A DATA-DRIVEN FEATURE SELECTION AND MACHINE-LEARNING MODEL BENCHMARK FOR THE PREDICTION OF LONGITUDINAL DISPERSION COEFFICIENT

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ABSTRACT

Longitudinal Dispersion (LD) is the dominant process of scalar transport in natural streams. An accurate prediction on LD coefficient ($D_l$) can produce a performance leap in related simulation. The emerging machine learning (ML) techniques provide a self-adaptive tool for this problem. However, most of the existing studies utilize an unproved quaternion feature set, obtained through simple theoretical deduction. Few studies have put attention on its reliability and rationality. Besides, due to the lack of comparative comparison, the proper choice of ML models in different scenarios still remains unknown. In this study, the Feature Gradient selector was first adopted to distill the local optimal feature sets directly from multivariable data. Then, a global optimal feature set (the channel width, the flow velocity, the channel slope and the cross sectional area) was proposed through numerical comparison of the distilled local optimums in performance with representative ML models. The channel slope is identified to be the key parameter for the prediction of LDC. Further, we designed a weighted evaluation metric which enables comprehensive model comparison. With the simple linear model as the baseline, a benchmark of single and ensemble learning models was provided. Advantages and disadvantages of the methods involved were also discussed. Results show that the support vector machine has significantly better performance than other models. Decision tree is not suitable for this problem due to poor generalization ability. Notably, simple models show superiority over complicated model on this low-dimensional problem, for their better balance between regression and generalization.

Keywords
Longitudinal dispersion coefficient · Feature selection · Feature gradient selector · Tree-structured Parzen Estimator · Benchmark

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1 Introduction

Streams are fragile systems which can be influenced by various physical, chemical and biological factors. In problems such as contaminant spills, sewage disposal or water disinfection, the understanding of longitudinal dispersion coefficient ($D_l$) is crucial\[1\]. $D_l$ is the core variable in the advection diffusion equation (ADE), which is often adopted to describe processes dominated by dispersion. The importance of $D_l$ has triggered various attempts on the prediction of $D_l$ with different methodologies.

Previous studies on LDC can be roughly divided into three branches according to the used methods (Fig. 1): the analytical\[2, 1, 3, 4\], the statistical \[5, 6, 7, 8\] and the machine learning (ML) driven research\[9, 10, 11\]. The ML-driven research can be further divided into explicit and implicit studies by whether a symbolic model can be proposed. Due to robust performance and applicability to big data, ML techniques have gained more interest in prediction of $D_l$ than the other two types of methods.

In ML-driven studies, the explicit method can distill symbolic models directly from data and cast more insight into the mechanism behind the phenomena (Table 1). However, the explicit method is unfriendly to high dimensional data\[9, 12\]. The lack of anti-overfitting strategies can also lead to a poor generalization ability\[13, 10\]. Moreover, the symbolic form of the distilled models restricts their predictive ability due to the disadvantage in complexity compared to the implicit ML-driven method\[14, 11\]. All these factors limit the use of explicit ML-driven methods in more complex problems. On the contrary, the implicit ML-driven method is more suitable for application (Table 2). Compared with symbolic models, the implicit ML-driven model has a huge advantage in model complexity, which can produce a leap in predictive performance. The generalization ability can be guaranteed through the mature control process of training. It can also deal with big data problems and recognize patterns from high dimensions. This advantage makes it become a hot topic and used frequently in the prediction of $D_l$ problem.

It is worth noting that the used feature combinations in most of studies are basically the same: the channel depth($d$), the channel width($w$), the flow velocity($U$) and the shear velocity($U^*$). This combination comes from a theoretical deduction. Parameters which have impact on dispersion can be categorized into three types: the channel geometrics, the flow properties and hydraulic conditions\[15, 16\]. Those parameters can be concluded as:

$$D_l = f (\rho, \mu, d, w, U, U^*, S_f)$$

(1)

where $\rho = \text{the fluid density}$, $\mu = \text{the fluid viscosity}$, $d = \text{the channel depth}$, $w = \text{the channel width}$, $U = \text{the flow velocity}$, $U_\ast = \text{the shear velocity}$, $S = \text{the channel slope}$.

Among them, $\rho$, $\mu$, $S_f$ and $S_n$ are usually dropped. For $\rho$ and $\mu$, they can form the Reynolds number($\rho U_d/\mu$). But the effect of Reynolds number is not obvious in turbulent flow, such as natural streams. However, $S$ is omitted because it is hard to collect. The influence of $S$ on $D_l$ remains unknown. Moreover, other possible candidates such as the discharge(Q) and the hydraulic radius(R) are not considered due to their correlation with $d$ and $w$. The frequently used feature set has not been compared with other possible combinations. These defects reduce the credibility of the frequently used feature set. Notably, the prediction performance of Environmental problems is not only dependent on
methodologies but also feature set used in development. A proper choice of features can bring advantages in cost and efficiency for prediction. But few studies evaluate the influence of feature sets.

Moreover, few studies have put attention on the comparison between different ML-driven models. The existing research focuses on the increase in performance achieved by various implicit ML-driven methods A numerical based comparative analysis is still lacking. The advantages and disadvantages of these methods are not compared comprehensively, which makes the proper choice of models in different application scenarios remain unknown.

