Abstract—Tunable diode laser absorption tomography (TDLAT) has emerged as a popular nonintrusive technique for simultaneous sensing of gas concentration and temperature. However, TDLAT imaging of concentration and temperature is an ill-posed, nonlinear inverse problem. Major challenges of TDLAT imaging include a highly nonlinear forward model, few projection measurements, and limited training data. We propose a novel model-based iterative reconstruction (MBIR) framework for TDLAT imaging. To do this, we formulate a nonlinear forward model for TDLAT that incorporates the physics of light absorbance through gaseous media, and we couple it with a non-Gaussian prior model based on a Gaussian mixture distribution that can be trained using a sparse training set. We show that the resulting MAP estimation problem can be solved using majorization minimization together with a novel multigrad optimization algorithm that solves the resulting optimization problem using an orthogonal basis set. Reconstructions using simulated TDLAT datasets show that our TDLAT-MBIR method can reduce reconstruction error while also resulting in a very computationally efficient algorithm.

Index Terms—Gaussian mixture models, GMM, non-convex optimization, non-homogeneous image model, tunable diode laser absorption spectroscopy, tunable diode laser absorption tomography, TDLAS, TDLAT, tomography.

I. INTRODUCTION

Simultaneous reconstruction of gas flow properties like concentration and temperature is a challenging nonlinear inverse problem [1] and appears in many applications including the monitoring of industrial exhaust [2] and diagnostics of engines [3]–[5]. Among different in situ gas flow diagnostic techniques, tunable diode laser absorption tomography (TDLAT) [6]–[10] has become popular because of its ability to track rapidly varying signals [11], [12], the high signal-to-noise ratio signals it can produce, and the wide availability of operationally simple tunable diode lasers [13].

Fig. 1 shows an illustration of a TDLAT measurement system for a single projection path. In TDLAT imaging of gases, tunable diode laser sources are employed to emit laser light at particular discrete frequencies [3], [14]. These frequencies correspond to quantum absorption transitions of a particular target molecule [15], [16]. The absorbance of light passed through the gaseous media is measured by using laser light detectors and is then used to reconstruct flow properties. The details of TDLAT measurement systems can be found in [13], [17].

Reconstruction of TDLAT data poses many challenges that make it quite different from traditional tomographic reconstruction of X-ray CT data [18], [19]. First, the TDLAT measurement model is highly nonlinear due to nonlinear dependence of light absorption on temperature. Second, TDLAT imaging systems typically only allow for a small number of projection measurements due to the physical limitations imposed by optical access and short lived combustion phenomenon [17]. For example, in a typical TDLAT system there may be only 10 to 100 measurements available to estimate 1000 to 10 000 pixel unknowns. Therefore, the reconstruction problem is highly ill-posed and nonlinear, so conventional tomographic techniques such as filtered back projection (FBP) [20], [21] are not appropriate.

In order to help constrain the solution, many restrictive assumptions have been used in the past. These include assuming uniform flow properties along the projection path [15], [22], assuming axisymmetric flow [23]–[25] and assuming different flow profiles [26]. However, these assumptions are often inappropriate for many applications that involve non-uniform and high speed turbulent gas flows [14], [17], [27]–[29]. Moreover, these simplistic assumptions do not allow for spatially resolved reconstruction of gas flow properties.

Some of the early studies to obtain spatially resolved gas flow properties without imposing restrictive assumptions were
based upon FBP together with a nonlinear inversion step [8], [11], [30]. However, these approaches require a large number of projection measurements at many different viewing angles (more than 500 projections). M. Ravichandran et al. worked on improving the quality of concentration and temperature reconstructions using a finite domain direct inversion (FDDI) method [31] and modified convolution back projection [32], both using more than 100 projections. In [9], a fan beam geometry was used to reconstruct concentration and temperature using a rotary mechanism to acquire 55 projections at different angles.

Perhaps more closely related methods to our work are the iterative reconstruction methods. For example, in [33] concentration and temperature are reconstructed by solving an optimization problem using 200 projection measurements and L2 regularization, or equivalently, a Gaussian Markov random field prior model. In [34], a principal component analysis (PCA) basis set for the concentration and temperature were used to perform reconstructions using 200 projection measurements. These bases were obtained by using 5000 simulated phantoms for each of the concentration and temperature fields. However, this approach did not take into account the correlation between the concentration and temperature fields. Both [33] and [34] use simulated annealing to solve their corresponding optimization problems which is computationally very expensive as is noted in their results.

An alternate approach to improve the accuracy of tomographic reconstructions is the use of model-based iterative reconstruction (MBIR) methods [35]–[39]. In MBIR, a model is specified for both the measurement process (forward model) and for the unknown image to be reconstructed (prior model). Typically, a maximum a posteriori (MAP) estimate of the unknown image is computed that optimally fits both the forward model and the prior model.

An important benefit of model based methods is that they allow for the incorporation of nonlinear forward models along with prior models that can be trained using representative images. For example, in TDLAT imaging, recently there has been a use of computational fluid dynamics (CFD) simulated images of molecular density and temperature fields which accurately capture the properties of gas flow [13], [40]. These CFD simulated images can potentially be used to improve the reconstruction quality by providing training examples for the prior model [6]. However, CFD simulation images are computationally expensive to compute and therefore usually very few of them are available for training. Moreover, typical CFD images are spatially non-homogeneous and tend to cluster in groups or modes with similar behavior. This makes it difficult to accurately represent them with typical prior models such as Markov random fields (MRF) [41]–[47].

In this paper, we propose a fast MBIR framework that we call TDLAT-MBIR for simultaneous reconstruction of 2-D molecular density and temperature fields of gaseous flow. There are four major contributions of our approach for TDLAT imaging.

1) A nonlinear physics-based forward model;
2) A Gaussian mixture model (GMM) as the prior model;
3) A majorization technique for computing the MAP estimate;
4) A multigrid algorithm for solving the required optimization.

Our MBIR approach incorporates a nonlinear forward model of the light absorption through the gaseous media. However, since the number of measurements is so small, we must also incorporate an advanced non-Gaussian prior model that can capture the multivariate distribution of the molecular density/temperature fields. We do this by training a Gaussian mixture model (GMM) model to model general non-Gaussian distributions of the combined molecular density and temperature fields. The GMM is particularly useful since it can model the empirical distribution of modes that typically occur in real flow fields.

In order to compute the MAP estimate, we introduce a majorization minimization technique for computing the surrogate cost function for the required optimization. To do this, we present a general theory for the creation of surrogate functions of multivariate mixture distributions that generalizes previous results for scalar Gaussian mixtures [48], [49]. Our final innovation is a multigrid algorithm that uses an orthogonal basis set to find a good solution to the resulting non-convex optimization problem.

