Deep Multi-Fidelity Active Learning of High-Dimensional Outputs

Shibo Li
shibo@cs.utah.edu

Robert M. Kirby
kirby@cs.utah.edu

Shandian Zhe
zhe@cs.utah.edu

School of Computing, University of Utah
Salt Lake City, UT, 84108

Abstract

Many applications, such as in physical simulation and engineering design, demand we estimate functions with high-dimensional outputs. The training examples can be collected with different fidelities to allow a cost/accuracy trade-off. In this paper, we consider the active learning task that identifies both the fidelity and input to query new training example so as to achieve the best benefit-cost ratio. To this end, we propose DMFAL, a Deep Multi-Fidelity Active Learning approach. We first develop a deep neural network based multi-fidelity model for learning with high-dimensional outputs, which can flexibly, efficiently capture all kinds of complex relationships across the outputs and fidelities to improve prediction. We then propose a mutual information based acquisition function that extends the predictive entropy principle. To overcome the computational challenges caused by large output dimensions, we use multi-variate Delta’s method and moment-matching to estimate the output posterior, and Weinstein-Aronszajn identity to calculate and optimize the acquisition function. The computation is tractable, reliable and efficient. We show the advantage of our method in several applications of computational physics and engineering design.

1 Introduction

Many applications require us to compute a mapping from low-dimensional inputs to high-dimensional outputs. For example, topology optimization [Rozvany, 2009] aims to find an optimal structure (i.e., high-dimensional output) given several design parameters (low-dimensional input). Physical simulation uses numerical solvers to solve partial differential equations (PDEs), which maps the PDE parameters and parameterized initial/bound conditions (low dimensional input) to the high-dimensional solution field on a mesh. The exact computation of these mappings is very costly. Hence, there is an urgent need to learn these mappings from data so that we can avoid calculating from scratch every time.

However, the collection of training examples can be restricted by the (computational) resources as well. To allow a trade-off between the cost and accuracy, we can query the training examples with different fidelities. Low fidelity examples are cheap to obtain but inaccurate while high-fidelity examples much more accurate yet expensive. Note that those examples can stay in different output spaces. For instance, in physical simulation, low-fidelity examples are often generated by running numerical solvers with coarse meshes. The output dimension is smaller than that of the high-fidelity examples produced with dense meshes.

To reduce the cost while maximizing the learning performance, we develop DMFAL, a deep multi-fidelity active learning approach that can identify both the fidelity and input location to query new training examples so as to achieve the best benefit-cost ratio. To our knowledge, this is the first work that incorporates multi-fidelity queries in active learning of high-dimensional outputs. Our major contributions are summarized as follows.

- First, we propose a highly expressive deep multi-fidelity model. We use a chain of neural networks (NNs) to model the outputs in each fidelity. Each NN first generates a low-dimensional latent output, and then projects it to the high-dimensional observational space. Both the original input and latent output are fed into the NN of the next fidelity so that we can efficiently propagate information throughout the fidelities and flexibly capture their complex relationships.
- Second, we propose an acquisition function based on the mutual information of the outputs between each fidelity and the highest fidelity (at which we produce our final predictions). This can be viewed as an extension of the predictive uncertainty principle for the tradi-
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Motivational example. When we look into the query at the highest fidelity, the acquisition function is reduced to the output entropy. We found empirically that our acquisition function outperforms the popular BALD principle [Houlsby et al. 2011] adapted to the multi-fidelity setting.

- Third, we address the challenges in computing and optimizing the acquisition function. Due to the large output dimension, it is very expensive or even infeasible to estimate the required covariance and cross covariance matrices with popular Monte-Carlo (MC) Dropout [Gal and Ghahramani 2016] samples. To address this problem, we consider the NN weights in the latent output layers as random variables and all the other weights as hyper-parameters. We develop a stochastic structural variational learning algorithm to jointly estimate the hyper-parameters and posterior of the random weights. Next, we use multi-variate Delta’ method to compute the moments of the hidden outputs in each fidelity, and use moment matching to estimate a joint Gaussian posterior of the hidden outputs. We then use Weinstein-Aronszajn identity to compute the entropy of their projection — the observed high-dimensional outputs. In this way, we can analytically calculate and optimize the acquisition function in a tractable, reliable and efficient way.

For evaluation, we examined DMFAL in three benchmark tasks of computational physics (solving the classical Burger’s, Heat and Poisson’s equations), a topology structure optimization problem, and a computational dynamic fluids (CFD) application that predicts the velocity field of a flow driven by rectangular boundaries. The output dimensions of these applications vary from hundreds to hundreds of thousands. Our method consistently achieves much better learning performance with the same query cost, as compared with using random query strategies, approximating the acquisition function with dropout samples of the latent outputs, and using other acquisition functions.

