \) because this section of the
domain contains regions that are dominated by premixed burning of the fuel-air mixture from the nozzle and the non-premixed burning of the products from the primary premixed flame zone, as discussed in Section 2.2. Next, we evaluate the generalization capabilities of the different algorithms by characterizing their performance on other sections of the flame.

We quantify model performance with two metrics of interest: the Jensen-Shannon divergence \[43\] \[44\] and the filtered progress variable source term. The Jensen-Shannon divergence measures the similarity between two PDFs and will characterize the error in predicting \( P(Z, c | \tilde{Z}, \tilde{Z}'', \tilde{c}, \tilde{c}'') \). It is a symmetric version of the Kullback-Leibler divergence \[45\].

The Jensen-Shannon divergence exhibits several advantages over the Kullback-Leibler divergence: PDFs do not need to have the same support, it is symmetric, \( J(Q||R) = J(R||Q) \), and it is bounded. The overall sub-filter PDF prediction accuracy of a model is characterized by the 90th percentile of all the Jensen-Shannon divergences, denoted \( J_{90} \). Examples of sub-filter PDF modeling using the \( \beta - \beta \) analytical model illustrate different Jensen-Shannon divergence values, Figure 7. This figure is similar to Figure 3, though it shows different realizations of \( P(Z, c) \). The \( \beta - \beta \) analytical model is not able to capture more complex sub-filter PDF shapes, such as bimodal distributions, leading to high Jensen-Shannon divergence values, Figure 7b, and it motivates the need for more accurate models. From these results, accurate predictions can be expected for \( J(P|P_m) < 0.3 \), whereas predictions with \( J(P|P_m) > 0.6 \) exhibit incorrect median values and overall shapes.

The second metric of interest characterizes the error in predicting \( \tilde{\omega} \) and is simply the normalized root mean square error (RMSE) of the model predictions,
\[ \tilde{\omega}_m : \]

\[
\text{RMSE}(\tilde{\omega}) = \frac{1}{\tilde{\Omega}} \sqrt{\frac{1}{|\mathcal{D}|} \sum_{i=1}^{[\mathcal{D}]} \left( \epsilon(\tilde{\omega}_i) \right)^2}, \tag{9}
\]

where \( \epsilon(\tilde{\omega}_i) = \tilde{\omega}_i - \tilde{\omega}_{m,i} \) is the error, \( \mathcal{D} \) is the data set over which the error is computed, and

\[
\tilde{\Omega} = \sqrt{\frac{1}{|\mathcal{D}_T|} \sum_{i=1}^{[\mathcal{D}_T]} \left( \tilde{\omega}_i \right)^2}, \tag{10}
\]

is the normalization constant, and \( \mathcal{D}_T = \bigcup_{i=1, \ldots, n} \mathcal{D}_i \). All metrics presented are computed with respect to the validation data sets.

### 3.1. Sub-filter probability density function predictions

ML models were trained using filtered DNS data from \( \mathcal{V}_3 \) (centered at \( z = 0.1025 \) m), i.e., the algorithms were trained on \( \mathcal{D}_3 \), and the metrics were evaluated on \( \mathcal{D}_3^v \). The random forests model training time for the 52920 PDFs
in $D^v_3$ was 1800 s on an Intel SandyBridge Xeon processor with 256 GB of memory. The DNN and CVAE training times were 2200 s and 3500 s on a NVIDIA Tesla K80 GPU.

Several example PDF predictions are shown in Figure 7, corresponding to low, medium, and high values of $J(P||P_m)$. The PDF and the cumulative density function for the Jensen-Shannon divergence of the predictions on the validation data, $J = J(P||P_m)$, where $P_m$ is the modeled sub-filter PDF, are presented in Figure 8. The three ML models exhibit similar PDF prediction errors with a narrow peak close to 0. The prediction error for the $\beta-\beta$ analytical model is larger than the prediction errors for the ML models; see Table 1. Additionally, comparing the training error, $J^t_{90}$, to the validation error, $J^v_{90}$, indicates that the random forests model overfits the training data (there is a large difference between the training and testing error), whereas the deep learning algorithms avoid overfitting; Table 1.

Model prediction times for each sub-filter PDF were computed for all models as:

$$t_m = \frac{1}{n_t |D^v_3|} \sum_{i=1}^{n_t} \text{time to evaluate } m(D^v_3)$$

where $n_t = 10$ predictions on the validation data set $D^v_3$, which contains 2940
samples, thereby necessitating 2940 model evaluations. Although the random forests model accuracy is similar to that of the neural networks, the model complexity required is such that the prediction time is approximately 20 times longer than the DNN and CVAE and the model size is more than 3000 times larger; see Table 1. The need for large amounts of memory for training and the slow prediction times illustrate the main drawback for the use of the random forests algorithm in production simulations from the standpoints of both training and prediction. Because the DNN and the CVAE decoder have similar architectures, their prediction time is similar. The $\beta$-$\beta$ model sub-filter PDF computations involve a discrete $\beta$ PDF evaluation in both $Z$ and $c$ and an outer product to compute the sub-filter PDF, leading to prediction times comparable with the random forests model. The $\beta$ PDF was computed through the SciPy library [46].