Experimental results using simulated TDLAT data generated using CFD phantoms show that our method can produce fast reconstructions of relatively high resolution images (i.e., $45 \times 45$) and very few projection measurements (i.e., 40 projection measurements obtained from 10 projection paths and 4 transition frequencies). Results show that the proposed prior model improves the reconstruction quality both visually and quantitatively by accurate modeling of non-homogeneous and non-Gaussian behaviors of the CFD images. Results also indicate that the proposed multigrid algorithm reduces the computation time by speeding convergence.

II. FORMULATION OF MAP COST FUNCTION

A typical approach to model-based inversion is to compute the MAP estimate of the unknown which is given as

$$\hat{x} = \arg \min_x \{ \log p(y|x) + \log p(x) \},$$

where $y$ is the measurement vector, $x$ is the joint vector of unknown molecular density and temperature, $p(y|x)$ is the probability of observing the data vector $y$ given the unknown $x$ (also called the forward model), and $p(x)$ is the probability of unknown $x$ (also called the prior model).

A. Forward Model

The TDLAT imaging technique yields projection measurements by measuring light absorbance through gaseous media, which in our case is water vapor in the air. Light intensity measurements are made along projection paths and at multiple discrete transition frequencies. Fig. 2 shows the optical projection path layout used in the simulations. Ten optical line of sight (LOS) paths indexed by $j \in \{1, 2, 3, \ldots, J\}$, for $J = 10$, are arranged in a rectilinear grid with non-uniform spacing. Laser light is swept over the optical frequency around four discrete transition frequencies indexed by $k \in \{1, 2, \ldots, K\}$, for
The linestrength function $S_k(T)$ [50] is given as

$$S_k(T) = S_k(T_0) \frac{Q(T_0)}{Q(T)} \exp \left[-\frac{hcE_k}{k_B} \left(\frac{1}{T} - \frac{1}{T_0}\right)\right] \times \left[\frac{1 - \exp(-hc\nu_k/k_BT)}{1 - \exp(-hc\nu_k/k_BT_0)}\right],$$

(5)

where $Q(T)$ is the partition function of the absorbing molecule [50], $k_B$ is the Boltzmann constant, $\hbar$ is Planck’s constant, $c$ is the speed of light, $E_k$ is the lower state energy level of the $k^{th}$ absorption transition, $\nu_k$ is the discrete transition frequency, and $T_0$ is the reference temperature. The partition function $Q(T)$ is a continuous function of temperature and is specific to the target molecule. Typically the partition function is calculated using a cubic spline polynomial. The estimation of cubic spline polynomial coefficients for the partition function is described in detail in Appendix B.

The absorbance of light follows from (3) by integrating over the projection path,

$$\ln \frac{I(\nu, 0)}{I(\nu, L_j)} = \phi_k(\nu) \int_{r_{1,j}}^{r_{2,j}} N(r) S_k(T(r)) \, dr,$$

(6)

$$\int_{r_{1,j}}^{r_{2,j}} \ln \frac{I(\nu, 0)}{I(\nu, L_j)} \, d\nu = \int_{r_{1,j}}^{r_{2,j}} N(r) S_k(T(r)) \, dr,$$

(7)

where $\Gamma_j$ is the $j$th projection path and (7) uses the fact that $\phi_k(\nu)$ is a unit area function. However, in practice the light intensity measurements are noisy due to a variety of noise sources including electronic noise, shot noise, digitization noise, beam steering, light scattering by particles and uncertainty in the spectrometric database [50]. To incorporate different sources of noise, we model the noise as additive white Gaussian noise with mean 0 and variance $\sigma^2$ [33], [34]. Consequently, the projection measurements are related to the light absorbance model by the following equation,

$$Y_{j,k} = \int_{r_{1,j}}^{r_{2,j}} N(r) S_k(T(r)) \, dr + W_{j,k},$$

(8)

$$= \int_{r_{1,j}}^{r_{2,j}} f_k(N(r), T(r)) \, dr + W_{j,k},$$

(9)

where $W_{j,k} \sim N(0, \sigma^2)$ is additive white Gaussian noise and $f_k(N(r), T(r)) = N(r) S_k(T(r))$ is a function defined for notational convenience.

For 2-D reconstruction of $N(r)$ and $T(r)$, the region of interest is discretized into a grid of $r_{ij}$ square pixels. Let $N = [N_1, N_2, \ldots, N_{r_{ij}}]^T$ and $T = [T_1, T_2, \ldots, T_{r_{ij}}]^T$ represent the unknown molecular density and temperature vectors and let $x = [N^T T^T]^T \in \mathbb{R}^p$ be the joint vector of unknowns. Equation (9) can then be approximated as

$$Y_{j,k} = \sum_{i=1}^{r_{ij}} H_{j,i} f_k(N_i, T_i) + W_{j,k},$$

(10)

where $H_{j,i}$ is the weighting coefficient for the $j$th projection path and $i$th pixel. Writing equation (10) compactly in terms of matrix-vector notation yields

$$Y = H[F(x)] + W,$$

(11)
where \( Y \in \mathbb{R}^{J \times K} \) are measurements, \( H \in \mathbb{R}^{J \times F} \) is the forward projection matrix, \( F(x) = [f_1(x) \ f_2(x) \ldots f_K(x)] \in \mathbb{R}^{F \times K} \), where \( f_k(x) = f_k(N,T) \in \mathbb{R}^F \) are column vectors such that each column \( f_k(x) \) represents the function \( f_k \) over the entire domain of interest for a particular absorption transition and \( W \in \mathbb{R}^{J \times K} \) is the white noise matrix such that \( [W]_{j,k} \sim \mathcal{N}(0,\sigma^2) \). Putting this together, the log likelihood of the measurements \( Y \) given the unknown \( x \) is given by

\[
\log p(Y|x) = -\frac{1}{2\sigma^2} ||Y - H[F(x)]||_2^2 + \epsilon, \tag{12}
\]

where \( \epsilon \) is a constant that does not depend on \( x \) and the norm in equation (12) is the Frobenius norm.

**B. Prior Model**

We model the joint distribution of the molecular density \( N \) and the temperature \( T \) using a Gaussian mixture model (GMM) with \( M \) mixture components. A major advantage of GMM prior over existing prior models like Markov random fields (MRF) and dictionary learning (DL) methods is that it models the non-homogeneous and non-Gaussian characteristics of the \( N \) and \( T \) fields. In contrast, MRFs and DL methods require the images to be modeled as stationary random processes. In this problem, modeling the non-homogeneous behaviors and the long-range correlations between the pixels of \( N \) and \( T \) are of crucial importance. The GMM prior model implemented in the eigenimage domain allows for these non-Gaussian and non-homogeneous dependencies to be captured effectively and can be trained with a sparse training dataset.

