Data efficient surrogate modeling for engineering design: Ensemble-free batch mode deep active learning for regression

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Abstract

In a computer-aided engineering design optimization problem that involves notoriously complex and time-consuming simulator, the prevalent approach is to replace these simulations with a data-driven surrogate that approximates the simulator’s behavior at a much cheaper cost. The main challenge in creating an inexpensive data-driven surrogate is the generation of a sheer number of data using these computationally expensive numerical simulations. In such cases, Active Learning (AL) methods have been used that attempt to learn an input–output behavior while labeling the fewest samples possible. The current trend in AL for a regression problem is dominated by the Bayesian framework that needs training an ensemble of learning models that makes surrogate training computationally tedious if the underlying learning model is Deep Neural Networks (DNNs). However, DNNs have an excellent capability to learn highly nonlinear and complex relationships even for a very high dimensional problem. To leverage the excellent learning capability of deep networks along with avoiding the computational complexity of the Bayesian paradigm, in this work we propose a simple and scalable approach for active learning that works in a student-teacher manner to train a surrogate model. By using this proposed approach, we are able to achieve the same level of surrogate accuracy as the other baselines like DBAL and Monte Carlo sampling with up to 40\% fewer samples. We empirically evaluated this method on multiple use cases including three different engineering design domains: finite element analysis, computational fluid dynamics, and propeller design.

1. Introduction

In the engineering and scientific community, surrogate modeling is a prevalent approach in the design process that involves computationally costly, complex simulators. Surrogate is a data-driven approximation for a physics-based simulation typically involving interpolation or regression on a set of data generated from the original simulator\cite{1}. Learning these highly complex nonlinear hyperplanes using learning models can assist human designers to find good designs much faster than traditional methods. The expected benefit of creating a surrogate is two folds: first, leverage the generalization capability of learning models to get a good approximate prediction on other designs in the design space, and second, parallel faster evaluation of design points, which will speed up the whole design decision process. Creating a surrogate for a reasonably sized design space for a complex simulation process has two main issues: first, since these simulation models and the simulation process have an iterative subroutine and consequently long simulation time, without any strategic sampling approach, the trivial randomized sampling approach to generate data becomes unavailing in high dimension design space because the number of data points needed to give reasonably uniform coverage rises exponentially- this phenomenon is infamously called the curse of dimensionality\cite{2}. The second issue is the step-sizing of the sampling i.e., without any prior information about the involved non-linearity in the solution space manifold, setting an arbitrary step size for sample selection consequently affects the quality of the collected data and trained surrogate.

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The utopian solution would be a dynamically adaptive step sizing to select samples with maximum informational value to learn these hyperplanes that produce an accurate surrogate in a few strategic samples. Traditional surrogate modeling approaches use learning models like kriging\cite{1}, Gaussian Process\cite{3}, etc., to do strategic adaptive sampling and step sizing but these learning models are not scalable for high dimensions or big design space. The recent advances in Machine Learning (ML) models, especially in Deep Learning (DL) have shown it as a promising paradigm in this scenario. Deep learning models have powerful learning capabilities, can learn in high-dimension space and automatically extract salient features, and have been used in various engineering surrogate problems\cite{1,2,3}. However, for using a deep learning model for surrogate modeling in a meaningful design space, we need to address the issue of strategic sampling and adaptive step sizing.

In most learning problem settings, we rely on theories for data modeling, which often assume that the data is provided by a source that we do not control, but we can sample from the data source. However, for a practical design problem, the data labeling/evaluation is left to the designer and which is relatively computationally expensive or slow in some complex engineering domains. In this scenario, the designer needs to be frugal and should select samples with the goal to learn as much as possible. To this end, a framework or algorithm is required that can objectively estimate the utility of candidate data points. The AL framework directly addresses this by estimating the utility of candidate data points. By combining DL with AL (this subfield of ML is called DeepAL\cite{7}), it is possible to retain the strong high dimensional learning capability of DL while also benefiting from strategic samples selected by AL. Compared with the multiple research work on Deep active learning for classification, there are only a few approaches for Deep active learning for a regression problem. For a classification problem, since the output is the probability of a class, that can be easily used with other statistical measures (like Shannon’s Entropy\cite{8} function) to create a query strategy. Many research work has leveraged it to create one or another flavor of query strategy. However, most scientific surrogate modeling problem involved in the design process are regression problems and their output is a scalar value or a vector of scalar values. In such cases, direct statistical measurement to give information about the quality of the sample cannot be deployed. To counter this, researchers took the route of the Bayesian framework to measure variance in estimation by an ensemble of predictors that can estimate uncertainty directly-such as the Bayesian Neural network\cite{9}, or to estimate uncertainty indirectly-by ensembling models\cite{10}. Bayesian methods become expensive when the number of samples is in thousands, or the input dimension exceeds 10. Ensemble methods require independent training of several models, which is also time-consuming. Another challenge in applying AL is that most AL framework works on a single sample per iteration. In contrast, retraining a neural network after each single data point is not computationally feasible. In such a scenario, although AL related-research on query strategy is quite rich, its direct application in the DL framework for a regression problems is complex. To solve adaptive sampling and step-sizing for training a deep learning model for regression problem, in this work we propose a scalable feedback-based learning architecture called ‘student-teacher’ architecture. It is an iterative learning process similar to AL paradigm in which the teacher is another neural network with the goal to find the regions where the student network is failing and can guide sampling and data generation in the next iteration. In the context of feedback-based learning, an analogy can be found in actor-critic based learning\cite{11} in Reinforcement learning\cite{12} literature.

Empirical evaluation of the proposed approach shows better accuracy of the trained surrogate model compared to other baseline methods in different engineering domains. The major contribution of this work is summarized below:

- Development of a noble approach of deep active learning for regression problems by selecting strategic samples during surrogate training to learn the input-output behavior of a function/simulator with fewer evaluations.
- Development of a scalable and easy-to-train batch mode DeepAL approach for surrogate training that is tractable as it needs to train only one main network called ‘student/learner’ and one small network called ‘teacher/guide’.
- Empirical evaluation of the proposed method on different real-world engineering design domains and comparison with other baseline methods to establish the performance gains from this novel approach in terms of sample efficiency or better accuracy.
To our knowledge, all active learning–based adaptive sampling approach for regression problem uses the Bayesian approach, which is not scalable or difficult to train for high dimensional design space. Our method of active sampling is scalable since it uses only one main network (student) and one small (in comparison to the student network) teacher network. It selects a batch of the most informative samples and automatically handles exploration-exploitation dilemmas during design exploration. This computationally scalable approach can make learning in a big design space possible, which was not possible with current approaches. Accordingly, surrogate training and trained model can make a big leap in the design automation process. We also observed that in high dimensional design space, on a given number of labeled samples the gap between the accuracy of our method and other baselines is wider in comparison to low dimensional design space. This is intuitive because space-filling sampling used in baseline methods needs combinatorial exponential samples while our approach is very strategic in labeling. The code and data used for our method is available publicly at [https://github.com/vardhah/epsilon_weighted_Hybrid_Query_Strategy](https://github.com/vardhah/epsilon_weighted_Hybrid_Query_Strategy).

The remainder of this paper is organized as follows: Section 2 talks about the related work in this field. In Section 3, we formalize the problem and discuss our methodology and baselines in detail. In Section 4, we present our experiments and evaluation of results. We conclude in Section 5 with a brief discussion of future work.