Besides, the importance of hyper-parameters is ignored in previous studies. The hyper-parameter refers to those values which control the learning process, such as the topology to NN and the kernel type to SVM. A different choice of hyper-parameters can make the model performance on a specific problem have a fluctuation range(Fig. 2). This will bring uncertainty into the established models and make the comparison between models unreliable. Previous studies choose the optimal hyper-parameters generally by hand. But such a strategy can be time-consuming and low-efficient. A proper method to tune hyper-parameters automatically is in pressing need.

Recently, an emerging technique called auto feature engineering has been utilized to build feature combinations in many problems. Feature Gradient selector is a typical one. It is based on the learnability of the data and can provide optimal

Table 1: Summary of explicit ML-driven formulas on LDC

| Author / Year          | The formula                                                                 | Features |
|------------------------|-----------------------------------------------------------------------------|----------|
| Sahay and Dutta / 2009 | \( \frac{D_s}{dU} = 2 \left( \frac{\pi}{2} \right)^0.190 \left( \frac{U}{d} \right)^{1.26} \) | d, w, U, U* |
| Li et al. / 2013       | \( \frac{D_s}{dU} = 2.2820 \left( \frac{\pi}{2} \right)^{0.1018} \left( \frac{U}{d} \right)^{1.475} \) | d, w, U, U* |
| Satter and Gharabaghi / 2015 | \( \frac{D_s}{dU} = a \left( \frac{\pi}{2} \right)^k \left( \frac{U}{d} \right)^c \) | d, w, U, U*, g |
| Wang and Huai / 2016   | \( \frac{D_s}{dU} = 17.648 \left( \frac{\pi}{2} \right)^{0.3610} \left( \frac{U}{d} \right)^{1.16} \) | d, w, U, U* |
| Wang and Huai / 2017   | \( \frac{D_s}{dU} = (0.718 + 47.9 \left( \frac{\pi}{2} \right)^{0.5}) \) | d, w, U, U* |
| Alizadeh et al. / 2017 | \( \frac{D_s}{dU} = 9.931 \left( \frac{\pi}{2} \right)^{1.85} \left( \frac{U}{d} \right)^{1.5} \) | d, w, U, U* |
| Riahi-Madvar et al. / 2019 | \( \frac{D_s}{dU} = 33.99 \left( \frac{\pi}{2} \right)^{0.5} \) + \( 8.497 \left( \frac{U}{d} \right)^2 \) | d, w, U, U* |
| Memarzadeh, R., et al. / 2020 | \( \frac{D_s}{dU} = \frac{27}{65} + \frac{27}{65} \) | d, w, U* |
| Riahi-Madvar et al. / 2020 | \( a = 1 + e^{-0.02w+0.39d+3.52U+11.37U^*−3.72} \) | d, w, U, U* |
| Ghaemi et al. / 2021   | \( D_t = 9.19 \exp \left( \frac{−d + 2U}{U_s} \right) + 0.33 \exp \left( \frac{−d + 2U}{U_s} \right) \) | d, w, U, U* |

* \( F_r \) - Froude number.
Table 2: Summary of implicit ML-driven formulas on LDC

| Author / Year                | Methods                | Features     |
|-----------------------------|------------------------|--------------|
| Tayfur and Singh/2005       | NN                     | d, w, U, U*  |
| Tayfur/2006                 | NN, fuzzy systems      | d, w, U, U*  |
| Toprak and Cigizoglu/2008   | NN                     | d, w, U, U*  |
| Noori et al. / 2009         | NN, SVM                | d, w, U, U*  |
| Adarsh / 2010               | SVM                    | d, w, U, U*  |
| Noori / 2011                | NN                     | d, w, U, U*  |
| Azamathulla and Wu / 2011   | SVM                    | d, w, U, U*  |
| Toprak et al. / 2014        | NN                     | d, w, U, U*  |
| Noori et al. / 2016         | SVM, NN, fuzzy systems | d, w, U, U*  |
| Alizadeh et al. / 2017      | NN, fuzzy systems      | d, w, U, U*  |
| Sefi and Riahi-Madvar / 2019| NN, GA                 | d, w, U, U*  |
| Ghiasi et al. / 2019        | Granular computing     | d, w, U, U*  |
| Ghiasi et al. / 2021        | Deep convolutional network | d, w, U, U* |
| Azar et al. / 2021          | SVM, ANFIS, optimization algorithm | d, w, U, U* |

* NN - the neural network; SVM - the support vector machine; ANFIS - the adaptive neuro fuzzy inference system.

sets of features under different quantities automatically. By further verifying the proposed feature set on representative ML models, a convincing global optimal set can be obtained.

Additionally, an emerging type of ML algorithm called ensemble learning has received more attention in predictive problems. Unlike other ML methods, ensemble learning utilizes a cluster of learning models to make the prediction. Importantly, this framework can often obtain a better and more stable model than other single learning methods[17].

For hyper-parameter tuning, the rise of Tree-structured Parzen Estimator(TPE) provides a solution for automatic tuning of hyper-parameters. TPE is a sequential algorithm which can estimate the model performance without hyper-parameter effects automatically. The time complexity of the algorithm is linear. This makes TPE a suitable choice for different practical problems.

Moreover,
The objectives of this paper are: (1) Based on the learnability of data, identify the optimal feature set from a multi-variable dataset for prediction of $D_l$ with the implementation of Feature Gradient selector. (2) The acquired local optimal set will be further validated with 5 popular machine learning models (NN, SVM, GDBT, DT and KNN) to distill the global optimal feature set. TSE will be implemented to avoid the negative influence of hyper-parameters.