2 Background

Problem setting. We assume that we can query training examples with M fidelities, which correspond to M mappings, \( \{ f_m(x) \in \mathbb{R}^{d_m} \}_{1 \leq m \leq M} \) where \( x \in X \) is an \( r \)-dimensional input, \( r \) is small, \( d_m \) is the output dimension, often very large, and \( d_m \) are not necessarily identical. In general, we assume \( d_1 \leq \ldots \leq d_M \). For instance, in structure design, the input can be the design parameters. The high fidelity examples correspond to high-resolution structures while the low fidelity ones low-resolution structures. We denote by \( \lambda_m \), the cost to query with fidelity \( m \). To perform active learning, we begin with a small set of training examples with mixed fidelities. Each step, we select both the fidelity and input location to query new training examples, so as to best balance the learning improvement and computational cost, namely, maximizing the benefit-cost ratio.

Dropout active learning. A very successful application of active learning with deep neural networks is image classification [Gal et al. 2017; Kirsch et al. 2019]. Typically, a pool of unlabeled input examples, i.e., images, is pre-collected. Each time, we rank the input examples according to an acquisition function computed based on the current model. We then query the labels of the top examples, and add them into the training set. There are two popular acquisition functions. The first one is the predictive entropy of the label,

\[
H[y|x, D] = - \sum_c p(y = c|x, D) \log p(y = c|x, D),
\]

where \( x \) is the input, and \( D \) are the training data. The other one is BALD (Bayesian active learning by disagreement) [Houlsby et al. 2011] — the mutual information between the label and model parameters,

\[
I[y, \theta|x, D] = H[y|x, D] - E_{p(\theta|D)} [H(y|x, \theta, D)],
\]

where \( \theta \) are the NN weights. The computation of these acquisition functions require us to first estimate the posterior of the NN output and weights. A popular approach is to use Monte-Carlo (MC) Dropout [Gal and Ghahramani 2016], which can be viewed as a variational inference method of Bayesian NNs. MC Dropout uses a probability \( p_i \) to randomly drop the neurons in each layer \( i \) (equivalent to zeroing out the corresponding weights) in the forward pass and performs backward pass over the remaining neurons. After training, the weights and output obtained from one such forward pass can be viewed as a sample of the approximate posterior. We can run Dropout multiple times to collect a set of posterior samples and calculate the acquisition functions by Monte-Carlo approximation.

3 Deep Multi-Fidelity Modeling for High-Dimensional Outputs

Despite its success, dropout active learning might be inappropriate for high-dimensional (continuous) outputs. When the output is a continuous vector, it is natural to use a multi-variate Gaussian posterior, \( p(y|x, D) \approx \mathcal{N}(y|\mu(x), \Sigma(x)) \), and the entropy \( H(y|x, D) \) in the acquisition functions (see [1] and [2]) require us to compute the log determinant of the covariance matrix, \( \log |\Sigma(x)| \). While we can use dropout samples to construct an empirical estimate \( \hat{\Sigma}(x) \), due to the large output dimension \( n \), the computation of this \( n \times n \) matrix and its log determinant is very expensive or even infeasible. One might seek to only estimate the variance of each individual output. However, this will ignore the strong, complex output correlations, which is critical to effectively evaluate the uncertainty and calculate the acquisition function. Furthermore, in our active learning task, we want to optimize the acquisition function to find the best input (rather than rank the inputs in a pre-collected pool). The empirical covariance estimation from random samples can
We place a standard Gaussian prior over the elements in $A$ where $\phi$ is the posterior inference and uncertainty reasoning. Given the training dataset $D = \{(x_{nm}, y_{nm})|m\}_{n=1}^{N_m}$, the joint posterior of our model is given by

$$p(W, Y|X, \Theta, s) = \prod_{m=1}^{M} \mathcal{N}(\text{vec}(W_m)|0, I) \cdot \prod_{n=1}^{N_m} \mathcal{N}(y_{nm}|A_m f_m(x_{nm}), \sigma_m^2 I),$$

where $W_m = \{W_m, \theta_m, A_m\}$ where $W_m$ is a $k_m \times l_m$ weight matrix in the latent output layer, $A_m$ is a $d_m \times k_m$ projection matrix, and $\theta_m$ the weights in all the other layers. Denote by $x_m$ the NN input, by $f_m(x)$ the latent NN output, and by $y_m(x)$ the observation. The model is defined by

$$x_m = [x; f_{m-1}(x)],$$

$$f_m(x) = W_m \phi_{\theta_m}(x_m),$$

$$y_m(x) = A_m f_m(x) + \epsilon_m,$$

where $\phi_{\theta_m}$ is the $l_m$ dimensional input to the latent output layer (therefore parameterized by $\theta_m$), and $\epsilon_m \sim \mathcal{N}(0, \sigma_m^2 I)$ is an isotropic Gaussian noise. We set $k_0 = 0$ and so $f_0(x)$ is empty; when $m = 1$, we have $x_m = x$. Note that $\phi_{\theta_m}$ can be viewed as a set of non-linear basis functions. Through their combinations via $W_m$ and $A_m$, we can flexibly capture the complex, strong relationships between the elements of $y_m$ to improve the prediction. Furthermore, the input $x_m$ is constructed by appending to the original input $x$ the latent output $f_{m-1}$, which can be viewed as a compact (or low-rank) summary of all the information up to fidelity $m - 1$. After a series of linear and nonlinear transformations, we obtain the latent output $f_m$ — the sum up to fidelity $m$ — and then generate the high dimensional observation $y_m$. In this way, we efficiently integrate the information from lower fidelities and capture the complex relationship between the current and previous fidelities by learning a nonlinear mapping, $f_m(x) = h(x, f_{m-1}(x))$, where $h(\cdot)$ is fulfilled by an NN.