The likelihood function of \( x = [N^T \ T^T]^T \) is given by

\[
p(x) = \frac{M}{m=1} \pi_m [B_m]^2 \exp \left\{-\frac{1}{2} \left||x - \mu_m\right||_B^2 \right\}, \tag{13}
\]

where \( \pi_m, \mu_m \) represent the prior probability and mean of the mixture component \( m \) and \( B_m \) represents the precision matrix of mixture component \( m \) or equivalently the inverse of the component covariance matrix \( R_m \).

1) Transformed Representation of \( x \): While the dimension \( p \) of the unknown \( x \) can be several thousand, \( x \) typically resides on a thin manifold in this higher dimensional space. In order to reduce the dimension of our problem, we will represent the image as

\[
x = Ez, \tag{14}
\]

where \( z \in \mathbb{R}^{\tilde{p}} \) is a lower dimensional representation of the image and \( E \) is a \( p \times \tilde{p} \) matrix with orthonormal columns. If \( x \) has a Gaussian mixture distribution, then it is easily shown that \( z \) must also have a Gaussian mixture distribution with parameters given by

\[
\bar{\pi}_m = \pi_m, \tag{15}
\]

\[
\bar{\mu}_m = E^T \mu_m, \tag{16}
\]

\[
\bar{R}_m = E^T R_mE, \tag{17}
\]

where \( \bar{\pi}_m, \bar{\mu}_m, \bar{R}_m \) are the prior class probability, class mean, and class covariance of the random vector \( z \) that shall be estimated from the data.

In order to avoid over fitting of the training data, we will constrain the covariance matrices \( \bar{R}_m \) to be diagonal. So the transformation, \( E \), must be chosen to diagonalize \( \bar{R}_m \) for each mixture component \( m \). We do this by first clustering the data \( x \) into the desired number of mixture components. Next, we hard classify each sample to a mixture component and subtract off the respective component mean from it giving us an approximate sample covariance matrix, \( \bar{R}_m \), for each mixture component. Once this is done, the columns of \( E \) can be computed to be the eigenimage vectors of the averaged component covariance matrix formed by

\[
\bar{R} = \sum_{m=1}^M \alpha_m \bar{R}_m, \tag{18}
\]

where \( \alpha_m \) is the number of hard classified samples in mixture component \( m \). Fig. 4 illustrates the effect of this diagonalization procedure for a 2-dimensional vector \( x \) with a Gaussian mixture distribution. Notice that using this technique, the coordinate bases are aligned with the axes of the mixture components. Appendix C explains this procedure in greater detail.

2) Training Procedure: Next, we used CFD simulated phantoms, shown in Fig. 5, to estimate the parameters \( \bar{\pi}_m, \bar{\mu}_m, \bar{R}_m \).
of the Gaussian mixture distribution. These training phantoms come in pairs of molecular density and temperature images. The training phantoms of Fig. 5 are representative of the typical CFD phantoms that we used for training the parameters. The complete set of the training phantoms is available in the supplementary material section of this paper. The GMM parameters are estimated using the EM algorithm software of [51] with the input data given by the $p$ dimensional vectors

$$z^{(i)} = E^T x^{(i)}, \quad \text{(19)}$$

where $x^{(1)}, \ldots, x^{(n)}$ are the $n$ CFD simulated phantom images used to train the model.

In order to improve the accuracy of the model, the EM algorithm is run with a number of constraints that reduce the number of parameters to be estimated. First, the covariance matrices $R_m$ are constrained to be diagonal. This helps in avoiding the over-fitting of the sparse training set. In addition, the diagonal covariance matrices $R_m$ provide a simpler cost function to minimize as compared to the non-diagonal covariance matrices. Second, for all coordinates greater than some value, $p_1$, the mean and the variance are constrained to be equal for all mixture components. Typically, $p_1$ is a small number such as $p_1 = 3$.

Lastly, to avoid singularities in estimating the parameters of GMM [52], each class is required to have at least two data samples assigned to it, so that, $\pi_m \geq 2/n$.

The prior likelihood of the unknown expressed in eigenimage basis set $E$ is then given as

$$p(z) = \sum_{m=1}^{M} \frac{\pi_m |B_m|^{\frac{1}{2}}}{(2\pi)^{\frac{1}{2}}} \exp \left\{ -\frac{1}{2} \| z - \mu_m \|_{B_m}^2 \right\}, \quad \text{(20)}$$

where $\tilde{B}_m$ is the inverse of $R_m$.

C. MAP Cost Function Expression

To derive the MAP cost function in eigenimage basis set $E$, we first give the MAP cost function in image domain using equation (1) as

$$c(x) = \frac{1}{2\sigma^2} \left\| Y - H [F(x)] \right\|_2^2 - \log \left( \sum_{m=1}^{M} \pi_m |B_m|^{\frac{1}{2}} \exp \left\{ -\frac{1}{2} \| x - \mu_m \|_{B_m}^2 \right\} \right), \quad \text{(21)}$$

where all the terms not depending on $x$ have been dropped. Next we use the transformation of equation (14) to write the MAP cost function in terms of the eigenimage basis set $E$ as

$$c(z) = \frac{1}{2\sigma^2} \left\| Y - H [F(Ez)] \right\|_2^2 - \log \left( \sum_{m=1}^{M} \frac{\pi_m |\tilde{B}_m|^{\frac{1}{2}}}{(2\pi)^{\frac{1}{2}}} \exp \left\{ -\frac{1}{2} \| z - \tilde{\mu}_m \|_{\tilde{B}_m}^2 \right\} \right). \quad \text{(22)}$$

Choosing large values for $p_1$ will result in over-fitting of the sparse training set as the number of GMM parameters increase as $M \times (2p_1 + 1) - 1$.

Additionally, we will constrain the reconstruction in the image domain inside the physically feasible region to ensure that all molecular density values $N \in \mathbb{R}^{T/2}$ are non-negative and all temperature values $T \in \mathbb{R}^{T/2}$ are greater than or equal to 296 Kelvins. Thus, the TDLAT-MBIR reconstruction is given as follows

$$\hat{z} = \arg\min_{z \in \Omega} c(z), \quad \text{(23)}$$

where

$$\Omega = \{ z \text{ s.t. } [N^T \ T]^T = Ez \ & N \geq 0 \ & T \geq 296 \}. \quad \text{(24)}$$

The MAP cost function of equation (22) is non-convex because of both the non-convex forward model term and non-convex prior model term.