2 Materials

2.1 Data pre-processing

The dataset (226 samples) used in this paper is from a review of literatures [18, 19, 20, 5, 1, 21, 22, 23, 24]. It contains both laboratory and field data of $D_l$ and its 8 influenced variables. Involved variables are: the width ($w$), the depth ($d$), the flow velocity ($u$), the shear velocity ($u_s$), the channel slope ($s$), the discharge ($Q$), the hydraulic radius ($R$) and the cross-sectional area ($A$).

A proper data pre-processing is carried out. Apart from duplication, the existence of outliers is a common problem among datasets. It can bring uncertainty into the modelling and make the model biased. To remove those errors, the inter quartile range (IQR) is introduced (Eq. 2).

$$IQR = Q_3 - Q_1$$

where for a $2n$ or $2n + 1$ set of samples, $Q_3$ = the median of the $n$ largest samples; $Q_1$ = the median of the $n$ smallest samples.

After removing duplication and outliers (By IQR), 191 samples are selected for further analysis. To have a basic understanding of this high-dimensional dataset, the visualization of pairwise relationship among parameters and the parameter distribution are carried out (Fig. 3). In Fig. 3, each subplot, except those on the diagonal, describes the pairwise relationship between the involved parameters. As for the diagonal subplot, it denotes the distribution of referred parameters.

It can be observed that all parameters are in normal distribution, which indicates data diversity. The $d$ and $R$ are in a linear relationship. The relationship between those remaining variables is not clear. Therefore, a spearman coefficient plot (Fig. 4) is further carried out to check the monotonic relationship between variables.

Results show that $Q$ has the strongest monotonic relationship with $D_l$ and $u$ the weakest. Noteably, $s$ is the only parameter in negative relationship with $D_l$, which makes it a unique input to the prediction of dispersion problem.

2.2 Subset selection

Selection of the testing set is pivotal to the development of models. A reliable testing set needs to have a similar distribution to the training set. For this purpose, Subset Selection of Kennard and Stone (SSKS) is deployed [25]. SSKS is a sample selection strategy, which can filter out subset with the greatest similarity with the original dataset. For a dataset $M_{x\times y}$ of $x$ samples with $y$ dimensions (Eq. 3), an absolute distance is defined between sample $u$ and point $v$ (Eq. 4).

$$D_{uv}^2 = \|m_u - m_v\|^2 = \sum_{i=1}^{n} (m_{ui} - m_{vi})^2, \text{ where } m_u = [m_{u1}, m_{u2}, \cdots, m_{un}]$$

After setting of the ratio between the training set and the testing set, $\alpha$, the selection begin. A pair of points, $a$ and $b$ with the maximum dissimilarity will be firstly chosen as the initial set, $I$ (Eq. 5).

$$D_{\text{max}}^2 = \max_{a,b} \|m_a - m_b\|^2, a \text{ and } b \in I$$
Figure 3: The visualization of the pairwise relationship between parameters
Figure 4: The visualization of the spearman coefficient between parameters

|     | d   | w   | u   | u_s | s   | Q   | R   | A   | D   |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| d   | 1.00| 0.82| -0.27| -0.12| -0.80| 0.85| 0.99| 0.96| 0.51|
| w   | 0.82| 1.00| -0.21| 0.03| -0.67| 0.92| 0.83| 0.93| 0.71|
| u   | -0.27| -0.21| 1.00| 0.52| 0.53| 0.01| -0.29| -0.25| 0.03|
| u_s | -0.12| 0.03| 0.52| 1.00| 0.62| 0.19| -0.12| -0.07| 0.41|
| s   | -0.80| -0.67| 0.53| 0.62| 1.00| -0.58| -0.80| -0.78| -0.26|
| Q   | 0.85| 0.92| 0.01| 0.19| -0.58| 1.00| 0.84| 0.90| 0.79|
| R   | 0.99| 0.83| -0.29| -0.12| -0.80| 0.84| 1.00| 0.97| 0.51|
| A   | 0.96| 0.93| -0.25| -0.07| -0.78| 0.90| 0.97| 1.00| 0.59|
| D   | 0.51| 0.71| 0.03| 0.41| -0.26| 0.79| 0.51| 0.59| 1.00|
Table 3: The statistical properties of training set and testing set

| Subset | Parameter | Min   | Max   | Med  | IQR  | STD  | Var  | MAD  | Skew  |
|--------|-----------|-------|-------|------|------|------|------|------|-------|
|        | d         | 0.034 | 17.466| 0.850| 1.798| 3.234| 0.731| 5.900|       |
|        | w         | 0.200 | 701.000| 24.300| 37.077| 67.116| 4504.522| 21.340| 7.798 |
|        | u         | 0.022 | 1.010 | 0.430 | 0.462 | 0.272 | 0.074 | 0.224 | 0.184 |
|        | u_s       | 0.001 | 0.180 | 0.040 | 0.051 | 0.037 | 0.001 | 0.024 | 1.001 |
|        | Q         | 0.006 | 6810.000| 2.605 | 15.934 | 588.144 | 345913.492 | 2.590 | 11.474 |
|        | R         | 0.029 | 16.700 | 0.850 | 1.866 | 1.703 | 2.902 | 0.786 | 5.893 |
|        | A         | 0.010 | 100.000| 0.872 | 17.639 | 24.294 | 590.194 | 0.857 | 2.133 |
|        | D         | 0.005 | 100.000| 12.500| 12.500| 22.527 | 411.662 | 11.260 | 2.269 |

Then the dissimilarity distance between a remaining point \( w \) and the selected set can be defined as:

\[
\Delta^2_w = \min \left\{ D^2_{1w}, D^2_{2w}, \cdots, D^2_{rw} \right\}, 1, 2, \cdots, r \in I
\]  \( (6) \)

To find next sample which has the maximum dissimilarity with \( f \), the following criterion will be used:

\[
\Delta^2_x = \max \left\{ \Delta^2_w \right\}
\]  \( (7) \)

Eq. 6 and Eq. 7 will be used repeatedly until the selection satisfies \( \alpha \).