2. Related Work

Surrogate modeling in engineering design that involve regression problems is a widely studied and prevalent approach where computationally complex engineering design domains are involved in the design process[1][13]. Most of the historical work in surrogate modeling is done using learning models like kriging[1], Gaussian process[3], support vector machines (SVM)[14], random forest[15], etc. All these methods have scalability issues either in terms of data or dimensionality of design space (computational complexity is not tractable for high dimension problems or bigger samples which are needed to create a surrogate model for a meaningful design space)[10]. Due to these challenges, the surrogate modeling approach is mostly utilized for very limited design space and has very limited utility for design optimization. However, the recent ML models especially DNN-based learning architecture, can play a major role in creating a surrogate model for a very large-scale design space. The deep learning model has demonstrated the capability to scale high dimensional data, and adding more data does not increase the training computational complexity[17]. In recent times, there are many examples of ongoing efforts for creating a deep learning-based surrogate model in various engineering domains[6][18][19][20]. Instead the full potential of DNN-based surrogate model is still untapped due to the absence of any guiding principle for data generation while training the neural network-based surrogate. Labeled data in some engineering design domains like FEA (Finite Element Analysis), CFD (Computational Fluid Dynamics), etc. are very costly. In such cases, traditional sampling or DOE bases methods for sample selection are not efficient since they do not select highly informative data points in the context of modeling the behavior using surrogates.

Active Learning [21] is a heuristic–based method dedicated to obtaining as much performance gain as possible by labeling as few samples as possible. The active learning paradigm offers sampling by utilizing an information–based query function has a long history [21][22][23]. However, applying these methods directly to Deep Learning (DL) is problematic as AL literature has little to offer when the parameters of learning models are large. There is plethora of ongoing research work in integrating DL with AL: DeepAL [7]. As classification problems dominate the DL arena, most work in DeepAL is done in the context of classification problems where direct probabilistic output makes creating information-based objective function much easier [24]. Uncertainly based query strategy [25] is an important direction of AL research, but finding correct uncertainty in DL prediction for regression problems is not directly known. In such cases, researchers have resorted to a Bayesian Neural Network(BNN), i.e. an ensemble of neural networks with weight as a probability distribution [26]. Additionally in [27], authors empirically show that the previous heuristic–based AL query strategy is invalid when it is applied to DL in batch settings. For such cases, creating a batch sample query strategy [27][28] that takes both the amount of information and the diversity of the batch into the account imposes the necessity to train a family of neural networks for BNNs, which has high computation cost. For regression problems, other Bayesian frameworks especially using Kriging and Gaussian Process models [1][3] are extensively used.
However, these models are not scalable on large data and high dimensional design space. An alternative formulation of deep active learning is done by [29] using one neural network where stochastic dropout is used during prediction for uncertainty estimation (which is a Bayesian approximation to representing model uncertainty in Deep Learning[26]). Even though [29] used only one DNN for surrogate modeling, it needs multiple runs using stochastic dropouts during prediction to get the distribution of uncertainty. This creates a bottleneck as it needs thousands of runs in sequentially to make prediction for one iterations.

Existing deep active learning approaches for regression problem is coupled with the Bayesian framework, which makes it computationally complex, especially when we need to train a surrogate for a large design space. Our work is inspired by [30, 31], in which an attempt is made to learn the failure probability in the context of rare event failures in RL agents.

3. Methodology

3.1. Problem statement

Let

\[ y = f(x), x \in \mathcal{X} \subset \mathbb{R}^n, y \in \mathcal{Y} \subset \mathbb{R}^m \] (1)

be an unknown function for which we want a surrogate approximation using the training data generated by a high-fidelity simulation process. Here, \( \mathcal{X} \) represents the unlabeled data set in the design space \( \mathcal{DS} \), and \( \mathcal{Y} \) represents the solution set evaluated by the simulation process. Accordingly, in the given \( \mathcal{DS} \), we view the simulator as a nonlinear function that maps the input space to the solution space (\( \text{simulator} : \mathcal{X} \rightarrow \mathcal{Y} \)) and whose behavior we want to model using a \( k \)-parameter DNN (\( \mathcal{NN} \)). For data-driven surrogate modeling, the first step is the generation of training data.

\[ \mathcal{D}^{\text{train}} = (x_j^{\text{train}}, y_j^{\text{train}}), j = 1, 2, ..., N_{\text{train}} \] (2)

Since most engineering simulators have scalar outputs, in this work, we are interested in regression problems. The training goal is to minimize a loss function \( l() \) by using \( \mathcal{D}^{\text{train}} \) along with getting acceptable prediction accuracy on test data \( \mathcal{D}^{\text{test}} \). As some numerical simulation process is computationally very costly, it is necessary to be strategic during the training data generation process to achieve acceptable accuracy in a minimal number of training data points. This problem can be formalized as:

\[ \arg\min_{\theta} \mathbb{E}_{(x,y)}[l(\mathcal{NN}(x,\theta)|\mathcal{D}^{\text{train}}) : \mathcal{D}^{\text{train}} \subseteq \mathcal{DS}, (x,y) \in \mathcal{D}^{\text{train}} \] (3)

\[ \min N_{\text{train}} \] (4)

subject to \( \mathcal{NN}(x,\theta) = y, \forall x \in \mathcal{DS} : y \approx y^* \) (5)

Instead of a given training data set (\( \mathcal{X} \)) and its label (\( \mathcal{Y} \)), we assume that we don’t have any data apriori and the designer has to select samples for labeling. To this end, we work in a pool-based setting, where an unlabeled pool data (\( \mathcal{U} \)) is given that contains a set of candidate points in \( \mathcal{DS} \) for simulation. The heuristic-based research field called AL, if used, it tries to choose the most informative sample for evaluation on which we want to run our simulations.

\[ \mathcal{U} = \{x_j, j = 1, 2, ..., N_{\text{pool}}\} , \mathcal{U} \subset \mathcal{DS} \]

As a subfield of machine learning, AL has been well-studied, and if deployed for training a learning model attempts to do it by evaluating the fewest samples possible. For such a purpose, AL methods rely on an acquisition function (\( \mathcal{A} \)) which computes a scalar score (\( s \in \mathbb{R}^+ \)) for a trained state of the model and unlabeled pool data (\( \mathcal{U} \)).

\[ \mathcal{A}(\mathcal{NN}, \mathcal{U}) : \mathcal{U} \mapsto \mathbb{R}^+ \] (6)

The acquisition function ranks the points in \( \mathcal{U} \), which indirectly measures the utility of data points for training the surrogate. The unlabeled candidate data point with a maximum score is most appealing for maximizing the model’s performance gain in the next iteration of model training and vice-versa. Therefore, the design of the acquisition function is crucial to the performance of AL methods. For a classification
problem, the output of regression is a relative probability in such case, Shannon’s entropy function \( \bar{\text{S}} \) can be used to measure the uncertainty measurement of samples and can guide the sampling in the next iteration:

\[
\mathcal{A} = -\sum_{i=1}^{k} p(y_i | x). \log(p(y_i | x)) : p(y_i | x) = \mathcal{N}(x) \forall x \in \mathcal{U} \tag{7}
\]