The PDF models were used to provide predictions of the reaction rate, $\tilde{\omega}$, by convoluting the predicted sub-filter PDF with the reaction rate, Equation 1, where $\langle \dot{\omega} | Z, c \rangle$ is from the same $32^3$ box as that used to generate $P(Z, c | \tilde{Z}, \tilde{Z}', \tilde{c}, \tilde{c}')$. This ensures that the errors observed in the predictions of $\tilde{\omega}$ can be exclusively attributed to the sub-filter PDF modeling. Table 1 and Figure 9 illustrate the different model performances in predicting $\tilde{\omega}$. The coefficient of determination, $R^2$, is above 0.95 for the three ML models, indicating a high model accuracy, whereas that of the $\beta$-$\beta$ model is significantly lower. The three different ML algorithms achieve similar results, Figure 9. The PDF of the error, $\epsilon(\tilde{\omega})$, is

| Model | $J^-_{90}$ | $J^-_{90}$ | $t_m$ (ms) | RMSE($\tilde{\omega}$) | $R^2(\tilde{\omega})$ | DoFs (million) | Memory (MB) |
|-------|------------|------------|-------------|------------------------|-----------------------|----------------|-------------|
| RF    | 0.03       | 0.12       | 0.932       | 0.22                   | 0.97                  | 5.2            | 82107       |
| DNN   | 0.11       | 0.11       | 0.036       | 0.23                   | 0.97                  | 1.1            | 27          |
| CVAE  | 0.11       | 0.12       | 0.038       | 0.22                   | 0.97                  | 2.3            | 36          |
| $\beta$-$\beta$ | 0.35       | 0.35       | 1.178       | 0.63                   | 0.75                  | –              | –           |

Table 1: Summary of model performance and size for $P(Z, c | \tilde{Z}, \tilde{Z}', \tilde{c}, \tilde{c}')$ and $\tilde{\omega}$. 


symmetric, indicating that the models are not biased toward under- or overpredicting. The $\beta$-$\beta$ analytical model has a broad range of prediction errors and tends to underpredict $\tilde{\omega}$ for $\tilde{\omega} > 5$ in this volume, Figure 9a.

### 3.2. Model generalization

In this section, we examine the performance of the models trained using different data sets and their ability to generalize to data from other regions of the
flame. An understanding of model generalization has important implications for the model’s applicability to other physical configurations. Because of the nature of the low-swirl burner flame, a wide range of different physical processes are encountered in different regions of the flame, and it is important to understand the conditions for a model’s applicability.

Three versions of the models were trained: (i) using \( D_{t,3} \) (volume centered at \( z = 0.0775 \) m); (ii) using data from a volume farther downstream, \( D_{t,5} \) (volume centered at \( z = 0.1025 \) m); and (iii) trained using data from every other volume \( D_{t} = \bigcup_{i=1,3,5,7,9} D_{t,i} \). Note that for the random forests trained on all volumes, the maximum depth size of the trees was reduced to 18 to avoid out-of-memory errors on a 256 GB node (the resulting model size exceeded 110 GB).

The difference between the PDFs in different volumes is quantified through the minimum of the pairwise Jensen-Shannon divergence between all PDFs belonging to \( V_i \) and all PDFs belonging to \( V_j \):

\[
r_{i,j} = \min_{k=1,\ldots,|D_{i,v}|} J(P_k\|P_l) \quad \forall P_k \in D_{i,v}, \forall P_l \in D_{j,v}.
\]

(12)

Low values of \( r_{i,j} \) indicate that \( \forall P_l \in D_{j,v} \) there is \( P_k \in D_{i,v} \), which has a small Jensen-Shannon divergence and, therefore, a similar shape. The 90\(^{th}\) percentile of \( r_{i,j} \), \( r_{90} \), for different data sets is presented in Figure 10. For \( V_3 \), it is clear that the PDFs in regions of the flame that are farther downstream or upstream are significantly different; however, models trained using data from every other volume, \( D_{t} \), have training data that are representative of the entire simulation domain.

Figure 11 presents the predictions for the three different model versions. For models trained using data from only one volume, the PDF prediction error is lowest for that volume and increases as the model is used on downstream or upstream volumes. All three types of ML algorithms predict similar generalization error profiles. This indicates that these models, including the generative algorithm, are unable to extrapolate to non-proximate regions of the flame. This is consistent with the observation that the training data are not representative of the entire flow, Figure 10. The RMSE(\( \bar{\omega} \)) decreases as a function of \( z \) because
the mean $\tilde{\omega}$ decreases as a function of $z$ as well. Models trained with $\mathcal{D}_e^i$ perform slightly better in the upstream portion of the domain, Figure 11b, because the PDFs in $\mathcal{V}_5$ are more representative of the upstream PDFs, but fail to capture those where the premixed burning at the nozzle is dominant ($z \approx 0.05$ m), Figure 10.