The \( \alpha \) used in this paper is 0.7, which means 134 samples (about 70% of the overall dataset) for training and 57 samples for testing (about 30% of the overall dataset). The statistical information of training and testing set is listed in Table 3.

Because of the high dimensions of data, it is challenging to assess the distribution and relationship between these two sets only by statistical information. Visualization is an alternative. Through implementation of t-SNE, a dimension reduction algorithm, the 8-D training and testing sets are plotted in a 3-D coordinate (Fig. 5). It is clear that the training and the testing set have similar distributions. The testing set is basically enveloped by the training set.

3 Methods

3.1 Feature Gradient selector

Feature Gradient selector is a gradient-based search algorithm for selection of features in the dataset. It originates from the research on estimation of learnability in data sub-regimes[26]. For the input \( X \in \mathbb{R}^{N \times D} \), the output \( y \in \mathbb{R}^N \), a setting integer \( k \), and the fitting coefficients \( \{a_i\}_{i=0}^{k-1} \) with \( a_i \in \mathbb{R} \), [26] proposes an estimation of learnability for a subset of features \( f \in \{0, 1\}^D \), which is given as:

\[
f(s) = \frac{y^\top y}{N} - \sum_{i=0}^{k-1} \left( \frac{a_i}{N} \right)^2 \operatorname{triu} \left( X \operatorname{diag}(s) X^\top \right)_{i+1} y
\]  \( (8) \)

This estimation is further expanded by Sheth and Fusi[27] through the following operation:

\[
\operatorname{triu} \left( zz^\top \right) y = \begin{pmatrix}
z_1z_2y + z_1z_3y_N + \cdots + z_1z_Ny_N \\
z_2z_3y + \cdots + z_2z_Ny_N \\
\vdots \\
z_{N-1}z_Ny_N \\
0
\end{pmatrix}
\]  \( (9) \)
Letting $u = zy$, a simplification can be obtained:

$$
\begin{align*}
y^\top \text{triud} \left( X \text{diag}(s)X^\top \right)^{i+1} y &= y^\top \left( \sum_{d=1}^{D} s_d \text{triud} \left( X:dX:d^\top \right) \right)^{i+1} y \\
&= y^\top \left( \sum_{d=1}^{D} s_d G_d \right) \cdots \left( \sum_{d=1}^{D} s_d G_d \right) y
\end{align*}
$$

(10)

Where $G_d \triangleq \text{triud} \left( X:dX:d^\top \right)$.

Eq. (10) can serve as an efficiently computable filter for grid search of feature subsets. By setting a specific positive integer $k$, the most informative $k$ features can be obtained through iterative computation. By testing the model performance under different proposed sets, the optimal feature set can be obtained.

### 3.2 Tree-structured Parzen Estimator

TPE is a sequential algorithm based on the Bayes Theorem, which can search the optimal hyper-parameter for the ML-driven model[28]. It already has many successful applications[29, 30]. Instead of evaluating the model directly, it will use a surrogate model to simplify the search process. For a ML model $m_I$, it defines the probability of model with loss $y$ under hyper-parameters $x$ as:

$$
P_{m_I}(y \mid x)
$$

(11)
The core criterion used in this algorithm is the Expected Improvement (EI) \[^{[31]}\]. It refers to the expectation of model \( m \) with hyper-parameters \( x \) exceeding some threshold \( y^* \).

\[
EI_{y^*}(x) := \int_{-\infty}^{\infty} \max(y^* - y, 0) p_M(y \mid x) dy
\]

(12)

For trained cases with random assignment of hyper-parameters within range \( R_h \), the median of \( y \) can be obtained. This median will be selected as the threshold \( y^* \). Two probability density(Eq. \[^{[13]}\]) can be trained according to \( y^* \). \( \ell(x) \) is the probability density of observations whose loss are less than \( y^* \) and \( g(x) \) is the probability density of the remaining observation.

\[
p(x \mid y) = \begin{cases} \ell(x) & \text{if } y < y^* \\ g(x) & \text{if } y \geq y^* \end{cases}
\]

(13)

Then An transformed optimization(Eq. \[^{[14]}\]) of EI can be obtained on the basis of Eq. \[^{[13]}\]

\[
EI_{y^*}(x) = \int_{-\infty}^{y^*} (y^* - y) p(y \mid x) dy = \int_{-\infty}^{y^*} (y^* - y) \frac{p(x \mid y)p(y)}{p(x)} dy
\]

(14)

Letting \( \gamma = p(y < y^*) \) and \( p(x) = \int_R p(x \mid y)p(y)dy = \gamma \ell(x) + (1 - \gamma)g(x) \). EI can be simplified into:

\[
EI_{y^*}(x) = \ell(x) \int_{-\infty}^{y^*} (y^* - y) p(y) dy = \gamma y^* \ell(x) - \ell(x) \int_{-\infty}^{y^*} p(y) dy
\]

(15)

and finally

\[
EI_{y^*}(x) = \frac{\gamma y^* \ell(x) - \ell(x) \int_{-\infty}^{y^*} p(y) dy}{\gamma \ell(x) + (1 - \gamma)g(x)} \propto \left( \gamma + \frac{g(x)}{\ell(x)}(1 - \gamma) \right)^{-1}
\]

(16)

Eq. \[^{[16]}\] shows that hyper-parameters \( x \) with high \( \ell(x) \) and low \( g(x) \) are needed to maximum the EI. The tree-structured relationship between \( \ell(x) \) and \( g(x) \) provides a method to select new candidates based on \( g(x) / \ell(x) \). Through iterations, the optimal topology \( x^* \) with the greatest EI can be obtained.