Here \( k \) is the number of possible output classes of an input sample. After training at each iteration, the samples’ output likelihood is estimated using a trained surrogate, and accordingly, the acquisition value is estimated using these probability measurements and equation \( \bar{\text{S}} \). Based on these acquisition function values, samples are selected from the unlabeled pool for the next iteration of training. However, this approach does not work for a regression problem which is our interest. In a regression problem, output prediction on an unlabeled sample using a trained surrogate is a scalar value (in case of single output) or a vector of scalars (in case of multi output). In such cases, researchers took the route of measuring uncertainty in prediction. A principle way to measure uncertainty in regression problem is to use Bayesian inference. For this purpose, we start with an informed or uninformed prior and compute the posterior distribution over the model parameters,

\[
p(\theta | D^{\text{train}}) \propto p(\theta) \prod_{i=1}^{N_{\text{train}}} p(y_i | x, \theta) \text{ where } (x, y) \in D^{\text{train}} \tag{8}
\]

then we compute the posterior predictive distribution \( p(y | x, D^{\text{train}}) = \int p(y | x, \theta)p(\theta | D^{\text{train}})d\theta \) for each test point \( x \in \mathcal{U} \). The full Bayesian inference (integration) is not computationally tractable for high dimensional parameter space on the entire distribution \( p(\theta | D^{\text{train}}) \). For computational reasons, the common approach is approximate the posterior distribution by various point estimates and ensemble their outcomes to replace the integral to summation. Another alternative and indirect approach to measure uncertainty is by ensemble the predictors trained on the separate subset of data. Both scenarios require training of multiple networks. Given a family of neural networks \( \mathcal{A} \mathcal{N} \) for \( i = \{1, 2, ..., n\} \), and the prediction made on an unlabeled sample (\( \mathcal{U} \)) after a iteration of training are \( p_i = \mathcal{A} \mathcal{N}_i(x) \) for \( i = \{1, 2, ..., n\} \), an acquisition function is created using the prediction as a function of mean and variance measurement and given as:

\[
\mathcal{A} = f(\mu_i, \sigma_i) : \mu_i = \frac{1}{n} \sum_{i=1}^{n} p_i & \sigma_i^2 = \frac{1}{n} \sum_{i=1}^{n} (x - \mu_i)^2 \forall x \in \mathcal{U} \tag{9}
\]

Some example function are maximum variance, Expected Improvement, etc. By estimating the acquisition values on \( \mathcal{U} \), new samples for labeling are selected for the next iteration of training. The problem with this approach is to train multiple neural networks. In complex behavior modeling, training even one network takes a very long time. Training a family of neural networks in such a scenario is computationally tedious. We propose a different approach for deep active learning in a regression problem to avoid this situation. The proposed approach is simple, scalable and called student-teacher-based surrogate modeling. We discuss it in the next section.

3.2. Student-teacher based surrogate modeling

For designing the acquisition function (\( \mathcal{A} \)), we propose to use two networks (one regressor and another classifier). These networks are called student and teacher networks based on their abstract purpose. The goal of the student network is to learn the simulator’s behavior (\( \text{student} : \mathcal{X} \rightarrow \mathcal{Y} \)), while the goal of the teacher network is to guide the sampling and labeling for the next iteration training based on the performance of the student network. Active learning is an iterative approach and at each iteration, we train teacher and student networks. For training the student network, we first split the already labeled data \( (\mathcal{X}^{\text{labeled}}, \mathcal{Y}^{\text{labeled}}) \) into train and test data. After completion of training the student network, we create a custom dataset based on the evaluation of the student network on already labeled train and test data. For evaluation purposes, we first define a threshold for fractional error called acceptable accuracy (aa : aa \( \in [0, 1] \))

\[
\text{fractional error} = \frac{|\mathcal{Y}^{\text{labeled}} - \mathcal{Y}^{\text{predicted}}|}{|\mathcal{Y}^{\text{labeled}}|} \tag{10}
\]
The threshold value ($aa$) is a user choice that indicates the permissible maximum percentage error in predictions made by a trained student network. We declare predictions made by the student to be accurate when the fractional error is less than $aa$ and vice-versa. We chose the value of $aa = 0.05 \pm 5\%$ error for all experiments. By using this evaluation report, we label each sample with a binary failure indicator ($F$), where $F = 0$, indicates student network is able to predict on the sample within an acceptable level of accuracy otherwise $F = 1$ (in case of multi-output regression problem, we can use logical and on all outputs to indicate a failure).

$$D_{labeled} = \{x_i, I(y_i - y^*_i) \geq aa* y^*_i \} \forall x_i \in X_{labeled}, \text{where } y_i = \text{prediction}, y^*_i : \text{true label} \quad (11)$$

Using the labeled binary failure outcome data ($D_{labeled}$), the teacher network is trained to learn a failure probability distribution of the student on the entire design space ($DS$). Due to 0/1 prediction, this problem is converted into classification problem. The failure probability guides the sampling in the next iteration to the regions in $DS$ on which the student network has poor performance/ high likelihood to fail. At each iteration of learning, we retrain the student and teacher networks on further evaluated samples at each iteration until we exhaust our budget for iterations (refer to figure 1).

$$S^* = \arg\max_x f_t(x) \forall x \in U \quad (12)$$

### 3.3. Batching

As mentioned above, the AL-based approach uses one-by-one sample selection, leads to the retraining of the neural network with a minimal change in the training data. There are two problems with this: first, retraining the entire network with one added sample will take a lot of training time and ruin the benefits gained from AL. Second, frequent retraining without adding much information to data can also easily lead to over-fitting\[7\]. To address this, at each active learning iteration, we want to select a batch of samples instead of only one sample. For this purpose, we score a batch of candidate unlabeled data samples $B = \{x_1, x_2, ..., x_b\} \subseteq U$. Based on the acquisition function $A$ that is derived by trained teacher, the goal is to select a batch of data samples $B^* = \{x^*_1, x^*_2, ..., x^*_b\}$ at each active learning iteration and can be formulated as

$$B^* = \arg\max_{B \subseteq U} P(B, f_t(x)) \quad (13)$$
Here \( P \) is a policy or algorithm or heuristic that chooses a batch of samples. In this work, we explored the following policies for batching drawn from current research in AL:

1. Top-b
2. Diverse Batched Active Learning (DBAL)
3. Epsilon(\( \epsilon \))-weighted Hybrid Query Strategy (\( \epsilon \)-HQS)
4. Batched Random

Now we will explain these policies of batching and its algorithms in details.

3.3.1. **Top-b**

It is a greedy strategy, here \( b \) is the batch size at each iteration. In this approach, after evaluating the failure probability score on all unlabeled samples \( U \), top-\( b \) samples are selected that have the maximum probability of failure. The selection policy, in this case, is defined as:

\[
B^*(P = \text{top–}b) = \arg\max_{B \subseteq U, |B| = b} \sum_{x \in U} f_t(x) ; x \in U
\]  

(14)

This is a naive approach to selecting a batch of samples, and this method considers each sample independently. In such a situation, it may select highly information-rich but similar samples which collectively do not add much information to the learning process. Without considering the correlation between the samples, it may result in a wastage of the evaluation budget and make the batch samples insufficiently optimized. The goal of the most optimal batch sampling should be to add collective maximum information to the learning process. For this purpose, the goal is to select information-rich but diverse samples. The pseudo-code of top-b algorithm is given in the algorithm 1.

**Algorithm 1** Top-b in student-teacher setting

1: Require: student network \( f_s(x, \theta) \), teacher network \( f_t(x, w) \), unlabeled sample pool \( U \), number of initial samples \( M \), number of AL iterations \( T \), acceptable accuracy \( aa \), and batch size \( b \)
2: Create training data for surrogate: \( S \leftarrow M \) examples drawn uniformly randomly from \( U \) and label it.
3: Train the student model to get \( \theta_1 \) on \( S \) by minimizing \( E_S[l_{\text{MAE}}(f_s(x; \theta), y)] \) \( \triangleright \) mean absolute error loss
4: Create labeled dataset: \( D_{\text{labeled}} = \{x_i, \mathbb{I}(y_i - y^*_i) \geq aa \times y_i \} \forall x_i \in S \)
5: Train the teacher model to get \( w_1 \) on \( D_{\text{labeled}} \) by minimizing \( E_{D_{\text{labeled}}}[l_{\text{CE}}(f_t(x; w), y)] \) \( \triangleright \) binary cross entropy error loss
6: for \( t = 1, 2, ..., T \) : do
7: For all examples \( x \) in \( U \setminus S \):
   1. Compute its failure probability \( p(x) = f_t(x) \)
   2. Select set \( S_t \) such that \( \arg\max_{S_t \subseteq U \setminus S, |S_t| = b} \sum_{x \in S_t} p(x) \) and label it.
8: \( S \leftarrow S \cup S_t \)
9: Train the student model to get \( \theta_{t+1} \) on \( S \) by minimizing \( E_S[l_{\text{MAE}}(f_s(x; \theta_t), y)] \)
10: Create labeled dataset: \( D_{\text{labeled}} = \{x_i, \mathbb{I}(y_i - y^*_i) \geq aa \times y_i \} \forall x_i \in S \)
11: Train the teacher model to get \( w_{t+1} \) on \( S \) by minimizing \( E_{D_{\text{labeled}}}[l_{\text{CE}}(f_s(x; w_t), y)] \)
12: end for
13: return surrogate student model and its weights \( \theta_{T+1} \)