We place a standard Gaussian prior over the elements in each $W_m$. Similar to (Snoek et al., 2015), we consider all the remaining parameters as hyper-parameters to ease the posterior inference and uncertainty reasoning. Given the training dataset $D = \{(x_{nm}, y_{nm})|m\}_{n=1}^{N_m}$, the joint probability of our model is given by

$$\mathcal{L}(q(W), \Theta, s) = \mathbb{E}_q \left[ \log \frac{p(W, Y|X, \Theta, s)}{q(W)} \right] = -\mathbb{KL}(q(W)||p(W)) + \sum_{m=1}^{M} \sum_{n=1}^{N_m} \mathbb{E}_q \left[ \log \mathcal{N}(y_{nm}|A_m f_m(x_{nm}), \sigma_m^2 I) \right],$$

where $\mathbb{KL}(\cdot||\cdot)$ is Kullback-Leibler divergence and $p(W)$ the prior of $W$. We maximize $\mathcal{L}$ to jointly estimate $q(W)$ and the hyper-parameters. While $\mathcal{L}$ is intractable, it is straightforward to use the reparameterization trick (Kingma and Welling, 2013) to generate parameterized samples for each $\text{vec}(W_m)$: $\mu_m + L_m \xi_m$ where $\xi_m \sim \mathcal{N}(0, I)$, substitute them into (5) to obtain a stochastic estimate of $\mathcal{L}$, and perform efficient stochastic optimization.

4 Multi-Fidelity Active Learning

4.1 Mutual Information based Acquisition Function

We now consider how to perform active learning with multi-fidelity queries. We assume that at each fidelity $m$, the most valuable training example is the one that can best improve our final prediction, namely, the prediction at the highest fidelity $M$. To this end, we propose our acquisition function

$$\text{Figure 1: Graphical representation of the deep multi-fidelity model. The low dimensional latent output in each fidelity $f_m(x)$ (1 ≤ m ≤ M) is generated by a (deep) neural network.}$$
based on the mutual information between the outputs at fidelity $m$ and $M$,

$$a(x,m) = \frac{1}{\lambda_m} \mathbb{H}(y_m(x)) \mathbb{H}(y_M(x)|D)$$

where $\lambda_m > 0$ is the cost of querying a training example with fidelity $m$. When $m = M$, we have $a(x,M) = \lambda_m \mathbb{H}(y_M(x)|D)$. Therefore, our acquisition function is an extension of the popular predictive entropy principle in conventional active learning. At each step, we maximize our acquisition function to identify a pair of fidelity and input location that give the biggest benefit-cost ratio.

### 4.2 Efficient Acquisition Function Calculation

To maximize the acquisition function (6), a critical challenge is to compute the posterior of the outputs $\{y_m\}$ in every fidelity, based on our model estimation results, $p(y_m|D) \approx q(y_m)$. Due to high dimensionality of each $y_m$ and the non-linear coupling of the latent outputs across the fidelities (see (3)), the computation is challenging and analytically intractable. To address this issue, we first consider approximating the posterior of the low dimensional latent output $f_m$, which can be viewed a function of the random NN weights $\Omega_m = \{W_1, \ldots, W_m\}$ (given the input x). We use multivariate Delta’s method (Oehler [1926], Bickel and Doksum [2013]) to compute the moments of $f_m$. Specifically, we approximate $f_m$ with a first-order Taylor expansion,

$$f_m(\Omega_m) \approx f_m(\mathbb{E}[\Omega_m]) + J_m (\mathbb{E}[\Omega_m] - \mathbb{E}[\eta_m]),$$

where the expectation is under $q(\cdot)$, $\eta_m = \text{vec}(|\Omega_m|)$, $J_m = \frac{\partial f_m}{\partial \mathbb{E}[\eta_m]}$ is the Jacobian matrix at the mean. The rationale is as follows. First, $f_m$ is linear to $W_m$, and the second-order derivative is simply 0. Second, as the NN output, $f_m$ is highly nonlinear to the random weights in previous layers, i.e., $W_j (j < m)$. Hence, we can assume the change rate of $f_m$ (e.g., gradient or Jacobian) is much greater scales than the posterior covariance of $W_j$ in the second-order term of the Taylor expansion. Note that $q(W_j)$ is much more informative and hence much more concentrated than the prior $N(0, I)$. The scale of the posterior covariance should be much less than 1. Integrating both cases, the first-order term can dominate the Taylor expansion and hence we ignore the higher order terms. Based on (7), we can easily calculate the first and second moments of $f_m$,

$$\alpha_m = \mathbb{E}[f_m] \approx f_m(\mathbb{E}[\Omega_m]),$$

$$\text{cov}(f_m) = \text{J}_m \text{cov}(\mathbb{E}[\eta_m]) \text{J}_m^\top,$$

where $\text{cov}(\mathbb{E}[\eta_m]) = \text{diag} \left( \{ \text{cov}(\text{vec}(W_j)) \}^{1 \leq j \leq m} \right)$. Then we use moment matching to estimate a joint Gaussian posterior, $q(f_m) = N(\alpha_m, \text{cov}(f_m), \text{V}_m, \text{V}_m^\top + \sigma_m^2 I)$.