### 3.3 Five machine learning models

Seven high-performance ML models are selected for further feature selection and validation. Both single(the neural network - NN, the support vector machine - SVM, the decision tree - DT) and ensemble algorithms(Gradient Boosting Decision Tree - GBDT, AdaBoost - Ada, Bagging Regressor - BR, Random Forest - RF) are involved. Details of these models can be referenced in supplementary materials.

### 3.4 Process and evaluation of models

#### 3.4.1 Model process

The process flow of models is shown in Fig. \[6\] The FG selector was first utilized to distill feature sets of different numbers. Then two representative models in single and ensemble learning were chosen to validate the obtained sets and filter the optimal set. On this basis, a performance benchmark on 7 popular ML models was established based on TPE. Baseline scores from simple linear regression, basic ML models and common ensemble ML models were obtained on the prediction of LDC under the optimal feature set. All involved models were implemented in Python 3.7 with the sklearn package \[^{[32]}\].

The tuning hyper-parameters of single and ensemble models were selected and listed in Table \[^{[4]}\] and Table \[^{[5]}\].

#### 3.4.2 Model evaluation

The metrics involved in evaluation are: R-square(\( R^2 \)), Mean Absolute Error(MAE), Root Mean Squared Error(RMSE), Discrepancy Ratio(DR) and accuracy.

1. R-square

\( R^2 \) is a model quality indication, which measure the variance proportion of the dependent variable from the independent variable. The definition of \( R^2 \) is:

\[
R^2 = 1 - \frac{\sum_{i=1}^{n} (y_{\text{pred}} - y_{\text{true}})^2}{\sum_{i=1}^{n} (y_{\text{pred}} - y_{\text{mean}})^2}
\]

(17)
Table 4: The hyper-parameters of single learning

| Model   | Parameter      | Type       | Range                      |
|---------|----------------|------------|----------------------------|
| NN      | The hidden size | Integer    | 1-1024                     |
|         | The learning rate | Choice    | 0.00000001,0.000001,0.001   |
|         | momentum        | Float      | 0-1                        |
| Decision Tree | Criterion    | Choice     | MSE, Friedman_MSE, MAE, Poission |
|         | Splitter       | Choice     | Best, Random               |
|         | Max_depth      | Choice     | 10,30,50,70,90,110,130,150 |
|         | Max_features   | Choice     | Auto, Sqrt, Log2           |
| SVM     | C              | Float      | 0.1-10                     |
|         | Kernel         | Choice     | Linear, RBF, Polynomial, Sigmoid |
|         | Degree         | Choice     | 1,2,3,4,5                  |
|         | Gamma          | Float      | 0.01-0.1                   |
|         | Coef0          | Float      | 0.01-0.1                   |

Figure 6: The visualization of training set and testing set
### Table 5: The hyper-parameters of ensemble learning

| Model         | Parameter        | Type      | Range          |
|---------------|------------------|-----------|----------------|
| GDBT          | num_leaves       | Integer   | 2-256          |
|               | The learning rate| Float     | 0.001-1.000    |
|               | num_iterations   | Choice    | 200,300,400    |
|               | bagging_fraction | Float     | 0.5-1.0        |
|               | bagging_freq     | Choice    | 1,2,4,8,10     |
|               | min_data_in_leaf | Integer   | 5-50           |
| Random Forest | n_estimators     | Choice    | 60,80,100,120,140 |
|               | criterion        | Choice    | MSE, MAE       |
|               | max_features     | Choice    | Auto, Sqrt, Log2 |
| Adaboost      | n_estimators     | Integer   | 5-100          |
|               | The learning rate| Float     | 0.01-1.00      |
|               | The loss         | Choice    | Linear, Square, Exponential |
| Decision Tree | n_estimators     | Integer   | 2-20           |
|               | max_samples      | Float     | 0.5-1.0        |
|               | max_features     | Choice    | 1,2,3,4        |

2. Mean Absolute Error

MAE is a measure of absolute error between predictions and observations. The definition of MAE is:

$$\text{MAE} = \frac{\sum_{i=1}^{n} |y_{\text{pred}} - y_{\text{true}}|}{n}$$  \hspace{1cm} (18)

3. Root Mean Squared Error RMSE is similar to MAE. It is defined as:

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (y_{\text{pred}} - y_{\text{true}})^2}$$  \hspace{1cm} (19)

4. Accuracy Accuracy in this paper is defined based on Discrepancy Ratio(DR). DR is a logarithmic form of prediction error, which is used to weaken the influence of noise. It is defined as:

$$\text{DR} = \log_{10} \frac{y_{\text{pred}}}{y_{\text{true}}}$$  \hspace{1cm} (20)

Generally, a good prediction will have DR between [-0.3, 0.3]. The accuracy is defined by the percentage of DR within the range of [-0.3, 0.3].