It may seem appealing to reconstruct the $N$ and $T$ fields in two stages by first reconstructing $f(x) \mid x$ and then reconstructing $N$ and $T$ [3], [8], [53]. However, this indirect approach typically does not yield good results because it is suboptimal. The Bayesian method models both the non-linear forward model and the joint prior distribution of $N$ and $T$ resulting in a single cost function that captures the synergy between the forward and the prior model. In comparison, the two-stage approach must also have a separate model for the functions $f(x)$. Another significant advantage of the Bayesian approach is that we can inform our prior model of $N$ and $T$ by using CFD simulations. It is also noteworthy that the 2-stage approach does not offer any computational advantages.

III. CONSTRUCTION OF SURROGATE COST FUNCTION

The MAP cost function of equation (22) is difficult to minimize since it is non-convex. In particular, the prior model term in the cost function is difficult to minimize directly as it has a mixture of exponentials inside the logarithm. Hence, we simplify the optimization problem by using the majorization minimization technique [18], [54] in which a quadratic surrogate function is used to upper bound the prior term. In order to use the majorization minimization approach, one must find a surrogate function $\hat{c}(z; z')$ such that

$$\hat{c}(z'; z') = c(z'), \quad \text{(25)}$$

$$\hat{c}(z; z') \geq c(z). \quad \text{(26)}$$

We can construct such a surrogate function using the following Lemma [55], [56], proved in Appendix D.

**Lemma:** Surrogate function for log of exponential mixtures

Let $s: \mathbb{R}^D \rightarrow \mathbb{R}$ be a function which takes the form,

$$s(z) = -\log \left( \sum_m w_m \exp \{-u_m(z)\} \right), \quad \text{(27)}$$

where $w_m \in \mathbb{R}^+, \sum_m w_m > 0$ and $u_m: \mathbb{R}^D \rightarrow \mathbb{R}$. Furthermore $\forall (z, z') \in \mathbb{R}^D \times \mathbb{R}^D$ define the function

$$G(z; z') = -s(z') + \sum_m w'_m \left( u_m(z) - u_m(z') \right), \quad \text{(28)}$$

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where \( w_m \) is the weight of the \( m \)th mixture component, and \( \{u_m(z')\} \) is the Gaussian mixture prior. Then \( \forall (z, z') \in \mathbb{R}^D \times \mathbb{R}^D \), \( G(z; z') \) satisfies the following two conditions,

\[
G(z'; z^*) = s(z') \tag{29}
\]

\[
G(z; z^*) \geq s(z). \tag{30}
\]

The conditions mentioned in (29) and (30) are sufficient to guarantee that \( G(z; z') \) is a surrogate function for \( s(z) \) and therefore that minimizing \( G(z; z') \) must also reduce the function \( s(z) \).

Comparing the prior log likelihood term in the MAP cost function of equation (22) with the function of equation (27), we define a quadratic surrogate function for the prior log likelihood term,

\[
\begin{align*}
g(z; z') &= -\log p(z') \\
&+ \sum_m d_m \left( \|z - \bar{\mu}_m\|_{B_m}^2 - \|z' - \bar{\mu}_m\|_{B_m}^2 \right), \tag{31}
\end{align*}
\]

where

\[
\begin{align*}
d_m &= \sum_j \pi_j \left\{ \sum_i \pi_i \left( \frac{1}{2} \|z' - \bar{\mu}_i\|_{B_i}^2 \right) \right\}, \tag{32}
\end{align*}
\]

and \( z' \) is the current state of the unknown. The resulting surrogate function for the MAP cost function \( c(z) \) is then given by

\[
\begin{align*}
\hat{c}(z; z') &= \frac{1}{2\sigma^2} \left\| Y - H [F(Ez)] \right\|_2^2 - \log p(z') \\
&+ \sum_m d_m \left( \|z - \bar{\mu}_m\|_{B_m}^2 - \|z' - \bar{\mu}_m\|_{B_m}^2 \right). \tag{33}
\end{align*}
\]

Since our goal is to minimize the cost with respect to \( z \), we may drop the terms involving \( z' \) to obtain an equivalent surrogate function given by

\[
\begin{align*}
c(z; z') &= \frac{1}{2\sigma^2} \left\| Y - H [F(Ez)] \right\|_2^2 + \frac{1}{2} \|z - \bar{\mu}\|_{\tilde{B}}^2, \tag{34}
\end{align*}
\]

where

\[
\tilde{B} = \sum_{m=1}^M d_m \tilde{B}_m, \tag{35}
\]

and

\[
\tilde{\mu} = \tilde{B}^{-1} \left( \sum_{m=1}^M d_m \tilde{B}_m \bar{\mu}_m \right). \tag{36}
\]

A typical example of a surrogate function for the prior term is shown for the case of a single coordinate in Fig. 6. The surrogate function has been constructed for a Gaussian mixture prior that has five mixture components and it is plotted for a single coordinate. Notice that in Fig. 6, while the original function corresponding to the GMM prior term is non-convex, the surrogate function is a convex function that forms an upper bound to the original function. It should be noted that the surrogate function of equation (34) is still a non-convex function due to the non-convex forward model term.

IV. OPTIMIZATION

In this section, we shall present a multigrid optimization algorithm to solve the MAP estimation problem. We shall also present a fixed-grid algorithm for comparison. Both the multigrid and the fixed-grid algorithms are designed to achieve a local minimum of the non-convex MAP estimation problem of equation (23). The multigrid algorithm, however, has much faster convergence as compared to the fixed-grid algorithm.

Multigrid algorithms can reduce the computational complexity of numerical problems by working on the data at different scales or grids. Multigrid algorithms have been used in many different applications including optical flow estimation [57], [58], signal/image smoothing [59], [60], image segmentation [61], interpolation of missing image data [62], and optical diffusion tomography [63], [64]. The main novelty in our multigrid algorithm is that we introduce a notion of grids using eigenimage basis functions.

Intuitively, the first few eigenimages are spatially smooth, whereas the latter ones have more spatial variation. We exploit this by cumulatively increasing the number of eigenimages as we move from coarse to fine grids. We start working on coarse grids first, gradually moving to finer grids, reducing the cost at each grid. This improves the convergence of the multigrid algorithm when compared with the fixed-grid algorithm.

A. Coordinate Update Method

The multigrid and fixed-grid algorithms both work by iteratively minimizing the cost function of equation (22) over individual coordinates \( z_i \) but with important differences. Both algorithms use the surrogate function formulation of equation (34) to reduce the 1-D cost. The cost function of equation (34) written as a function of the \( i \)th coordinate only is given as,

\[
\begin{align*}
c(z_i; z') &= \frac{1}{2\sigma^2} \left\| y - H [Ez' + E_{z_i}(z_i - z'_i)] \right\|_2^2 \\
&+ \frac{1}{2} \left( z_i - \bar{\mu}_i \right)^2 \tilde{B}_{i,i}, \tag{37}
\end{align*}
\]

where \( z' \) is the current value of the unknown and \( E_{z_i} \in \mathbb{R}^{D \times 1} \) is the \( i \)th eigenimage.