3.3.2. **Diverse Batched Active Learning (DBAL)**

The general approach to impart batched collective maximum information in AL literature is to include diversity in the sample selection. Wei et al.\(^{32}\) include diversity by formulating a submodular function on the distances between samples and selecting a batch of unlabeled samples, which optimizes the submodular function. Another approach to include diversity is attempted \(^{25}\) as a core-set selection problem, i.e. choosing
a set of points such that a model learned over the selected subset is competitive for the remaining data points. For this purpose, they defined a loss function called core-set loss, which is the difference between the average empirical loss over the labeled set of points and the average empirical loss over the entire data set, including unlabelled points. Since we do not have access to all the labels, the core-set loss reduction is not directly computable, consequently [25] gave an upper bound for this objective function which we can optimize. This upper bound for the loss function of the core-set selection problem is optimized by minimizing its equivalent to the k-Center problem (minimax facility location [33]). A similar approach is taken by Zhdanov [34], who proposed the batched active learning using the clustering approach and proposed to solve it as a facility location problem. Since the direct solution to the facility location problem is NP-hard, the alternative formulation using the k-center/ k-medoid algorithm is used in both [25] [34]. We took the Zhdanov [34] formulation to include diversity in the batched sample selection. K-mean cluster minimizes the below objective function to find the center of cluster \( \mu_b \) and the cluster assignment \( z_{i,b} \).

\[
\sum_{x_i \in \mathcal{U}} \sum_{b} z_{i,b} ||x_i - \mu_b||^2
\]

This clustering approach is further given informativeness about its probability to fail i.e. failure probability estimation \( p(x) : p(x) \in [0,1] \) for every unlabeled sample in \( \mathcal{U} \). This informativeness gives weight-age of different samples in clustering and the modified objective for minimization problem is defined as:

\[
\sum_{x_i \in \mathcal{U}} \sum_{b} z_{i,b} p_i(x) ||x_i - \mu_b||^2
\]

This is solved by a weighted K-means clustering algorithm. In order to improve the scalability of this approach, a pre-filtering process is adopted to select \( \beta b \) most informative samples before clustering. The good choice of \( \beta \) would depend upon data and batch size. For this experiment, we selected the same \( \beta \) values (\( \beta = 10 \) & 50) that are used in Zhdanov [34] and called it DBAL-10 and DBAL-50. The complete pseudo-algorithm is given in algorithm 2.

**Algorithm 2** DBAL in student-teacher setting

1. **Require**: student; network \( f_s(x, \theta) \), teacher network \( f_t(x, w) \), unlabeled sample pool \( \mathcal{U} \), number of initial samples \( M \), number of AL iterations \( T \), batch size \( b \), acceptable accuracy \( aa \), and parameter \( \beta \)
2. Create training data for surrogate: \( S \leftarrow M \) examples drawn uniformly randomly from \( \mathcal{U} \) and label it.
3. Train the student model to get \( \theta_1 \) on \( S \) by minimizing \( E_S[l_{\text{MAE}}(f_s(x; \theta), y)] \) \( \triangleright \) mean absolute error loss
4. Create labeled dataset: \( \mathcal{D}_{\text{labeled}} = \{ x_i, \mathbb{I}(y_i - y^*_i) \geq aa \times y_i \} \setminus x_i \in S \)
5. Train the teacher model to get \( \theta_1 \) on \( \mathcal{D}_{\text{labeled}} \) by minimizing \( E_{\mathcal{D}_{\text{labeled}}}[l_{\text{CE}}(f_t(x; w), y)] \) \( \triangleright \) binary cross entropy error loss
6. **for** \( i = 1, 2, ..., T \) **do**
   1. For all examples \( x \) in \( \mathcal{U} \setminus S \):
      1. Compute its failure probability \( p(x) = f_t(x) \)
      2. Pre-filter the top \( \beta b \) informative samples (\( I_s \)): \( \arg \max \sum_{x_i \in \mathcal{U} \setminus S|I_s| = \beta b} p(x) \)
   3. Cluster \( b \) clusters on \( I_s \) using weighted K-Means: \( \sum_{x_i \in \mathcal{U}} \sum_{b} z_{i,b} p_i(x) ||x_i - \mu_b||^2 \)
   4. \( S_t \) = select \( b \) samples closest to the cluster centers and label it.
7. \( S \leftarrow S \cup S_t \)
8. Train the student model to get \( \theta_{i+1} \) on \( S \) by minimizing \( E_S[l_{\text{MAE}}(f_s(x; \theta_i), y)] \)
9. Create labeled dataset: \( \mathcal{D}_{\text{labeled}} = \{ x_i, \mathbb{I}(y_i - y^*_i) \geq aa \times y_i \} \setminus x_i \in S \)
10. Train the teacher model to get \( \theta_{i+1} \) on \( S \) by minimizing \( E_{\mathcal{D}_{\text{labeled}}}[l_{\text{CE}}(f_t(x; w_i), y)] \)
11. **end for**
12. **return** surrogate student model and its weights \( \theta_{T+1} \)
3.4. Epsilon(ε)-weighted Hybrid Query Strategy

One new batched sample selection policy is proposed in this work which capitalizes on the solution proposed to solve the exploration versus exploitation dilemma in reinforcement learning literature [12] [35]; we call this ε-HQS. The role of a teacher in the student-teacher framework is to estimate the performance of the trained surrogate in the design space \( f_t : x \mapsto [0,1] \forall x \in DS \) by providing a failure estimate. At each iteration of training, we want to estimate the following:

\[
f^*(x) = P(f_s(x) \geq aa \ast y^*), \quad x \in DS, y^* = true \ label
\]

(17)

where \( f^* \) is the true failure probability of the student surrogates in the design space \( DS \) at the end of training. However, since we do not have true labels \( (y^*) \) for all unlabeled points in \( U \). In such a case, the goal of a teacher is to learn an approximation \( f_t \approx f^* \). We want this approximation to be as accurate as possible. However at each iteration of training, we have a limited amount of labeled data, consequently, \( D_{labeled} \) has limited information about the design space \( DS \) (a maximum up to training and testing data).

\[
f_t(x) = P(f_s(x,w)|D_{labeled}), \quad \forall x \in DS
\]

(18)

In such a case, we can only approximate \( f^* \) up to some relative accuracy (\( \rho \) approximation of \( f^* \)). It results in the biased estimation of the performance of the student network by the teacher network. The estimation/bound on \( \rho \) is an open research question, but we can increase the robustness of the teacher network and can reduce the sensitivity of mismatch between the distribution of \( f_t \) and \( f^* \). For this purpose, we introduce a two-step process: first, we filter all samples with the teacher’s prediction (likelihood to fail) more than a threshold value (samples with high probability of failure), and second, we introduce a belief weight-age on the teacher network. For this end, we introduce two hyperparameters- threshold and \( \epsilon \). Since the output layer of the teacher network is sigmoid function, we kept standard threshold of 0.5 for all experiments (i.e. select all \( x \) if \( f_t(x) \geq 0.5 \ \forall x \in DS \)). \( \epsilon \) is a belief factor, that we assign to the teacher network. \( \epsilon \) is a scalar real value ranging between 0 (indicates complete dis-belief in the teacher network’s estimate) and 1 (indicates a complete belief in teacher’s estimation) \( (\epsilon \in [0,1]) \).