To synthesize the above metrics, a weighted score(WS) which has range from 0 to 1 score was defined. It is established with the above metrics by normalization under maximum and minimum(Eq. 21).

$$x_n = \frac{x - x_{\text{min}}}{x_{\text{max}} - x_{\text{min}}}$$  \hspace{1cm} (21)

The definition of WS is:

$$\text{SCORE} = 0.3(R_n^2 + ACC_n) + 0.2(MAE_n + RMSE_n)$$  \hspace{1cm} (22)

More weights are given to $R^2$ and $ACC$ because $MAE$ and $RMSE$ are basically the same kind of measures for predictive errors.

However, only evaluating the test performance of model will make the result biased to lessfitting cases. Similarly, focusing on training performance can lead to a result which tends toward overfitting cases. Therefore, weighted scores(WS) of each case in training and testing were both calculated and combined at the rate of 4:6 to obtain a more comprehensive model performance metric. This metric is called final weighted score(FWS) in this paper(Eq. 23).

$$\text{FWS} = 0.4WS_{\text{train}} + 0.6WS_{\text{test}}$$  \hspace{1cm} (23)

Moreover, TSE will build hundreds of candidate models to distill the optimal hyper-parameters. Depended on the computing power, the optimal hyper-parameter result can be different in distinct attempts. Thus, it is necessary to learn about both the average and the optimal performance of those cases developed by TSE to give an objective comparison. Hence, the top 5% and the optimal FWS are adopted for further evaluation in validation and benchmarking.
Table 6: FG result

| Notation | Num of Features | Combinations |
|----------|----------------|--------------|
| I        | 1              | w            |
| II       | 2              | w, A         |
| III      | 3              | w, u, A      |
| IV       | 4              | w, u, s, A   |
| V        | 5              | d, w, u, s, A|
| VI       | 6              | u, u, s, Q, R, A |
| VII      | 7              | w, u, u, s, Q, R, A |
| VIII     | 8              | w, d, u, u, u, s, Q, R, A |

Table 7: Validation on NN

| Feature Set | Type | R2_train | MAE_train | RMSE_train | ACC_train | R2_test | MAE_test | RMSE_test | ACC_test | WS_train | WS_test | FWS |
|-------------|------|----------|-----------|------------|-----------|---------|----------|-----------|----------|----------|---------|-----|
| NN-I        | optimal | 0.439 | 0.604 | 0.916 | 51.493 | 0.585 | 0.221 | 0.319 | 56.140 | 0.116 | 0.636 | 0.428 |
| NN-I        | average | 0.575 | 0.601 | 0.911 | 47.388 | 0.588 | 0.219 | 0.307 | 58.333 | 0.087 | 0.646 | 0.415 |
| NN-II       | optimal | 0.709 | 0.500 | 0.487 | 70.896 | 0.271 | 0.665 | 1.017 | 40.351 | 0.066 | 0.254 | 0.427 |
| NN-II       | average | 0.675 | 0.432 | 0.554 | 67.537 | 0.281 | 0.662 | 1.045 | 40.351 | 0.626 | 0.264 | 0.409 |
| NN-III      | optimal | 0.930 | 0.140 | 0.287 | 88.806 | 0.275 | 0.857 | 1.271 | 47.386 | 0.860 | 0.199 | 0.463 |
| NN-III      | average | 0.936 | 0.139 | 0.215 | 92.090 | 0.237 | 0.959 | 1.414 | 45.138 | 0.903 | 0.132 | 0.440 |
| NN-IV       | optimal | 0.999 | 0.000 | 0.001 | 123.000 | 0.020 | 0.998 | 2.136 | 49.123 | 0.999 | 0.024 | 0.527 |
| NN-IV       | average | 0.999 | 0.007 | 0.012 | 99.627 | 0.300 | 0.913 | 1.282 | 45.175 | 0.995 | 0.017 | 0.510 |
| NN-V        | optimal | 0.999 | 0.006 | 0.011 | 97.254 | 0.119 | 0.889 | 1.276 | 43.866 | 0.995 | 0.014 | 0.514 |
| NN-V        | average | 0.999 | 0.007 | 0.027 | 99.352 | 0.308 | 0.955 | 1.342 | 40.000 | 0.991 | 0.035 | 0.488 |
| NN-VI       | optimal | 0.999 | 0.016 | 0.013 | 100.000 | 0.240 | 1.030 | 1.606 | 49.123 | 0.996 | 0.081 | 0.447 |
| NN-VI       | average | 0.999 | 0.011 | 0.018 | 99.502 | 0.209 | 1.070 | 1.504 | 42.105 | 0.992 | 0.074 | 0.441 |
| NN-VII      | optimal | 0.999 | 0.011 | 0.022 | 99.254 | 0.284 | 0.975 | 1.374 | 47.386 | 0.991 | 0.155 | 0.491 |
| NN-VII      | average | 0.999 | 0.010 | 0.025 | 99.840 | 0.292 | 0.954 | 1.340 | 41.667 | 0.991 | 0.154 | 0.489 |
| NN-VIII     | optimal | 0.999 | 0.000 | 0.001 | 100.000 | 0.302 | 0.898 | 1.236 | 49.123 | 0.999 | 0.021 | 0.527 |
| NN-VIII     | average | 0.999 | 0.007 | 0.012 | 99.627 | 0.300 | 0.913 | 1.282 | 45.175 | 0.995 | 0.017 | 0.510 |
| NN-VIII     | optimal | 0.999 | 0.015 | 0.038 | 99.000 | 0.379 | 0.980 | 1.138 | 37.088 | 0.986 | 0.202 | 0.515 |
| NN-VIII     | average | 0.999 | 0.030 | 0.077 | 98.257 | 0.338 | 0.971 | 1.204 | 36.466 | 0.991 | 0.164 | 0.486 |
| NN-O        | optimal | 0.944 | 0.142 | 0.260 | 89.532 | 0.340 | 0.899 | 1.194 | 35.088 | 0.871 | 0.189 | 0.462 |

4 Results and Discussions

As mentioned, the commonly used 4-feature combination is: \(d, w, u\) and \(u_s\). It will serve as the comparison baseline, notated as set \(O\), in further validations to check the rationality of the feature sets proposed by FG.