To reduce this 1-D cost function, we propose a fast and robust coordinate update method. We fit a quadratic
function through the 1-D cost function by selecting three points, $(z_i - \epsilon_i, z_i, z_i + \epsilon_i)$ and minimize this quadratic. We choose the step size $\epsilon_i$ for each coordinate in an adaptive manner corresponding to the variation in the coordinate;

$$\epsilon_i \leftarrow \delta \sqrt{\tilde{R}(i,i)},$$

(38)

where $\tilde{R}$ is the inverse of the equivalent precision matrix in equation (35) and $\delta$ is usually picked between $10^{-5}$ to $10^{-3}$. This procedure is known as inverse parabolic interpolation [65].

A typical example of the quadratic fit is shown in Fig. 7.

The quadratic fit to the true cost function is not necessarily a strict upper bound to the true cost function as shown in Fig. 7, therefore we must check if the true cost is reduced as a result of minimizing the quadratic fit. In rare cases, the true cost could increase, so then we revert to Brent’s method that alternates between golden section iterations and quadratic fits [65]. Fig. 8 shows an example where Brent’s method is used to reduce the 1-D cost function.

Finally, at each coordinate update, we ensure that the reconstruction $z$ remains inside the physically feasible region $\Omega$. If after a coordinate update, the reconstruction in the image domain goes out of the feasible region, we project it onto the boundary of the feasible region by changing the value of eigenimage coordinate using a bisection method. More precisely, we iteratively bisect the interval between the optimum value and the old value of the eigenimage coordinate until we satisfy the physical feasibility constraints, while at the same time achieving the minimum 1-D cost under these constraints.

B. Fixed-Grid Optimization

In the fixed-grid algorithm, we reduce the cost function on a single grid that consists of all the eigenimage basis vectors. To minimize the cost function, we use the ICD update strategy [66]. ICD, which is related to Gauss-Seidel method and has been found to be suitable for CT applications [67], works by optimizing over each coordinate one by one until some stopping criterion is met. Fig. 10 shows the pseudocode of fixed-grid algorithm.

C. Multigrid Optimization

In the multigrid algorithm, we work at different grids having a different number of eigenimages to be optimized over. At the coarsest grid, we start from the first column vector, $E_{1,1}$, of the eigenimage basis set $E$ and optimize over it. Next, as we move to the fine grids, we increase the number of eigenimages by a factor of $\rho$ at each grid until we include the final eigenimage, $E_{\tilde{p},\tilde{p}}$, at the finest grid. At each grid, we optimize over a fixed number of eigenimages. This process is repeated in a loop until the stopping condition is met. The pseudocode of multigrid optimization algorithm is presented in Fig. 11 and the coordinate update pattern of the multigrid algorithm is shown in Fig. 12.

V. EXPERIMENTAL RESULTS

We now present our TDLAT-MBIR image reconstruction results by performing reconstructions of a simulated TDLAT
dataset. To test our proposed Gaussian mixture prior model and multigrid optimization algorithm, we perform reconstructions on CFD simulated phantoms. These CFD phantoms are obtained by running simulations for a single axial plane of an engine having a diameter of 12 inches. The CFD simulated phantoms are used to produce simulated projection measurement data using the measurement layout of Fig. 2. This simulated measurement dataset is then used in all the experiments.

First, we compare the reconstruction results of the proposed prior model with the results of two different prior models; Gaussian model (GM) [6] and Gaussian Markov random field (GMRF) model [41] and also with the reconstruction results of the proper orthogonal decomposition (POD) approach of [34]. We compare the reconstructions both visually and using an objective criterion of normalized root mean squared error (NRMSE). The NRMSE between two images \( X \) and \( Z \) is defined as

\[
\text{NRMSE}(X, Z) = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (X_i - Z_i)^2} / \max_i (Z_i) - \min_i (Z_i). \tag{39}
\]

We provide some reconstruction results for visual comparison and also provide a table that shows the average results of all the reconstructions.

\[\text{A. Comparison of Reconstruction Results}\]

To test our proposed GMM prior model, we perform reconstruction experiments using CFD simulated phantoms. A total of 42 CFD phantoms are available, so we perform 42 reconstruction experiments, where in each experiment, we keep one phantom for testing and train the prior model on the rest of the 41 phantoms. The image array size in the reconstructions is kept at \( 45 \times 45 \); however, since the region of interest is a circle, the total number of unknowns \( p = 3194 \). The TDLAT measurements are simulated using (12) with an average SNR of 30 dB. This corresponds to a value of noise standard deviation \( \sigma \), which is roughly 3% of the mean value of forward projections representing practical scenarios. Also, for these simulations \( J = 10 \) and \( K = 4 \), so \( Y \in \mathbb{R}^{10 \times 4} \).

We set \( M = 5 \) and \( p_1 = 3 \), since we found that using these values in the experiments yielded the lowest average NRMSE results. We estimate the parameters of the mixture model in the eigenimage basis space \( E \) using expectation-maximization algorithm. We constrain the mixture component covariance matrices \( \hat{R}_m \) to be diagonal.

Fig. 13(a) shows the scatter plot of the training data using eigenimage basis domain. In this figure, the blue dots represent the training data, the red dots represent the means of the estimated Gaussian mixture components. The green dot represents mean of estimated Gaussian distribution. The length of the red and green segments corresponds to the standard deviation of the corresponding eigenimage coordinates. (b) Shows the mesh plot of probability density function of Gaussian mixture model.

Finally, we perform convergence experiments to compare our multigrid optimization algorithm with conventional fixed-grid optimization algorithm. We compare the speed of convergence using two different metrics. One of them is the MAP cost, whereas the other is the normalized root mean squared error (NRMSE) between the current state and the converged state of the unknown fields \( N \) and \( T \). We present the plots of MAP cost and NRMSE between current and converged state of the unknown fields \( N \) and \( T \).

\[\text{Fig. 11. Pseudocode of multigrid algorithm.}\]

```matlab
function [\( \hat{Z} \)] = MULTIGRID(y, z', G, \( \rho \))

/* Inputs: Measurements y, Initial condition \( z' \), Total number of grids G, Factor for calculating grid coefficients \( \rho \) */

/* Output: MAP estimate \( \hat{Z} \) */

\( \hat{Z} \leftarrow z' \)

while Stopping criterion is not met do

for \( j = 0 \) to \( G - 1 \) do /* For each grid level */

for \( i = 1 \) to \( \rho^j \) do

Compute \( \hat{B} \) and \( \hat{\mu} \) using eq. (32), (35), (36)

\( \hat{z}_i \leftarrow \arg \min_{\zeta} c(z_i; \zeta) \) /* Reduce cost of eq. (37) */

\( z' \leftarrow \hat{z}_i \) /* Update the current state */

end for

end for

end while

end function
```