\( \epsilon - \text{greedy} \) based policy is inspired by RL [12] literature, the \( \epsilon \) factor controls the balance between exploration and exploitation. Since, the teacher network does not know what it does not know - the exploration versus exploitation dilemma exists in this situation similar to RL, i.e., the search for a balance between exploring the design space to find regions where we have not explored while exploiting the knowledge gained so far by the teacher network. The fixed value of \( \epsilon \) expresses linear belief in the teacher prediction. Another famous approach is to let \( \epsilon \) go to one with a certain rate to increase our belief in the teacher with more and more labeled data available for its training in later iterations. It turns out that at a rate of \( \frac{1}{T} \) (\( T \) = number of training iterations) proved to have a logarithmic bound on the regret (maximum gain) [36]. \( \epsilon - \text{greedy} \) rule [12] is a simple and well-known policy for the bandit problem. At each iteration of active sampling, this policy selects \( \epsilon \times b \) number of samples from the filtered unlabeled data (samples that have a likelihood to fail more than the threshold) and the rest of the samples \( (1-\epsilon) \times b \) is selected uniformly randomly from leftover unlabeled samples. The complete pseudo-code for this approach is given in the algorithm[3].

3.5. Batched Random sampling

This algorithm samples a batch of random samples \( B \) from the unlabeled pool \( U \) and label it at each iteration of training. The probability distribution for the random sample selection is assumed to be a uniformly distributed within the interval \( [x_l, x_h] \) and given by :

\[
p(x) = \frac{1}{x_h - x_l}
\]

(19)

Where \( x_h \) and \( x_l \) is highest and lowest values in each dimension of design space. This is the simple batched sampling approach and has a computational complexity of \( O(1) \).

In the next section, we empirically evaluate and compare all the above-mentioned methods to train neural network-based surrogate model in three different engineering domains.
Algorithm 3 $\epsilon$-HQS

1: Require: student network $f_s(\theta)$; teacher network $f_t(x; w)$; unlabeled sample pool $\mathcal{U}$; number of initial samples $M$; number of AL iterations $T$; batch size $b$, acceptable accuracy $aa$, hyper-parameter $\epsilon$
2: Create labeled data: $S \leftarrow M$ examples drawn uniformly randomly from $\mathcal{U}$ and label it.
3: Train the student model to get $\theta_1$ on $S$ by minimizing $E_S[l_{MAE}(f_s(x; \theta), y)]$
4: Create labeled data: $D_{labeled} = \{x_i, \|y_i - y_i^*\| \geq aa \times y_i\} \forall x_i \in S$
5: Train the teacher model to get $w_1$ on $D_{labeled}$ by minimizing $E_{D_{labeled}}[l_{CE}(f_s(x; w), y)]$
6: for $t = 1, 2, ..., T$ do
7:   For all examples $x$ in $\mathcal{U}$ \ $S$
8:      1. Compute its failure probability $p(x) = f_i(x)$
9:      2. $X_f = \{x \mid p(x) \geq 0.5\}$ \ samples with high failure probability
10:     3. $X_{sel} = \text{Choose } (\epsilon \times b) \text{ number of samples uniformly randomly from } X_f.$
11:     4. $S \leftarrow S + X_{sel}$
12:     5. $X_{rest} = \text{Choose } (1 - \epsilon) \times b \text{ number of samples uniformly randomly from } \mathcal{U} \ \setminus X_{sel}$
13:     6. $S \leftarrow S + X_{rest}$
14:    end for
15: return surrogate student model and its weights $\theta_{T+1}$

4. Experiments and Evaluation

4.1. Experimental setup

In each experiment, we follow the same procedure as explained below. Since we are interested in a pool-based setting where we assume that we already have collected a pool of unlabeled input data ($\mathcal{U}$) and during the selection process of data for training, we remove the budgeted data per iteration ($b$) from the pool and label it. For a given total number of iterations of the active learning ($T$), entire procedure is outlined as below:

1. Warm-up stage: Selection of initial data set (selected randomly from the pool) and get its label to create a training data $D_{train}$. Initialize the training weights, bias, and learning hyper-parameters. Initialize AL iteration counter $t$.

2. For each iteration of the AL :
   While $t \leq T$:
   (a) The student network is trained on $D_{train}$. After completion of training, the train and test data is evaluated on the trained student model.
   (b) The labeled data set is created and used to train the teacher network.
   (c) The score/ failure probability is computed using the trained teacher network on leftover pool data $\mathcal{U}$.
   (d) The query policy is deployed on the computed failure probability to select the new batch of candidate samples ($S_{candidate}$) for training in the next iteration.
   (e) Exclude $S_{candidate}$ from corresponding $\mathcal{U}$ : $\mathcal{U} := \mathcal{U} \ \setminus S_{candidate}$
   (f) Get the label ($L$) for $S_{candidate}$ and create newly added data. $D_{new} = S_{candidate}, L_{candidate}$
   (g) Add $D_{new}$ to $D_{train}$: $D_{train} := D_{train} \cup D_{new}$
For evaluating the performance of trained student surrogate, we used the left-over data ($U \setminus D_{train}$) as our test data and evaluated the student surrogate after each iteration of active learning. To rigorously evaluate our approach and to ensure the performance consistency, we ran each algorithm multiple times (every time with different random seeds) and averaged their result.

4.2. Metrics

For testing the performance of the trained surrogate model, we choose our evaluation metric as fraction of test predictions that are within acceptable accuracy, we defined a regression output as acceptable if it is within 5% of error (+/- 5% error) i.e.,

$$\text{Accuracy} = \frac{\sum_{i=1}^{N_{test}} I(|y_i - y^*_i| \leq 0.05 \times |y^*_i|)}{N_{test}}$$

(20)

Here $y_i$ is a prediction on $i^{th}$ test sample with ground truth $y^*_i$ and $N_{test}$ is the total number of samples in the test data. Since other accuracy metrics like MSE/MAE do not explain whether the error value is due to a generalization error or outliers, our chosen metric gives a better understanding of prediction results. During the surrogate training, we choose $L1$ loss (MAE) as our optimization objective for the student network. We treated the optimization objective as a hyper-parameter, tested both $L1$ loss (MAE) and $L2$ loss (MSE) and observed better performance on test data using MAE. For training the teacher network, our loss function was binary cross-entropy, since the teacher’s goal is to create a pass-fail (0-1) probabilistic map.

4.3. Surrogate modeling in Engineering design domains

We take three different use cases of real-world engineering problems (multi input - single output regression problem) of surrogate modeling. The pool data is accumulated either by generating data from the available open-source simulators or taken from already collected baseline data from prior works. In the Finite Element Analysis (FEA) domain, we took the data generated by Vardhan et al. [4]. It uses FreeCAD[37] which is a toolbox for parametric 3D CAD designs and has numerical solvers like CalculiX for the FEA analysis. In the propeller design domain, we used the pool data generated by [6]. It uses the openProp numerical simulation tool for designing a propeller. OpenProp[38] is a computational tool for designing and analyzing marine propellers and horizontal-axis turbines based on the vortex lattice lifting line methods. In the CFD domain, data generation is done using an integrated tool chain comprises of FreeCAD[37] (for CAD modeling) and OpenFOAM[39] (for computational fluid dynamics solver). In all three cases, we want to replace a physics-based simulation process with a computationally cheap DNN-based surrogate model for a given design space ($DS$). For this end, we want to model the relationship between input (design parameters) and output (behavior of interest) by a neural network. By training a neural network in a given design space, we want to capitalize on the excellent generalization capability of the neural network and can make predictions on other designs in the design space without running the actual simulation. Accordingly, it will result in huge savings in computational cost and can get the design’s behavior of interest in almost negligible time in comparison to running simulation. In the FEA domain, the learning goal is to train a surrogate to predict the maximum Von-mises stress (which determines the hull’s integrity when submerged at a depth) in the capsule-shaped pressure vessel used in an underwater vehicle [4]. In the propeller domain, the goal is to train a surrogate to predict the propeller’s efficiency on the given requirement and geometric design [6]. In the CFD domain, the surrogate learning goal is to predict the drag force on a given UUV (Unmanned Underwater vehicle) hull shape defined by hull parameters. The size of the design space (dimensionality and the extension) dictates the amount of data required for training in each domain. Larger and high-dimensional design spaces need more labeled samples for surrogate training and vice versa. For all experiments, we chose a reasonable big-size design space and collected or labeled a reasonable amount of data for experimentation. We aim to evaluate the performance of all the above-mentioned sampling approaches in these real-world design domain problems.