The outcome entropy is $\mathbb{H}(y_m|D) = \frac{1}{2} \log |\text{A}_m \text{V}_m \text{V}_m^\top + \sigma_m^2 I| + dm \log 2 \pi e \sigma_m^2$. However, directly computing the log determinant of a $d_m \times d_m$ matrix is very expensive. We further use the Weinstein-Aronszajn identity (Kato 2013) to derive

$$\mathbb{H}(y_m|D) = \frac{1}{2} \log |\sigma_m^{-2} \text{A}_m^\top \text{A}_m + I| + dm \log \sqrt{2 \pi e \sigma_m^2}.$$

Now, the log determinant is calculated on a much smaller, $k_m \times k_m$ matrix, which is very cheap and efficient.

Using a similar approach, we can calculate the joint posterior of $f_m = [f_m; f_M]$ and then $y_m = [y_m; y_M]$. First, we view $f_m$ as a function of all the random weights, $W = \{W_1, \ldots, W_M\}$. We use the multivariate Delta’s method and moment matching to estimate a joint Gaussian posterior, $q(f_m) = N(\bar{f}_m, \mathbb{E}[V], \mathbb{V}_m)$. Specifically, we approximate $f_m$ with a first-order Taylor expansion,

$$f_m(\Omega_m) \approx f_m(\mathbb{E}[\Omega_m]) + J_m (\mathbb{E}[\Omega_m] - \mathbb{E}[\eta_m]),$$

where $\bar{A}_m = \text{diag}(\tilde{A}_m, \tilde{A}_m)$ and $\tilde{\epsilon}_m = [\epsilon_m; \epsilon_M]$. Therefore, the joint posterior of $\bar{y}_m$ is

$$q(\bar{y}_m) = N(\bar{y}_m | \bar{A}_m \bar{f}_m + \bar{\epsilon}_m, \bar{A}_m \mathbb{V}_m \bar{A}_m^\top + \mathbb{S}_m),$$

where $\mathbb{S}_m = \text{diag}(\sigma_{A_1}^2 I_{d_1}, \ldots, \sigma_{A_M}^2 I_{d_M})$. Again, we use Weinstein-Aronszajn identity to simplify the entropy computation of $y_m$ (i.e., $y_m$ and $y_M$).

$$\mathbb{H}(y_m,y_M|D) = \frac{1}{2} \log |\mathbb{S}_m^{-1} \bar{A}_m \bar{V}_m \bar{A}_m^\top + I| + \xi_m,$$

where $\xi_m = dm \log \sqrt{2 \pi e \sigma_m^2} + dm \log \sqrt{2 \pi e \sigma_M^2}$ and the log determinant is computed from a $(k_m + k_M) \times (k_m + k_M)$ matrix, which is cheap and efficient. Note that we can use matrix blocks to compute $\bar{A}_m \mathbb{S}_m^{-1} \bar{A}_m = \text{diag}(\sigma_{A_1}^2 A_1 \mathbb{A}_1, \ldots, \sigma_{A_M}^2 A_M \mathbb{A}_M)$.

Now, based on (10) and (12), we can calculate our acquisition function (6) in an analytic and deterministic way. For each fidelity $m$, we maximize $a(x, m)$ w.r.t to $x$ to find the optimal input. We can use automatic differential libraries to calculate the gradient and feed it to any optimization algorithm, e.g., L-BFGS. We then use the optimal input at the fidelity that has the largest acquisition function value to query the next training example. Our deep multi-fidelity active learning is summarized in Algorithm 1.
Algorithm DMFAL $\langle D, T, \{\lambda_m\}_{m=1}^M \rangle$

1: Train the deep multi-fidelity model $\mathbb{H}$ on the initial dataset $D$ with stochastic structural variational learning.

2: for $t = 1, \ldots, T$ do
3: Based on $\mathbb{G}$ and $\mathbb{H}$, calculate and optimize the acquisition function $a(x, m)$ to find

$$ (x_t, m_t) = \operatorname*{argmax}_{x \in X, 1 \leq m \leq M} a(x, m). $$

4: Query the output $y_t$ with fidelity $m_t$.
5: $D \leftarrow D \cup \{(x_t, y_t)\}_{m_t}$.
6: Re-train the deep multi-fidelity model on $D$.
7: end for

4.3 Algorithm Complexity

The time complexity of training our deep multi-fidelity model is $O\left(N\left(\sum_{m=1}^{M}(k_m^2 + F)\right)\right)$ where $N$ and $F$ are the total number of training examples and NN parameters, respectively. The space complexity is $O(F + \sum_{m=1}^{M}k_m^2)$, which is to store the NN parameters, and posterior mean and covariance of each random weight matrix $W_m$. The time complexity of calculating the acquisition function is $O(\sum_{m=1}^{M}d_m^2k_m^2 + k_m^2)$. Since $k_m \ll d_m$, the complexity is linear to the output dimensions. Due to the usage of the learned variational posterior $q(W)$, the space complexity of computing the acquisition function is the same as that of training the multi-fidelity model.