4.1 FG results

The result of Feature Gradient selector is shown in Table 6. Various combinations under different numbers of features are distilled by the FG selector. Among them, \(w\) and \(A\) show the highest frequency, which indicates the importance of these two features.

4.2 Verification

In validation, representative models in single learning (NN) and ensemble learning (GBDT) are both utilized. The statistical results are shown in Table 7 and Table 8. It is worth noting that the statistics listed are sorted results according to \(FWS\), which are different to results only considering the training process.

Visualizations of different feature sets with baseline of set \(O\) are also carried out on NN (Fig. 7) and GDBT (Fig. 8). These visualizations reveal that a similar pattern can be found in both models (Figure 7). At beginning, the model performance score soars with the increase in feature number and reaches peak at the set of \(w, u, s\) and \(A\). Then the performance tends to decline and keep fluctuating. In general, the model performance is in normal distribution.

The initial performance enhancement accompanies the rise in the feature number. This is because when parameters used are too few, the information contained in samples is not enough to carry out reliable predictions. During this stage, the increase in the feature number can impose a positive impact on the prediction until the global optimal feature set: \(w, u, s\) and \(A\). However, the further increase in the feature number weakens the model performance. This could be caused by the noise in the dataset. Although data pre-processing has removed some outliers, there are still some undetected errors left. The introduce of new features can bring in more noise and bring a negative impact to the prediction. When the
Table 8: Validation on GDBT

| Feature Set | Type    | R2_train | MAE_train | RMSE_train | ACC_train | R2_test | MAE_test | RMSE_test | ACC_test | WS_train | WS_test | FWS |
|-------------|---------|----------|-----------|------------|-----------|---------|----------|-----------|----------|----------|---------|-----|
| GDBT-I      | optimal | 0.168    | 0.730     | 1.049      | 64.179    | 0.388   | 0.297    | 0.341     | 70.175   | 0.287    | 0.599   | 0.474|
| GDBT-I      | average | 0.177    | 0.719     | 1.043      | 62.896    | 0.355   | 0.296    | 0.350     | 66.396   | 0.288    | 0.577   | 0.462|
| GDBT-II     | optimal | 0.249    | 0.603     | 0.997      | 48.039    | 0.499   | 0.247    | 0.309     | 64.912    | 0.274    | 0.603   | 0.490|
| GDBT-II     | average | 0.268    | 0.658     | 1.004      | 52.242    | 0.373   | 0.280    | 0.344     | 61.084    | 0.312    | 0.572   | 0.468|
| GDBT-III    | optimal | 0.253    | 0.597     | 0.926      | 43.776    | 0.409   | 0.263    | 0.335     | 57.895    | 0.336    | 0.577   | 0.480|
| GDBT-III    | average | 0.273    | 0.680     | 1.003      | 56.418    | 0.399   | 0.280    | 0.337     | 64.702    | 0.304    | 0.590   | 0.476|
| GDBT-IV     | optimal | 0.239    | 0.663     | 1.004      | 65.072    | 0.394   | 0.296    | 0.340     | 73.684    | 0.335    | 0.612   | 0.501|
| GDBT-IV     | average | 0.241    | 0.658     | 1.002      | 65.104    | 0.370   | 0.298    | 0.346     | 69.965    | 0.334    | 0.592   | 0.489|
| GDBT-V      | optimal | 0.235    | 0.675     | 1.006      | 65.672    | 0.388   | 0.300    | 0.341     | 73.684    | 0.331    | 0.609   | 0.498|
| GDBT-V      | average | 0.242    | 0.671     | 1.001      | 65.624    | 0.371   | 0.301    | 0.336     | 69.614    | 0.335    | 0.609   | 0.498|
| GDBT-VI     | optimal | 0.454    | 0.533     | 0.850      | 62.887    | 0.321   | 0.283    | 0.360     | 50.877    | 0.447    | 0.520   | 0.491|
| GDBT-VI     | average | 0.325    | 0.625     | 0.943      | 52.776    | 0.365   | 0.267    | 0.337     | 58.526    | 0.342    | 0.562   | 0.474|
| GDBT-VII    | optimal | 0.227    | 0.692     | 1.012      | 65.672    | 0.369   | 0.304    | 0.347     | 70.175    | 0.324    | 0.591   | 0.484|
| GDBT-VII    | average | 0.257    | 0.677     | 0.996      | 65.075    | 0.322   | 0.308    | 0.359     | 68.982    | 0.336    | 0.570   | 0.476|
| GDBT-VIII   | optimal | 0.168    | 0.711     | 1.050      | 64.179    | 0.303   | 0.252    | 0.307     | 66.667    | 0.291    | 0.639   | 0.500|
| GDBT-VIII   | average | 0.210    | 0.682     | 1.023      | 49.104    | 0.474   | 0.252    | 0.316     | 59.509    | 0.269    | 0.607   | 0.472|
| GDBT-V     | optimal | 0.300    | 0.589     | 0.921      | 61.940    | 0.249   | 0.312    | 0.383     | 39.649    | 0.393    | 0.309   | 0.462|
| GDBT-V     | average | 0.180    | 0.717     | 1.040      | 65.254    | 0.326   | 0.308    | 0.358     | 67.088    | 0.298    | 0.566   | 0.459|