4.3.1. Pressure vessel design problem using Finite Element Analysis

Problem setting and numerical method: Static stress analysis is the most common type of structural integrity analysis of the sub-sea pressure vessel. A subsea pressure vessel contains dry components like electronics, batteries, sensors, and various underwater equipment. During the design phase of the vessel, these pressure
vessels are tested by subjecting it to external pressure to test the integrity of the design during sub sea operation and to find an optimal vessel design that can withstand the operating pressurized environmental conditions (generally optimal designs are the thinnest possible design). For the parametric design of the vessel, \[4\] chose a cylindrical vessel with hemispherical end-caps. This simplified geometry allows for an efficient distribution of the external pressure. Cylindrical Pressure vessel has wide applications in thermal and nuclear power plants, process and chemical industries, space and ocean depths, and fluid supply systems in industries[10]. The material that is used in this research study is aluminum alloy (\(Al - 6061T6\)) which is a widely used material for sub-sea pressure vessel design with material properties (density= 2700 Kg/m\(^3\), Young’s modulus= \(69 \times 10^6\) Pa, Poisson ratio=0.33) \[4\]. The accuracy of the FEA is highly dependent on the mesh employed. For getting an accurate result, an automated process of refining the mesh and evaluating the results is carried on until the result stabilizes and further refinement does not change the output\[4\].

These design parameters and the depth of the sea (which determines the applied external pressure to the vessel) are parameterized and a combination of these parameters creates a design space. For estimation of applied crush pressure, the following formulation is being used with water density as open sea density 1027 kg/m\(^3\):

\[
\text{External pressure} = \rho \times g \times \text{depth} \times \text{safety factor}
\]  

The value of the safety factor is taken to 1.5. For a given internal radius of the cylinder (\(a\)), uniform thickness of vessel (\(t\)) , the outside radius (\(b = a + t\)) , the internal pressure by \(p_i\), and the external pressure by \(p_o\) the tangential and radial stresses are given by \[41\]:

\[
\sigma_t = \frac{p_i a^2 - p_o b^2 + a^2 b^2 (p_i - p_o) / r^2}{b^2 - a^2} \tag{22}
\]

\[
\sigma_r = \frac{p_i a^2 - p_o b^2 - a^2 b^2 (p_i - p_o) / r^2}{b^2 - a^2} \tag{23}
\]

These equations of radial and tangential stress as a function of radius are known as Lamé’s equations. Axial or longitudinal stress for this closed-end cylinder can be found by force equilibrium condition and is given by:

\[
\sigma_l = \frac{p_i a^2 - p_o b^2}{b^2 - a^2} \tag{24}
\]

In this experiment setting, it assumed to have only external pressure i.e. \(p_i = 0\). In such a case, the stress equations as a function of radius can be written as :

\[
\sigma_t = \frac{-p_o b^2}{b^2 - a^2} \left[ 1 + \frac{a^2}{r^2} \right] \tag{25}
\]

\[
\sigma_r = \frac{-p_o b^2}{b^2 - a^2} \left[ 1 - \frac{a^2}{r^2} \right] \tag{26}
\]

\[
\sigma_l = \frac{-p_o b^2}{b^2 - a^2} \tag{27}
\]
| Parameter          | Symbol | Minimum | Maximum |
|--------------------|--------|---------|---------|
| Depth of the sea   | $D_{sea}$ | 0 m   | 6000 m |
| Length             | $L$    | 50 mm  | 600 mm |
| Radius             | $a$    | 1 mm   | 1850 mm|
| Thickness          | $t$    | 50 mm  | 600 mm |

Table 1: Design Space: Range of design parameters for surrogate modeling - FEA domain

All these three stresses represent the three principal stresses acting on a cylinder. Hence the Von-mises stress (also known as equivalent stress $\sigma_{equ}$) is estimated by using three principal stresses and given by:

$$\sigma_{equ} = \sqrt{\frac{(\sigma_l - \sigma_i)^2 + (\sigma_i - \sigma_r)^2 + (\sigma_r - \sigma_l)^2}{2}}$$  \(28\)

Figure 3 shows the outcome of one of the simulation experiments using a UUV hull design simulation outcome in OpenFOAM using above mentioned setting and methodology.

Figure 3: Example FEA simulation experiment result. (tested at sea depth =500 meters, the applied crushing pressure is calculated for open seawater density with safety factor 1.5 resulting in crushing pressure of 7.5MPa. The estimated maximum Von-mises stress was 37MPa which is much less than the yield stress of ($Al-6061T6$) which is 69MPa). The Hull shape parameter for this design: L: 100 mm, $a$: 40 mm, $t$: 10 mm, and $D_{sea}$: 500 meters.

Design space and data generation  The design space for this experiment is composed of 4 variables ($D_{sea}, L, R, t$) (refer table 1). From this design space, 11311 randomly sampled data points and ran the FEA simulation to get the maximum Von-mises stress. We use this as our pool data. The sample labeling cost in terms of evaluation time is 200 sec/sample. At each iteration of training the surrogate model, we chose 50 samples ($b = 50$) from the pool of collected data and conducted 50 AL iterations on all above mentioned approaches, that resulted in 2500 evaluated samples used for training the surrogate.

Results: Figure 3 and table 2 shows the accuracy result of trained surrogates on the test data using different strategic sampling methods. It can be seen that all $\epsilon$-HQS methods (with different values of $\epsilon$) perform better than other strategic sampling-based surrogate models. DBAL and Top-B methods perform worse than the batched random sampling method due to not handling bias and diversity properly during sample selection.
In the figure 5, we show the comparison between batched random sampling strategy with the $\epsilon$ method with logarithmic varying $\epsilon \ (\epsilon - \text{greedy})$. It is empirically observed in this domain to get similar surrogate accuracy as the best-performing baseline (batched random) we need 42% fewer samples. Since the time for training of teacher network and making inferences on prediction is very cheap (approx 120 seconds per iteration) in comparison to the simulation time (200 Sec), it saves days of sample labeling/simulation time. Since the time for training of teacher network and making inferences on prediction is very cheap (approx 120 seconds per iteration) in comparison to the simulation time (approx 200 seconds per sample), it saves days of sample labeling/simulation time.