5 Related Work

Active learning is an important and classical machine learning topic (Settles, 2009; Dasgupta, 2011; Hanneke et al., 2014). Many methods have concentrated on active learning with kernel based models, such as Support Vector Machines (SVMs) (Cortes and Vapnik, 1995) and Gaussian processes (Rasmussen and Williams, 2006). For example, Schohn and Cohn (2000); Tong and Koller (2001) select samples that are close to the decision boundary. The labels of these samples are viewed as most uncertain to the SVM classifiers. Joshi et al. (2009) extract probabilistic outputs from SVMs and select the examples to be labeled via “Best-versus-Second-Best(BvSB)” in multi-class classification tasks. The BvSB score can be viewed as a greedy approximation to the predictive entropy. Krause et al. (2008) developed a Gaussian process active learning method for sensor placement, where the optimal locations (i.e., new input) are found by a mutual information measurement. Li and Guo (2013) used Gaussian processes to obtain an information density measure, and combine it with the entropy measure to actively query new examples for image classification. Huang et al. (2010) proposed a selection criteria that considers both the (label) uncertainty and representativeness, and performs well for SVM active learning.

Recent research in active learning focus more on deep neural networks. An important work by Gal et al. (2017) first uses Monte-Carlo (MC) Dropout (Gal and Ghahramani, 2016) to perform variational inference for Bayesian neural networks. The dropout samples can be viewed as the posterior samples of the output. These samples are then used to compute an information measure, such as predictive entropy and BALD (Bayesian Active Learning by Disagreement) (Houlsby et al., 2011), to select unlabeled examples to query. This method has achieved a great success in image classification. Following this work, Kirsch et al. (2019) developed a greedy approach to select a batch of unlabeled examples each time, so as to improve the efficiency of active learning. There are also other excellent works along this line. For example, Geifman and El-Yaniv (2017); Sener and Savarese (2018) select representative examples based on core-set search. Gissin and Shalev-Shwartz (2019) select maximally indistinguishable samples from the unlabeled pool, and the idea is reminiscent of generative adversarial networks (Goodfellow et al., 2014). Ducoffe and Precioso (2018) uses adversarial samples to calculate the distance to the decision boundary and select examples accordingly to label. Ash et al. (2019) measure the uncertainty in terms of the gradient magnitude and select a disparate batch of inputs in a hallucinated gradient space.

Our work differs from the existing studies in several aspects. First, most methods are pool-based active learning — first collect a pool of unlabeled examples, and each time it only select the examples from the pool. This is reasonable when the training input is high-dimensional or hard to generate, e.g., image classification. On the contrary, our work focuses on learning mappings from low-dimensional inputs to high-dimensional outputs, which are common in physical simulation and engineering design. To find the best training example, we optimize the acquisition function in the entire domain rather than limit the search in a discrete set. Second, most methods assume a uniform fidelity (or quality) of the training examples and so the query cost does not need to be taken into account. Our work considers the case that the training examples can be queried with multiple fidelities, resulting in different trade-offs between the cost and quality. Our goal is to best balance the cost and benefit in active learning. To our knowledge, this is the first work about multi-fidelity active learning of high-dimensional outputs. In the mean time, the large number of outputs bring in challenges of modeling, inference, and acquisition function computation, which stimulate our major contributions.

6 Experiment

6.1 Solving Partial Differential Equations

We first evaluated DMFAL in standard computational physics tasks. Specifically, we used DMFAL to predict the solution fields of three commonly used partial differential equations (PDEs): Burgers’ , Poisson’s and Heat equations (Olsen Kettle, 2011). The training examples are collected by running a numerical solver with different meshes. The more the nodes/steps to create the mesh, the higher the fidelity. The input includes the PDE parameters and/or parameterized initial or boundary conditions. The output consists of the
solution values at the mesh used in the solver. For example, a 50 × 50 mesh corresponds to a 2,500 dimensional output vector. To perform active learning, we considered two-fidelity queries for all three equations, where the sizes of the corresponding output fields are 16 × 16 and 32 × 32. In addition, we considered a three-fidelity setting for Poisson’s equation, denoted by Poisson-3, and the sizes of the output fields of the three fidelities are 16 × 16, 32 × 32, and 64 × 64, respectively. For the two-fidelity active learning, we uniformly sampled the inputs, and queried 10 training examples at the first fidelity and 2 at the second fidelity. We used those examples as the initial training dataset. Similarly, for Poisson-3, we collected 10, 5 and 2 examples in the first, second, and third fidelity as the initial training set. We generated 500 samples for test, where the test inputs were uniformly sampled from the domain. The outputs are calculated by running the solver with an even denser mesh — 128 × 128 for Burger’s and Poisson’s equations, and 100 × 100 for Heat equation — and interpolating the solution values at the target grid (Zienkiewicz et al., 1977) (this is the standard approach in physical simulation and the accuracy does not change). More details are given in the supplementary material. We ran the solvers at each fidelity for many times and calculated the average running time. We then normalized the average running time to obtain λ1 = 1, λ2 = 3 and λ3 = 10.