Fig. 12. Coordinate update pattern in one full iteration of Multigrid algorithm using \( \rho = 1 \) and \( \tilde{\rho} = 40 \).

\[\text{Fig. 13. Illustration showing the multi-modal nature of the distribution of the CFD training data. (a) Shows the scatter plot of the CFD training data expressed in eigenimages. The blue dots are the data samples and the red dots are the means of the estimated Gaussian mixture components. The green dot represents mean of estimated Gaussian distribution. The length of the red and green segments corresponds to the standard deviation of the corresponding eigenimage coordinates. (b) Shows the mesh plot of probability density function of Gaussian mixture model.}\]

\[\text{We provide some reconstruction results for visual comparison and also provide a table that shows the average results of all the reconstructions.}\]

\[\text{2Our implementation of POD approach is similar to [34], however, unlike [34], we do not use the simulated annealing algorithm. We use our proposed multigrid algorithm of Fig. 11 without imposing any bounds on the eigenimage coordinate values.}\]

\[\text{Finally, we perform convergence experiments to compare our multigrid optimization algorithm with conventional fixed-grid optimization algorithm. We compare the speed of convergence using two different metrics. One of them is the MAP cost, whereas the other is the normalized root mean squared error (NRMSE) between the current state and the converged state of the unknown fields N and T. We present the plots of MAP cost and NRMSE between current and converged state of the unknown fields N and T.}\]
distribution. Modeling this data using a Gaussian distribution does not capture different empirical modes evident in the scatter plot. Fig. 13(b) shows the probability density function of the Gaussian mixture model whose parameters are trained from the CFD training data.

For all the experiments, the initial condition for GMRF reconstructions is a constant image for both the $N$ and $T$ fields, the initial condition for GM and POD reconstructions is the mean of the training data, and the initial condition for GMM reconstruction is the end result of GM reconstruction. The initial conditions were chosen in an effort to achieve lowest possible final value of MAP cost function after convergence of the optimization procedure. The regularization level was chosen for GMRF, GM, and GMM to achieve the lowest NRMSE, whereas in POD there is no regularization parameter to be set.

For POD, GM, and GMM reconstructions, we run 3 iterations of multigrid optimization algorithm using the eigenimage basis as described in Section IV. The coarsest grid has only 1 eigenimage coefficient, the finest grid has 40 and $\rho = 1.8$. For the GMRF reconstructions, we use a multi-resolution approach by performing reconstructions on three different scales, where, at each finer scale, we use the end result of the next coarser scale as an initial condition.

Table I shows NRMSE results averaged over all 42 reconstructions. It is evident that overall the GMM prior gives the lowest NRMSE results. The GMRF prior model gives the highest NRMSE results. This could be because the GMRF is not a very expressive prior model particularly for CFD phantoms; and with a sparse measurement set, the prior serves an important role in avoiding the estimation of a reconstruction that is unlikely to occur.

It appears from the reconstructed example results in Figs. 15 and 16 that the GMM prior model and the GM prior model produce the best reconstruction results, however, only the reconstructions with the GMM prior model capture the dense patches in the molecular density fields. The POD technique gives false dense patches in the molecular density reconstructions. This might be because the POD technique does not model the correlation between concentration and temperature. Although smooth, the GMRF reconstructions fail to capture the essential structure in $N$ and $T$ fields. It seems that with the very sparse measurement set, GMRF tends to overly smooth the reconstructions.

We also studied the effect of changing the number of Gaussian mixture components $M$ in GMM prior model. With 41 CFD phantoms available for training, we found out that $M = 5$ mixture components gave us the best results. Fig. 14 shows the average NRMSE of 42 reconstructions as a function of the number of mixture components.

### B. Convergence Results

We compared the convergence speed of our multigrid optimization algorithm with our fixed-grid optimization algorithm by running 42 reconstruction experiments using a Gaussian mixture prior model. The initial condition for these reconstructions is the end result of reconstructions with the Gaussian prior model. For each reconstruction, we first run the algorithm for a sufficiently large number of iterations to achieve a “fully converged” result. We then run the same reconstructions again and at each coordinate update we compute the MAP cost and the NRMSE between the current and the converged state of the unknown fields $N$ and $T$. Both multigrid and fixed-grid algorithms use eigenimage bases. In the case of the multigrid algorithm, the coarsest grid has 1 eigenimage coordinate, the finest grid has 40 eigenimage coordinates and $\rho = 1.8$.

Fig. 17(a) shows a comparison of cost plots averaged over 42 reconstructions. It is evident that the cost drops much more quickly with the multigrid algorithm. This makes sense since the multigrid algorithm spends much more computation on eigenimage coefficients which are expected to have more variation in the eigenimage domain.

In Fig. 17(b) and 17(c) we present % NRMSE plots between current and converged state of the unknown molecular density and temperature fields averaged over 42 reconstructions. It is clear from the figures that the multigrid algorithm converges much faster than the fixed-grid algorithm. Typically for these reconstructions, a 1% NRMSE criterion is enough to guarantee sufficient convergence. In Fig. 18, we observe the speed-up as a function of % NRMSE between the current and converged result. We define the speed-up as

\[
\text{speed-up (r)} = \frac{\text{Average fixed-grid iterations to achieve } r \% \text{ NRMSE}}{\text{Average multigrid iterations to achieve } r \% \text{ NRMSE}}.
\]

(40)

Hence speed-up at $r$ % NRMSE would be the relative decrease in the computation that one gets by using the multigrid algorithm as opposed to the fixed-grid algorithm to achieve an

<table>
<thead>
<tr>
<th></th>
<th>% NRMSE (N)</th>
<th>% NRMSE (T)</th>
<th>Avg. NRMSE</th>
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<tr>
<td>POD</td>
<td>9.89</td>
<td>12.13</td>
<td>11.01</td>
</tr>
<tr>
<td>GMRF</td>
<td>10.00</td>
<td>13.50</td>
<td>11.75</td>
</tr>
<tr>
<td>GM</td>
<td>6.15</td>
<td>5.51</td>
<td>5.83</td>
</tr>
<tr>
<td>GMM</td>
<td>6.14</td>
<td>5.14</td>
<td>5.64</td>
</tr>
</tbody>
</table>

NRMSE(N) is Average NRMSE in Molecular Density. NRMSE(T) is Average NRMSE in Temperature. Avg. NRMSE is Average of the NRMSE in Molecular Density and Temperature.
Fig. 15. Example 1 of TDLAT reconstructions. The scale of $N$ is $0 \times 10^{17}$ molecules-cm$^{-3}$ and the scale of $T$ is 0 to 1000 Kelvins. Both GM and GMM produce good reconstruction results, however, GMM captures the dense region in molecular density reconstruction, whereas, GM does not. POD seems to suffer from a lot of artifacts, whereas, GMRF seems to overly blur the details.