4.3.2. **Propeller design using lifting line method using openprop**

**Problem setting and Numerical method:** A propeller is a widely used mechanical design that converts rotational energy into thrust. The performance of a propeller depends upon its geometrical characteristics...
### Table 2: Accuracy of trained surrogate after exhausting the training budget in FEA domain: after iteration=50,budget/iteration=50 (Total budget = 2500)

| Sampling strategy | Accuracy |
|-------------------|----------|
| Random            | 83.76%   |
| top-b             | 83.11%   |
| DBAL-10           | 57.28%   |
| DBAL-50           | 47.92%   |
| ϵ-greedy         | 86.47%   |
| ϵ = 0.25        | 85.85%   |
| ϵ = 0.50        | 87.01%   |
| ϵ = 0.75        | 86.96%   |
| ϵ = 1.0         | 87.56%   |

and physical parameters. For example, [38] considers the number of blades (Z), propeller’s diameter (D), chord radial distribution (C/D), pitch radial distribution (P/R), and hub diameter (Dhub) as geometrical characteristics and thrust coefficient (Ct), power coefficient (Cp) and advance ratio (J) as governing physical parameters. For a given thrust requirement at well-defined operational points (e.g., cruising speed and the actuator’s spinning rate (RPM)), the goal of a designer is to search for the optimal geometric characteristics than can fulfill the thrust requirement at maximum efficiency (E). The numerical tool used for propeller design in this work is openprop [38]. Openprop is a moderately-loaded lifting line theory-based propeller blade design method with trailing vorticity aligned to the local flow velocity. The goal of the propeller design optimization procedures in openprop is to determine the optimum circulation distribution along the span of the blade on given inflow conditions and blade 2D section properties. For a given required thrust $T_S$, the openprop uses Coney’s formulation [42] to determine produced torque $Q$, thrust $T$, and circulation distribution $\Gamma$. For optimization, an unknown Lagrange multiplier ($\lambda_1$) is introduced to perform circulation optimization to get an optimal design. For this purpose, an auxiliary function is defined as below:

$$H = Q + \lambda_1(T - T_s)$$  \hspace{1cm} (29)

If $T = T_S$ then a minimum value of $H$ coincides with a minimum value of $Q$. To find the minimum, the partial derivative with respect to unknowns are set to zero.

$$\frac{\partial H}{\partial \Gamma(i)} = 0 \text{ for } i = 1, 2, ..., M$$  \hspace{1cm} (30)

$$\frac{\partial H}{\partial \lambda_1} = 0$$  \hspace{1cm} (31)

These $M$ system of equations are non-linear and an iterative approach is used to solve it by freezing other variables and linearizing the system of equations with linearized unknowns $\Gamma, \lambda_1$. The system of equations 30 and 31 are solved for the linear $\Gamma, \lambda_1$, and the new linearized circulation distribution $\hat{\Gamma}$ is used to update the flow parameters. This process is repeated until convergence which does yield an optimized circulation distribution and a physically realistic design. For more details on numerical methods, refer [38, 42].

**Design space and data generation:** We used the design space used by Vardhan et al [6]. Since the evaluation of each design is cheap and the dimensionality of the problem is high (14 dimensions), [6] generated approximately 200000 valid designs as pool data. For surrogate training, at each iteration of training, we chose 50 samples and trained the surrogate for 50 iterations same as FEA domain.

**Results:** Figure 7 and table 3 show the accuracy result of trained surrogates on the test data using different strategic sampling methods. It can be seen that all $\epsilon$ weighted methods perform better than other strategic sampling-based surrogate modeling. DBAL50, DBAL10, and Top-B perform worse than the random batch uniform sampling method. Figure 8 shows the comparison between batched random sampling strategy when compared with our proposed method with logarithmic varying $\epsilon$ (no parameter). It is empirically observed
in this domain to get similar surrogate accuracy as the best performing baseline (batched random) but with 32% fewer samples. It can be also seen that the prediction accuracy gap between the best $\epsilon - HQS$ method and the best baseline method (batched random in this case) is more than 12%. In this domain, the labeling cost is not much but the goal of inclusion of this domain was to analyze the performance of this approach in high dimensional problems. A wider gap in this example domain reflects that in high dimension problems (14 dimensions in this case) the $\epsilon - HQS$ based $\epsilon$-greedy is more sample efficient while sample labeling by taking strategic samples.

4.3.3. **UUV hull design using CFD analysis**

*Problem setting and Numerical method:* In the design process of a UUV’s hull, the drag resistance has most dominant effect and the goal of design optimization is to minimize the drag resistance for a given set of design
Figure 8: The mean and variance of test accuracy using $\epsilon$-greedy ($\epsilon$ - HQS with logarithmic increasing $\epsilon$) and DBAL50 (Diverse Batch Active Learning with $\beta=50$) strategy

| Sampling strategy | Accuracy |
|-------------------|----------|
| Random            | 55.07%   |
| Top-b             | 31.83%   |
| DBAL-10           | 35.84%   |
| DBAL-50           | 36.66%   |
| $\epsilon$-greedy | 63.9%    |
| $\epsilon = 0.25$ | 67.18%   |
| $\epsilon = 0.50$ | 63.9%    |
| $\epsilon = 0.75$ | 60.92%   |
| $\epsilon = 1.0$  | 58.01%   |

Table 3: Accuracy table in propeller design domain: iteration=50,budget/iteration=50 (Total budget = 2500)

requirements. For the design of the hull, we used the most common modern hull design, the “Myring” type hull profile. It has three components - nose, tail, and cylindrical body. The shape of the nose and tail are parameterized and given by equations:

$$r_1(x) = \frac{1}{2}D \left[ 1 - \left( \frac{x-a}{a} \right)^2 \right]^{\frac{1}{4}}$$ \hspace{1cm} (32)

$$r_2(x) = \frac{1}{2}D - \left[ \frac{3D}{2c^2} - \frac{\tan \theta}{c} \right] (x - a - b)^2 + \left[ \frac{D}{c^3} - \frac{\tan \theta}{c^2} \right] (x - a - b)^3$$ \hspace{1cm} (33)

For drag estimation of a hull design, Computational Fluid Dynamics (CFD) based numerical simulation that solves the Navier-Stokes equation, or its variant is used. In this research work, we used the time-averaged variant of the Navier-Stokes (NS) equation called Reynolds Averaged Navier Stokes (RANS) with $k – \omega$SST turbulence model for drag estimation. For this purpose, an open-source simulation tool called OpenFOAM is used. The continuity equation and Navier–Stokes equation for an incompressible are described as

$$\rho \frac{d\vec{v}}{dt} = -\nabla p + \mu \nabla^2 \vec{v} + \rho \vec{g}$$ \hspace{1cm} (34)

$$\nabla \cdot \vec{v} = 0$$ \hspace{1cm} (35)
with \( v \) as the velocity field, \( \mu \) as the fluid’s viscosity, \( p \) as the pressure, \( \rho \) as the density, and \( g \) as the gravitational acceleration. For turbulence physics, \( k - \omega \) shear stress transport (\( k - \omega \) SST) mathematical formulation was used. The mathematical model of the \( k - \omega \) SST model used in OpenFOAM is given by \[45\] and formulated below:

\[
\frac{\partial (\rho k)}{\partial t} + \frac{\partial (\rho U_i k)}{\partial x_i} = P_k - \beta^* \rho k \omega + \frac{\partial}{\partial x_i} \left[ (\mu + \sigma_k \mu_t) \frac{\partial k}{\partial x_i} \right]
\]

(36)

\[
\frac{\partial (\rho \omega)}{\partial t} + \frac{\partial (\rho U_i \omega)}{\partial x_i} = \alpha \rho S^2 - \beta \rho \omega^2 + \frac{\partial}{\partial x_i} \left[ (\mu + \sigma_\omega \mu_t) \frac{\partial \omega}{\partial x_i} \right] + 2(1 - F_1)\rho \sigma_{w2} \frac{1}{\omega} \frac{\partial k}{\partial x_i} \frac{\partial \omega}{\partial x_i}
\]

(37)

The blending function \( F_1 \) is defined by:

\[
F_1 = \tanh \left\{ \min \left[ \max \left( \sqrt{k} \beta^* \omega \frac{500v}{y^2 \omega}, \frac{4\rho \sigma_{w2} k}{CD_{k\omega} y^2} \right) \right] \right\}^4
\]

(38)

with \( CD_{k\omega} = \max \left( 2\rho \sigma_{w2} \frac{1}{\omega} \frac{\partial k}{\partial x_i}, 10^{-10} \right) \) and \( y \) is the distance to the nearest wall.