Competing methods. We compared DMFAL with the following active learning approaches. (1) MF-BALD, a straightforward extension of BALD (Houlsby et al., 2011) to integrate multi-fidelity queries. The acquisition function is
\[
a_{\text{MF-BALD}}(x, m) = \frac{1}{\lambda_m} \mathbb{E}(y_m(x) \mid D)
\]
\[
= \frac{1}{\lambda_m} \left( \mathbb{H}(y_m(x) \mid D) - \mathbb{E}_{p(y_m(x) \mid D)} \left[ \mathbb{H}(y_m(x) \mid W, D) \right] \right)
\]
\[
= \frac{1}{\lambda_m} \left( \mathbb{H}(y_m(x) \mid D) - \frac{d_m}{2} \log(2\pi e\sigma_m^2) \right).
\]

Note that conditioned the NN parameters, the entropy of the observed output y_m is only determined by the noise variance \( \sigma_m^2 \). (2) Dropout-latent, where we use MC dropout (Gal et al., 2017) for variational inference, each time draw 100 dropout samples for the low dimensional latent outputs \( \{f_i(x)\ldots,f_M(x)\} \) to estimate multi-variate Gaussian posteriors for each \( f_m \) and \( f_m = \{f_m; f_M\} \) (via empirical means and covariance matrices), and then follow Section 4.2 to calculate and optimize the acquisition function (6). Note that we have also used Dropout-latent. Instead, it was way worse than Dropout-latent and MF-BALD. See the details in the supplementary material. (3) MF-Random, where each time we randomly select a fidelity and then an input to query. (4) Random-F1, (5) Random-F2, and (6) Random-F3, where we stick to the first, second and third fidelity, respectively, and randomly sample an input to query each time.

Settings and results. We introduced a two-layer NN for each fidelity and used \text{tanh} as the activation function. The layer width was chosen from \{8, 16, 32, 64, 128\}. We set the same dimension for the latent output in each fidelity and used \{5, 10, 15, 20\}. For Dropout-latent, we tuned the dropout rate from \{0.1, 0.2, 0.3, 0.4, 0.5\}. All the methods were implemented with PyTorch (Paszke et al., 2019). We used ADAM (Kingma and Ba, 2014) for stochastic optimization, where the learning rate was tuned from 0.001 to 0.0001.
\{10^{-4}, 5 \times 10^{-4}, 10^{-3}, 5 \times 10^{-3}, 10^{-2}\}. We set the number of epochs to 2,000, which is enough for convergence. We conducted five runs for each method, and in each run, we queried 100 examples. We report the average normalized root-mean-square-error (nRMSE) vs. the accumulated cost in Fig. 2 and 3. The shaded region shows the standard deviation. We can see that at the beginning, all the methods have the same or comparable performance. Along with more queries, DMFAL quickly achieves better prediction accuracy, and continues to outperform all the other methods by a large margin. Therefore, DMFAL can perform much better with the same cost or achieve the same performance with the smallest cost. It is interesting to see that in Fig. 2a, while all the competing approaches have saturated early, DMFAL keeps improving its prediction accuracy. Dropout-latent and MF-BALD consistently outperform random querying strategies, demonstrating the effectiveness of the information-based acquisition functions. However, MF-BALD only computes the predictive entropy in each single fidelity (plus the entropy of the noise, see (13)), and does not consider how the low-fidelity training examples influence the final predictions (i.e., at the highest fidelity). Its inferior performance to DMFAL indicates that a straightforward extension to the original BALD can be suboptimal. The worse performance of Dropout-latent than DMFAL implies that our structural variational inference can give a better posterior estimation for the latent outputs than the stochastic estimations constructed from the dropout samples. Overall, these results have demonstrated the advantage of our deep multi-fidelity active learning approach.

6.2 Topology Structure Optimization

Next, we applied DMFAL in topology structure optimization. A topology structure is a layout of materials, e.g., alloy and concrete, in some designated spatial domain. Given the input from the outside environment, e.g., external force, we want to find an optimal structure that achieves the maximum (or minimum) interested property, e.g., stiffness. Topology structure optimization is crucial to many engineering design and manufacturing problems, including 3D printing, and design of air foils, slab bridges, aerodynamic shapes of race cars, etc. The conventional approach is to solve a constraint optimization problem that minimizes a compliance objective subject to a total volume constraint (Sigmund, 1997). However, the numerical computation is usually very costly. We aim to use active learning to learn a model that directly predicts the optimal structure, without the need for running numerical optimization every time.