Fig. 16. Example 2 of TDLAT reconstructions. The scale of $N$ is $0 \times 10^{17}$ molecules-cm$^{-3}$ and the scale of $T$ is 0 to 1000 Kelvins. Both GM and GMM produce good reconstruction results, however, GMM captures the dense region in molecular density reconstruction, whereas, GM does not. POD seems to suffer from a lot of artifacts, whereas, GMRF seems to overly blur the details.

Fig. 17. Comparison of convergence speed of fixed-grid and multigrid algorithm. All three plots represent an average from 42 reconstructions. These plots are representative of the typical behavior. It can be seen from all three plots that multigrid algorithm converges faster than fixed-grid algorithm. (a) MAP cost plot. (b) $\%$NRMSE between current and converged value of $N$. (c) $\%$NRMSE between current and converged value of $T$.

Fig. 18. Average relative decrease in computational time when using the multigrid algorithm as opposed to fixed-grid algorithm. To achieve a $1\%$ NRMSE between the current and the converged result, multigrid algorithm requires about 0.27 seconds, whereas fixed-grid algorithm requires about 0.73 seconds on a computer with an Intel core i7 processor and 32 GB memory using MATLAB. NRMSE of $r\%$ in both $N$ and $T$ fields. It is clear from Fig. 18 that the multigrid algorithm is almost uniformly better than the fixed-grid algorithm. The speed-up seems to converge at about a factor of 1.8 for very conservative criterion of NRMSE, whereas for a more practical convergence criterion i.e., $1\%$ NRMSE, there is a speed-up factor of 2.7.

VI. CONCLUSION

We have proposed a novel framework that we have named TDLAT-MBIR for reconstruction of TDLAT dataset. We first derived a forward model based upon physics of light absorbance through gaseous media. Next, we proposed a Gauss-
sian mixture model as a prior model for images that can capture non-homogeneous and multimodal behaviors of the image distributions. We presented a methodology for training the parameters of this model. Finally, we proposed a multigrid optimization algorithm using eigenimage basis functions along with a robust 1-D optimization strategy. Reconstruction results using CFD simulated phantoms indicate that the proposed GMM prior model improves the quality of reconstructions and the multigrid optimization algorithm improves convergence.

APPENDIX A

SELECTION OF ABSORPTION LINE SPECTRUM

In hyperspectral TDLAT, more than a single absorption line spectrum, typically more than two, are analyzed to collect data [33]. This increases the information content by adding more measurements at different discrete optical frequencies. This is important to offset the very low number of LOS projection measurement paths. There are many factors that determine the absorption lines to be chosen. For example, strength of absorption, spectral separation between absorption lines, temperature sensitivity of absorption lines, effects of boundary layers and lack of interference from nearby absorption lines [16]. Other factors that affect the selection of lines include expected sensor operating conditions and hardware capabilities [22].

In this paper, we are using water as our target molecule because of its natural availability as a major combustion product, strong rovibrational transitions [13] and wide range of transition frequencies. Therefore, the transition frequencies are chosen according to the properties of the water molecule. The four different absorption transition lines that are used in this work are given in Table II. These absorption transitions lines are same as the ones used in [40].

APPENDIX B

ESTIMATION OF SPLINE COEFFICIENTS FOR Q FUNCTION

The partition function $Q(T)$ acts as a normalizing constant for the probability of occupation of a particular quantum state at temperature $T$ [68]. In practice, even for simple molecules like H$_2$O, the partition function is difficult to calculate. Typically, the partition function is approximated using cubic spline polynomials which are fit to laboratory derived values that are usually very accurate [16]. In this study, we used the calculations of the partition function for water done by Gamache et al. [68]. We fit cubic splines to the data to get a smooth, twice differentiable curve as seen in Figs. 19, 20(a) and (b).

The original cubic spline polynomial coefficients, that were made available to us to approximate the partition function were such that the resulting fit was not twice differentiable. Table III shows the cubic spline polynomial coefficients that were provided to us in the beginning. To understand the role of each of the coefficients in the provided tables, we provide the representation of the partition function in a temperature range from $T_0$ to $T_1$, such that the resulting fit was not twice differentiable. Table III shows the cubic spline polynomial coefficients that were provided to us in the beginning. To understand the role of each of the coefficients in the provided tables, we provide the representation of the partition function in a temperature range from $T_0$ to $T_1$.

$$Q(T) = a + b T + c T^2 + d T^3$$, \quad $T_0 \leq T < T_1$. \hspace{1cm} (41)

Using the coefficients in Table III, the resulting first and second derivatives are discontinuous at temperature values where a change of polynomial occurs. In order to ensure that the approximated partition function is twice differentiable, we corrected the value of the polynomial coefficients given in Table III and also minimized the overall error using the tabulated values of partition function made available by R. R. Gamache [68]. Following were the steps that were taken to ensure that the resulting cubic spline polynomial coefficients give a twice differentiable curve.

1) We ensure the continuity of the second derivative by adjusting the value of coefficient $c$ such that on points where the change of polynomial occurs, the difference in the values of $Q''(T)$ is 0.

2) We adjust the values of coefficient $b$ such that on points where the change of polynomial occurs, the difference in the values of $Q'(T)$ is 0. This ensures the continuity of the first derivative of $Q$ function.

3) We adjust the values of coefficient $a$ such that on the points where change of polynomial occurs, the difference in the values of $Q(T)$ is 0. This gives us a continuous $Q$ function.

The above procedure gives us a continuous, twice differentiable $Q$ function. Finally, to reduce the overall error between

<table>
<thead>
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<th>TABLE II</th>
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</thead>
<tbody>
<tr>
<td>ABSORPTION SPECTROSCOPIC LINE PARAMETERS</td>
</tr>
<tr>
<td>Transition Frequency $\nu_i$ (cm$^{-1}$)</td>
</tr>
<tr>
<td>7181.156</td>
</tr>
<tr>
<td>7161.410</td>
</tr>
<tr>
<td>7185.597</td>
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<td>7179.752</td>
</tr>
</tbody>
</table>

Fig. 19. Plot of partition function using cubic spline polynomial approximation.

Fig. 20. Derivatives of partition function calculated using cubic spline polynomial approximation. (a) First derivative of $Q$ function. (b) Second derivative of $Q$ function.