\( F_1 \) is equal to zero away from the surface (\( k - \epsilon \) model) and switches over to one inside the boundary layer (\( k - \omega \) model). The turbulent eddy viscosity is defined as follows:

\[
v_t = \frac{a_1 k}{\max(a_1 \omega, SF_2)}
\]

(39)

where \( S \) is the invariant measure of the strain rate and \( F_2 \) is a second blending function defined by:

\[
S = \frac{1}{2} \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right)
\]

(40)

\[
F_2 = \tanh \left[ \left[ \max \left( \sqrt{\frac{2}{\beta^* \omega y}}, \frac{500v}{y^2 \omega} \right) \right]^2 \right]
\]

(41)

A limiter is used in the \( k - \omega \) SST model to prevent the build-up of turbulence in stagnation regions:

\[
P_k = \mu_t \frac{\partial U_i}{\partial x_j} \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \rightarrow \tilde{P}_k = \min(P_k, 10 \beta^* \rho k \omega)
\]

(42)

All the constant are computed by a blend from the corresponding constants of \( k - \epsilon \) and \( k - \omega \) model via \( \alpha = \alpha_1 F + \alpha_2 (1 - F) \) etc. the constant for this model are: \( \beta^* = 0.09, \alpha_1 = 0.31, \beta_1 = 0.075, \sigma_{k1} = 0.85, \sigma_{\omega1} = 0.5, \alpha_2 = 0.44, \beta_2 = 0.0828, \sigma_{k2} = 1, \sigma_{\omega2} = 0.856 \). The standard Dirichlet boundary conditions
were used for all simulations. The inlet velocity inlet boundary condition is applied at the inflow, and a zero pressure at the outlet boundary condition was applied at the outflow. A no-slip boundary condition was applied to the hull surface and the remaining surfaces, consisting of the side wall, symmetry wall, and far field, were set to symmetry. Simulations were performed at a flow speed of 2 m/s and the assumed inflow intensity level was 4%, assuming medium turbulence since it is a low-speed flow. Initial values for \( k \) and \( \omega \) is the estimated approximately \( = 0.01 \text{ m}^2/\text{s}^2 \) and 57 per sec. We assumed the Newtonian model which assumes constant kinematic viscosity and we assigned this value to 1.7 mm$^2$/sec.

**Design space and data generation** We tried to cover the design space for a small UUV shape. We used a Myring hull-based parametric design, and for data generation, the hull shape parameter is randomly sampled from the design space from the range mentioned in the design space (refer to table 4). The number of generated data points was 3021.

Since, in this case, we have a small data pool, at each iteration of training, we chose 10 samples from the pool of collected data. We conducted this iterative training for 50 iterations, which resulted in 500 samples. While choosing samples at each iteration, we deployed all the policies mentioned above for batching.

![Output steady state pressure field of one of the simulation.](image)

**Table 4:** Design Space: Range of design parameters for surrogate modeling-CFD domain

| Parameter                  | Symbol | Minimum | Maximum |
|----------------------------|--------|---------|---------|
| Diameter of middle section | \(d\)  | 50 mm   | 200 mm  |
| Length of nose section     | \(a\)  | 50 mm   | 600 mm  |
| Length of middle section    | \(b\)  | 1 mm    | 1850 mm |
| Length of tail section      | \(c\)  | 50 mm   | 600 mm  |
| Index of nose shape         | \(n\)  | 1.0     | 5.0     |
| Tail semi-angle             | \(\theta\) | 0°     | 50°     |
| Total length                | \(l = a + b + c\) |

Results: Figure 11 and table 5 shows the accuracy result of trained surrogates on the test data using different sampling methods. It can be seen that all \( \epsilon - HQS \) methods have better accuracy on test data than other sampling approaches for surrogate modeling. In this domain, DBAL-50 performed slightly better than the batched random sampling but still less than all \( \epsilon - HQS \) methods. The Top-B approach performs worse than all other approaches due to a lack of consideration of diversification in sample selection. Figure 12 shows the accuracy of DBAL-50 sampling strategy-based trained surrogate and \( \epsilon - HQS \) with logarithmic varying \( \epsilon \) sampling-based trained surrogate on multiple runs across all iterations. It shows the mean accuracy as well as the variance in accuracy prediction. The predicted test accuracy performance suggests that empirically in
Figure 11: The comparison of expected/mean test accuracy of trained surrogate in CFD domain using all proposed approaches at the different iterations of training. DBAL50 (Diverse Batch Active Learning with $\beta=50$), DBAL10 (Diverse Batch Active Learning with $\beta=10$), random (batch uniformly random), $\text{ep}_{0.25}$ ($\epsilon$-HQS with constant $\epsilon=0.25$), $\text{ep}_{0.5}$ ($\epsilon$-HQS with constant $\epsilon=0.5$), $\text{ep}_{0.75}$ ($\epsilon$-HQS with constant $\epsilon=0.75$), $\text{ep}_{1}$ ($\epsilon$-HQS with constant $\epsilon=1.0$), $\text{ep}_{\text{greedy}}$ ($\epsilon$-HQS with logarithmic increasing $\epsilon$).

Figure 12: The mean and variance of test accuracy using $\text{ep}_{\text{greedy}}$ ($\epsilon$-HQS with logarithmic increasing $\epsilon$) and DBAL50 (Diverse Batch Active Learning with $\beta=50$) strategy.
### Table 5: Accuracy table in CFD design domain: iteration=50, budget/iteration=10 (Total budget = 500)

| Sampling strategy | Accuracy |
|-------------------|----------|
| Random            | 94.27%   |
| top-b             | 88.33%   |
| DBAL-10           | 90.55%   |
| DBAL-50           | 95.09%   |
| ϵ-greedy          | 96.81%   |
| ϵ = 0.25          | 95.93%   |
| ϵ = 0.50          | 96.97%   |
| ϵ = 0.75          | 96.67%   |
| ϵ = 1.0           | 97.09%   |

This domain, to get similar surrogate accuracy as alternative policy-based best-performing approach (DBAL-50), $\epsilon - HQS$ with non-parametric $\epsilon$-greedy approach needs approx 20% fewer samples. Since the time for training of teacher network and making inferences on prediction is very cheap (approx 120 seconds per iteration) compared to the simulation time (approx 300 seconds per sample), it saves days of sample labeling/simulation time.

### 5. Conclusion and Future Work

In this work, we developed and evaluated a novel deep active learning approach for data-efficient surrogate modeling in regression problems. This method is computationally tractable and scalable since it does not uses an ensemble of learning models for query design. We brought knowledge and approaches from the current research works in active learning to increase collective information/diversity in a batch learning setting and designed algorithms based on it. When we compared these methods with different benchmarks and generated data sets, we found that $\epsilon - HQS$ outperforms all of them in all cases. We also observed that as the dimension of the problem increases, the performance gap between $\epsilon - HQS$ and other baseline become wider. This is a new paradigm for deep active learning in a regression problem. For future work, there are multiple directions that would be interesting to look into:

1. To understand the effect of batch size on the performance of this approach. In this work, we kept a fixed batch size and a reasonable budget. We believe a smaller batch size will improve the performance by increasing collective information, although it may increase the training computational cost. To study and find an approach for selecting an ideal batch size would be interesting and useful.

2. To provide a theoretical guarantee or bounds (upper and lower) on the performance of the $\epsilon - HQS$ approach.

3. To design and work towards new batching policies or algorithms that can further improve sample efficiency.

4. To test this approach on various other use cases like multi-output regression problems, image based regression problems etc.

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