![Figure 4: Prediction accuracy of active learning in topology structure optimization.](image)

![Figure 5: The predicted topology structures for 8 different loads.](image)

We considered the stress experiment in (Keshavarzadeh et al., 2018) with an L-shape linear elastic structure. The structure is subjected to a load (i.e., input) on the bottom right half and is discretized in a \([0, 1] \times [0, 1]\) domain. The load is represented by two parameters, the location (in \([0, 1]\)) and angle (in \([0, \pi]\)). The goal is to find the structure that achieves the maximum stiffness given the load. Op-
We used two fidelities to query the training examples. One uses a $50 \times 50$ mesh, the other $75 \times 75$. Correspondingly, the output dimensions are 2,500 and 5,625. The costs are measured by the average running time: $\lambda_1 = 1$, $\lambda_2 = 3$. We randomly generated 500 structures for test, where the internal solver uses a $100 \times 100$ mesh. Initially, we randomly queried 10 examples at the first fidelity and 2 at the second fidelity. We then ran all the active learning methods to query 100 examples. We conducted the experiments for five times, and report the average nRMSE along with the cost in Fig. 4. As we can see, DMFAL achieves much better prediction accuracy than the competing approaches (with the same cost). That implies our predicted structures are much closer to the optimal structures. While the performance of the other methods tended to converge early, DMFAL’s performance kept improving and the trend did not stop even when all the queries were finished. It is worth noting that MF-BALD is even worse than random query strategies. This might because the acquisition function [13] does not take into account the relationships between the fidelities, which are critical for this task.

To perform a fine-grained comparison, we visualize eight structures predicted by all the methods, after the active learning is finished. As shown in Fig. 4, DMFAL predicted much more accurate structures, which capture both the global shapes and local details, and the density of the materials is closer to the ground-truth. Although Dropout-latent captures the global shapes as well, its predictions are more blurred and miss many local details, e.g., the second to seventh structure in Fig. 4. The other methods often provided wrong structures (e.g., the first and last structure in Fig. 4), e, and f) and insufficient density (e.g., the second, third and sixth structure in 4).

### 6.3 Predicting Fluid Dynamics

Finally, we applied DMFAL in a computational fluid dynamics (CFD) problem. The task is to predict the first component of the velocity field of a flow within a rectangular domain in $[0,1] \times [0,1]$. The flow is driven by the boundaries with a prescribed velocity (i.e., input) [Bozeman and Dalton 1973]. Along with time, the local velocities inside the fluid will vary differently, and eventually result in turbulent flows. Computing these fields along with time requires us to solve the incompressive Navier-Stokes equations [Chorin 1968], which is known to be challenging to solve because of their complex behaviors under big Reynolds numbers. We considered active learning with two-fidelity queries to predict the first component of the velocity field at evenly spaced 20 time points in $[0,10]$ (temporal domain). The examples in the first fidelity were generated with a $50 \times 50$ mesh in the spatial domain (i.e., $[0,1] \times [0,1]$), and the second fidelity $75 \times 75$. The corresponding output dimensions are 50,000 and 112,500. The input is a five dimensional vector that consists of the prescribed boundary velocity and Reynold number. Fig. 6 shows examples of the field at three time points. To collect the test dataset, we randomly sampled 256 inputs and computed the solution with a $128 \times 128$ mesh. The test outputs are obtained by the cubic-spline interpolation. At the beginning, we randomly queried 10 and 2 training examples in the first and second fidelity, respectively. Then we ran each active learning method with 100 queries. We repeated the experiments for five times. The average nRMSE along with the accumulated cost is shown in Fig. 7. It can be seen that during the training, DMFAL consistently outperforms all the competing methods by a large margin. On the other hand, to achieve the same level of accuracy, DMFAL spends a much smaller cost. That means, our methods requires much less (high-fidelity) simulations to generate the training examples. This is particularly useful for large-scale CFD applications, in which the simulation is known to be very expensive.

![Figure 6: Examples of the first component of the velocity field (with contour lines) at three time points.](image)
7 Conclusion

We have presented DMFAL, a deep multi-fidelity active learning approach for high-dimensional outputs. Our deep neural network based multi-fidelity model is flexibly enough to capture the strong, complicated relationships between the outputs and between the fidelities. We proposed a mutual information based acquisition function that accounts for multi-fidelity queries. To calculate and optimize the acquisition function, we developed an efficient and reliable method that successfully overcomes the computational challenges due to the massive outputs.

References


8 Experimental Details

8.1 Solving Partial Differential Equations

Burgers’ equation is a canonical nonlinear hyperbolic PDE, widely used to model various physical phenomena, such as nonlinear acoustics (Sugimoto [1991]), fluid dynamics (Chung [2010]), and traffic flows (Nagel [1996]). Due to its capability of developing discontinuities (i.e., shock waves), Burger’s equation is used as a benchmark test example for many numerical solvers and surrogate models ([Kutluay et al., 1999], [Shah et al., 2017], [Raissi et al., 2017]). The viscous version of Burger’s equation is given by

\[ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = v \frac{\partial^2 u}{\partial x^2}, \]

where \( u \) is the volume, \( x \) is a spatial location, \( t \) is the time, and \( v \) is the viscosity. We set \( x \in [0, 1] \), \( t \in [0, 3] \), and \( u(x, 0) = \sin(x\pi/2) \) with a homogeneous Dirichlet boundary condition. The input parameter is the viscosity \( v \in [0.001, 0.1] \). Given the input, we aim to predict the solution field (i.e., the values of \( u \)) in the spatial-temporal domain \( [0, 1] \times [0, 3] \). To obtain the training and test datasets, we solve the equation using the finite element (Cabal [2014]) with hat functions in space and backward Euler in time domains on a regular mesh.