Models trained using every other volume achieve errors that are approximately half the error of the $\beta-\beta$ analytical model, Figure 11c. This indicates that the models are capable of interpolating the sample space across the entire physical domain while using only a small subsection of the samples in the domain. The ML models achieve very good accuracy and approximate the conditional means of $\tilde{\omega}$, which is the optimal estimator using these data, Figure 12. Significant overpredictions in the $\beta-\beta$ model are observed. These are driven by errors in upstream volumes, Figure 11c, particularly at high $\tilde{Z}$ and $\tilde{c}$, Figure 12. Sample PDFs where $\tilde{\omega} > 15$ are shown in Figure 13 for different Jensen-Shannon divergences computed on the DNN model. Bimodal distributions are accurately predicted by the ML models, and, even for the worse case, Figure 13c, the shapes in $Z$ and $c$ are well modeled.

In addition to demonstrating the accuracy of the ML algorithms, these results illustrate that the 90th percentile of $r_{i,j}$ is a good metric for characterizing PDF similarity and provides a model generalization criteria, $r_{90} < 0.2$, for an a-priori assessment of model performance on new data. Models trained using a data set that has an $r_{90} < 0.2$ with another data set will produce joint sub-filter PDFs exhibiting $J_{90} < 0.2$ and, consequently, accurate $\tilde{\omega}$ predictions. As a demonstration, a DNN model was trained using samples from the negative $x$-half of the volume $\mathcal{V}_3$ of the axisymmetric flame (centered at $x = y = 0$ m), i.e., $\mathcal{D}_x^t = \{s \mid s \in \mathcal{D}_x^t, x_s < 0 \text{ m}\}$, and validated on predictions of samples in the positive $x$-half of the other volumes, $\mathcal{D}_x^v = \{s \mid s \in \mathcal{D}_x^v, x_s > 0 \text{ m}, i = 1, \ldots, n_v\}$. This model performs accurately on PDF predictions in nearby volumes, e.g., $J_{90} \approx 0.15$ in $\mathcal{V}_2$ and $\mathcal{V}_3$, and performs poorly at locations farthest downstream, e.g., $J_{90} = 0.63$ in $\mathcal{V}_7$.

The results in this section illustrate (i) the importance of using data repre-
Figure 11: $J_{90}$ and RMSE($\tilde{\omega}$) as a function of height using ML algorithms trained with data from different sections of the flame. Red squares and solid: RF; green diamonds and dashed: DNN; blue circles and dash-dotted: CVAE; orange pentagons and short dashed: $\beta$-$\beta$ model.

sentative of the extent of the physical processes present in the simulation and (ii) the potential to develop in situ ML modeling capabilities, where the model is developed during the simulation, without adversely affecting the simulation time because the most accurate models were trained using data from less than 4% of the total DNS domain volume.

4. Conclusion

In this work, we used three different ML algorithms representative of different types of ML (traditional methods, deep learning, and generative learning) to design presumed PDF models for combustion applications. We showed that models designed through ML are better able to capture the complexity of these sub-filter PDFs than analytical models. Although the random forests model predicts results similar to those of the deep learning models, this model is not suitable for in situ training and modeling because of the model complexity, which
Figure 12: Reaction rate predictions for models trained on $D' = \bigcup_{i=1,3,5,7,9} D'_i$. Red squares and solid: RF; green diamonds and dashed: DNN; blue circles and dash-dotted: CVAE; orange pentagons and short dashed: $\beta$-$\beta$ model; black solid: DNS.

Figure 13: Marginal sub-filter PDFs for median and high Jensen-Shannon divergence values for models trained on $D' = \bigcup_{i=1,3,5,7,9} D'_i$. Red solid: RF; green dashed: DNN; blue dash-dotted: CVAE; orange short dashed: $\beta$-$\beta$ model; black solid: DNS.
leads to high memory requirements and high prediction times. The deep learning algorithms were able to achieve the same high accuracy with fast prediction times and low model complexity. Generative learning models, which present advantages in many deep learning applications through the use of a latent space representation, do not provide increased accuracy or better generalization characteristics compared to feed-forward neural networks. Additionally, the deep learning models provide fast predictions relative to the $\beta$-$\beta$ model, indicating that these methods might at the very least be efficient encoders of $\beta$-$\beta$ tabulation models by using DNS as a source of training data, resulting in encodings that provide more useful forms of the joint sub-filter PDF not expressible by the $\beta$-$\beta$ model. Our results illustrate methodologies that can be successfully leveraged to derive accurate deep learning models for a wide range of applications. The results exhibited throughout this work indicate that deep learning models can be advantageously used for in situ modeling of turbulent combustion flows. These deep learning algorithms are readily integrated with scientific computing codes through PyTorch’s C++ API for future a-posteriori model evaluation.

This work — including neural network models, analysis scripts, Jupyter notebooks, and figures — can be publicly accessed at the project’s GitHub page[^1]. Traditional ML algorithms were implemented through scikit-learn [20] and the deep learning algorithms through PyTorch [39].

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[^1]: https://github.com/NREL/ml-combustion-pdf-models
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