---

3We estimated the cubic spline polynomial coefficients to get a partition function $Q(T)$ that is twice differentiable up to 64-bit double precision.


\[
\text{Temp. Range} \quad a \quad b \quad c \quad d \\
T < 500 \quad -18.221850000000000 \quad 0.423075200000000 \quad 7.703331000000000 \quad 6.185911000000000e-9 \\
500 \leq T < 1000 \quad -65.94119999999993 \quad 0.694587000000000 \quad 2.468241000000000e-4 \quad 3.484234000000000e-7 \\
1000 \leq T < 1350 \quad -61.853600000000000 \quad 0.697335600000000 \quad 2.183511000000000e-4 \quad 3.699410000000000e-7 \\
1350 \leq T < 1425 \quad 1.16661815424874e5 \quad -2.51101921239251e6 \quad -6.640078900000000e-4 \quad 5.875034666666668e-7 \\
1425 \leq T < 2500 \quad -1.311191000000000e3 \quad 3.214013000000000 \quad -0.001522213000000 \quad 7.885534200000000e-7 \\
2500 \leq T < 5000 \quad -4.529464000000000e3 \quad 7.314166000000000 \\
\]

Table III
Cubic Spline Coefficients for Q Function Provided in the Beginning

Fig. 21. Plot of percent error in Q function.

experimentally determined values of Q function and the computed values of Q function using the cubic splines, we fit a cubic function to the error and adjust the coefficients \(a, b, c\) and \(d\) to reduce the error. The error for our final cubic spline fit was below 2% for a range of temperature values given by 300 Kelvin to 3010 Kelvin as shown in Fig. 21. The final cubic spline coefficients that give a continuous, twice differentiable Q function are provided in Table IV.

APPENDIX C
Orthonormal Basis Estimation Procedure

Let \(x^{(1)}, \ldots, x^{(n)}\) be the CFD training vectors, where each \(x^{(i)}\) is a \(p\) dimensional vector. Without any loss of generality, assume that the mean of all the training vectors is 0. Let \(X\) be the \(p \times n\) training matrix containing all the training images given by

\[
X = [x^{(1)}, \ldots, x^{(n)}].
\]  

We can write the SVD of the matrix \(X\) as

\[
X = E_1 \Sigma_1 V_1^T,
\]  

where \(E_1, \Sigma_1, V_1\) are the left-singular vectors, singular values and right-singular vectors of \(X\). We assume that the singular values are ordered in descending magnitude along the diagonal of the matrix \(\Sigma_1\).

We need to obtain an orthonormal basis set \(E\) that diagonalizes the class covariance matrices for all the mixture components. We obtain this basis set by applying a rotation transform on \(E_1\). The need of rotation arises from the fact that \(E_1\) computed through SVD ignores the possibility of different mixture components in the distribution of unknown \(x\).

First we represent the CFD data in eigenimage basis set \(E_1\) as vectors \(z^{(1)}, \ldots, z^{(n)}\) and estimate the mixture parameters \(\{\pi'_m, \mu'_m, R'_m\}_{m=1}^M\). Next, we bring each mixture component onto the origin by subtracting the component mean off from every data sample. We do this by performing a maximum a posteriori classification of each of the data samples to a mixture component. So let \(c_i\) be the MAP classified mixture component of the \(i\)th data sample, so,

\[
c_i = \arg \max_{1 \leq m \leq M} p \left( z^{(i)} \text{ belongs to } m^{th} \text{ component } | z^{(i)} \right).
\]

Let \(Z'\) be the matrix in which each column consists of a training data sample after subtracting off the component mean, so,

\[
Z' = [z^{(1)} - \mu_{c_1}^{(1)}, \ldots, z^{(n)} - \mu_{c_n}^{(n)}].
\]

Since we constrain all the mixture components to have a common mean and covariance for all coordinates greater than \(p_1\), we only need to rotate the first \(p_1\) coordinates of the data samples. Therefore, let \(Z''\) be the matrix that consists of first \(p_1\) rows of \(Z'\). The rotation \(E_2 \in \mathbb{R}^{p_1 \times p_1}\) that rotates the first \(p_1\) coordinates of the data samples is computed by performing an SVD decomposition on \(Z''\),

\[
Z'' = E_2 \Sigma_2 V_2^T,
\]

Finally the rotation transform that aligns the GMM components with eigenimage vectors is given as

\[
E_3 = \begin{bmatrix} E_2 & 0 \\ 0 & I_{p-p_1} \end{bmatrix} \in \mathbb{R}^{p \times p},
\]  

where \(I_{p-p_1}\) is an \((p - p_1) \times (p - p_1)\) identity matrix. After obtaining the rotation transform, we recompute the new eigenimage basis vectors set \(E\) as

\[
E = E_1 \times E_3.
\]

APPENDIX D
Proof of Lemma

\[
\log p(x) = \log p(x') + \log \left( \frac{p(x)}{p(x')} \right) = \log p(x') + \log \left( \frac{1}{p(x')} \sum_i w_i \exp \{-u_i(x)\} \right)
\]
\[ = \log p(x') + \log \left( \frac{\sum_i w_i \exp(-u_i(x))}{\sum_i w_j \exp(-u_j(x))} \right) \]

\[ = \log p(x') + \log \left( \frac{\sum_i w_i \exp(-u_i(x))}{\sum_i w_j \exp(-u_j(x))} \right) \]

\[ \times \exp(-u_i(x) + u_i(x')) \]

\[ \geq \log p(x') + \log \left( \sum_i \tilde{\pi}_i \times \exp(-u_i(x) + u_i(x')) \right) \]

We have used Jensen’s inequality to derive the result in the last inequality. Multiplying by \(-1\) on both sides of the last inequality results in the expression:

\[ -\log p(x) \leq -\log p(x') + \sum_i \tilde{\pi}_i \times (u_i(x) - u_i(x')) \]

\[ = G(x; x') . \]

Finally if we put \(x = x'\), this results in \(-\log p(x') = G(x'; x')\).

ACKNOWLEDGMENT

The authors would like to thank Dr. Mark Hagenmaier of the Air Force Research Laboratory, Wright-Patterson AFB, OH for use of the CFD solutions.

REFERENCES


{\small TABLE IV

<table>
<thead>
<tr>
<th>Temp. Range</th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>d</th>
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<td>T &lt; 500</td>
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<td>0.36653379313569</td>
<td>8.10262127972126e-4</td>
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<tr>
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<td>-0.003361406906565</td>
<td>1.040923104631856e-6</td>
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</table>

The table shows the estimated cubic spline coefficients that produce twice differentiable Q function. The coefficients are given for different temperature ranges. The coefficients are used to model the temperature distribution in the flow using cubic splines. The coefficients are ordered by their position in the temperature range, with the lowest temperature range first.
et al.  


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