Poisson’s equation is an elliptic PDE and commonly used to model potential fields, e.g., electrostatic and gravitational fields, in physics and mechanical engineering ([Chapra et al., 2010]). The equation used in our experiment is given by

\[ \Delta u = \beta \delta(x - c), \]

where \( \Delta \) is the Laplace operator (Persides [1973]), \( u \) is the volume, \( \delta(\cdot) \) is the Dirac-delta function, and \( c \) is the center of the domain. We used a 2D spatial domain, \( x \in [0, 1] \times [0, 1] \), and Dirichlet boundary conditions. We used the constant values of the four boundaries and \( \beta \) as the input parameters, each of which ranges from 0.1 to 0.9. We solved the equation using the finite difference method with the first order center differencing scheme and regular rectangle meshes.

Heat equation is a fundamental PDE that models heat conduction over time. It is also widely used in many other areas, such as probability theory (Spitzer [1964], Burdzy et al. [2004]) and financial mathematics (Black and Scholes [1973]). The equation is defined as

\[ \frac{\partial u}{\partial t} + \alpha \Delta u = 0, \]

where \( u \) is the heat, \( \alpha \) the thermal conductivity, and \( \Delta \) the Laplace operator. In our experiment, we used a 2D spatial-temporal domain \( x \in [0, 1], t \in [0, 5] \) with the Neumann boundary condition at \( x = 0 \) and \( x = 1 \), and \( u(x, 0) = H(x - 0.25) - H(x - 0.75) \), where \( H(\cdot) \) is the Heaviside step function. We considered three input parameters — the flux rate \( \in [0, 1] \) of the left boundary at \( x = 0 \), the flux rate \( \in [-1, 0] \) of the right boundary at \( x = 1 \), and \( \alpha \in [0.01, 0.1] \). To generate the training and test examples, we solve the equation with the finite difference in the space domain and backward Euler in the time domain.

8.2 Predicting Fluid Dynamics

We also examined DMPAL in predicting the velocity field of a flow within a rectangular domain with a prescribed velocity along the boundaries (Bozeman and Dalton [1973]). This is a classical computational fluid dynamics (CFD) problem. The simulation of the flow involves solving the incompressible Navier-Stokes (NS) equation (Chorin [1968]),

\[ \rho(u \cdot \nabla)u = -\nabla p + \mu \nabla^2 u, \]

where \( \rho \) is the density, \( p \) is the pressure, \( u \) is the velocity, and \( \mu \) is the dynamic viscosity. The equation is well known to be challenging to solve due to their complicated behaviours under large Reynolds numbers. We set the rectangular domain to \( [0, 1] \times [0, 1] \), and time \( t \in [0, 10] \). The input includes the tangential velocities of the four boundaries and the Reynolds number \( \in [100, 50000] \). The output are the first component of the velocity field at 20 equally spaced time steps in \( [0, 10] \). To generate the training and test examples, we used the SIMPLE algorithm (Caretto et al. [1973]) with a stagger grid (Versteeg and Malalasekera [2007]), the up-wind scheme (Versteeg and Malalasekera [2007]) for the spatial difference, and the implicit time scheme with fixed time steps to solve the NS equation.
8.3 Using Full Dropout

In the experiment of Section 6.1 of the main paper, we have also applied MC dropout to directly generate the posterior samples of the final output in each fidelity \( \{y_m\}_{m=1}^M \). We generated 100 samples. We used these high-dimensional samples to calculate the empirical means and covariance matrices, based on which we estimated a multi-variate Gaussian posterior for each \( y_m \) and \( \bar{y}_m = [y_m, y_M] \) via moment matching. These posterior distributions are then used to calculate and optimize our acquisition function (Eq. (6) of the main paper), and multi-fidelity BALD (Eq. (13) of the main paper), in the active learning. We denote these methods by **Dropout-full** and **MF-BALD-Dropout**. We report their nRMSE vs. cost in Fig. 8 and 9 along with all the other methods. As we can see, in all the cases, **Dropout-full** is far worse than **Dropout-latent**, and even inferior to random query strategies. The prediction accuracy of **MF-BALD** is always much better than **MF-BALD-Dropout** except that in Fig. 8a, they are quite close. Those results demonstrate that the posterior distributions of the high-dimensional outputs, if fully estimated by a small number of dropout samples, are far less accurate and reliable than our method. Also, the computation is much more costly — we need to directly compute an empirical covariance matrix based on these high-dimensional samples, and calculate the log determinant.