Figure 7: The performance score of NNs with different feature combinations

Figure 8: The performance score of NNs with different feature combinations
Table 9: The feature sets with similar physical meaning with the optimal set

| Notation | Num of Features | Combinations |
|----------|----------------|--------------|
| 1        | 4              | \(d, w, u, s\) |
| 2        | 5              | \(w, s, Q\) |

Figure 9: The performance score of NNs with different feature combinations

negative impact of the increase in feature numbers surpasses its positive impact, the performance score begins to decline. Depending on the anti-noise ability of different models, the final performance of different models can vary slightly.

The best feature combination is a 4-feature set of \(w, u, s\) and \(A\). Compared with the classic combinations: \(d, w, u\) and \(u, s\), the main difference is the use of \(s\). As shown in the plot of spearman coefficient among 8 features as well as the corresponding LDC(Fig. 4), \(s\) is the only unique feature which is in negative correlation with the LDC. Moreover, the relationship between \(s\) and other features is weak. This indicates that the information hidden behind \(s\) matters for the prediction of LDC.

Besides, a notable change is the introduce of \(A\) to the feature set. \(A\) refers to the cross-sectional area, which is in close relationship with \(d\) and \(w\) in physics. Therefore, a possible feature combination can be \(d, w, u\) and \(s\). Moreover, another possible combination is \(w, s\) and \(Q\) due to \(Q = uA\). These two sets are listed in Table 9 and notated with 1 and 2.

However, those sets show no superiority in learnability over the optimal combination according to FG results, although the physical meaning behind them is similar. To verify this, further experiments are carried out on those combinations with NN(Fig. 9) and GBDT(Fig. 10).

Results show that the combination of \(w, u, s\) and \(A\) is still the optimal one, which is in consistence with the result of FG. This phenomenon could be caused by two factors: suitability and freedom of features. Among sets of \(d, w, u, s\) and \(w, u, s, A\), FG and experiments reveal that the combination of \(w, A\) is more suitable for application of ML techniques than \(d, w\). This is mainly determined by the black-box nature of ML-techniques. Those techniques make predictions based on the correlation between inputs and outputs rather than prior knowledge of physics. Different feature combinations are likely to have different suitability for the learning process. As a result, those feature sets with similar physical meaning could vary significantly in prediction. And results show that \(w, A\) is better. For set of \(w, s, Q\), the performance decline results from the use of \(Q\). Although \(Q\) contains information of \(u\) and \(A\) physically, this representation bounds \(u\) and \(A\) together, which severely restricts the feature freedom. Instead, the application of \(u, A\) can bring in more manipulations and operations on the information behind those features and proposes a better prediction.

The above analysis indicates although ML-techniques are powerful tools for prediction, a careful feature selection is still crucial. It can have a serious impact on model performance. The improvement in feature selection can achieve an enhancement in prediction.
4.3 The model benchmark

The main goal of the model benchmark is to evaluate the performance of popular ML models for the prediction of LDC under the global optimal feature set. This evaluation can establish a reference on model selection for related practical engineering projects.

In this benchmark, the linear model is utilized to function as the baseline. Single learning (NN, DT and SVM) and ensemble learning models (RF, GDBT, Ada and BR) are both involved. The statistical result is listed in Table 10.

A visualization is also carried out (Fig. 11). For comprehensive comparison, the training and testing scores of these models are also plotted.

It can be observed that the best prediction model is the SVM and the worst DT. The remained models achieve similar prediction results.

In training, single learning models have higher scores than ensemble models. All models outperform linear models. This indicates that all models can learn patterns of different degrees from the data. The top performer is NN and the worst one GDBT. However, this doesn’t mean single learning has stronger predictive ability. The illustrated training score is a result obtained through sort based on $FWS$, a compromise of training and testing. Therefore, this result is not an indication of upper limit on learning ability but the trend of overfitting on dataset with hundreds of samples. It reveals that single learning models are less likely to overfit and give biased results on a relatively small dataset. This is caused by the stronger regression ability of ensemble models[17]. This characteristic makes ensemble models easily influenced by the noise behind the data.
In testing, the opposite result is obtained. Single learning models, except SVM, perform poorly. DT achieves a negative score, which is even lower than the linear model. On the contrary, ensemble models show a stable and excellent performance. This phenomenon indicates ensemble models have an advantage in generalization ability.

The result shows that SVM is the best choice for the prediction of $D_l$ on a dataset with hundreds of samples. Due to weak generalization ability, DT is not suitable for the prediction of $D_l$ and other similar problems. The remaining models have similar predictive abilities. NN shows advantage in fitting but weakness in generalization ability. The ensemble model has good generalization ability but tends to overfit on relatively small dataset, hundreds of samples in our cases.

5 Conclusions

A novel feature combination and a benchmark of different ML models for prediction of LDC were proposed in this paper. The feature selection utilizes the Feature Gradient selector for search and the Tree-structured Parzen Estimator for validation. The establishment of benchmark involves multiple popular ML models, both single learning and ensemble learning. It can serve as a guideline of model choice for predictive problems like $D_l$ and other similar problems.

The detailed conclusions are as follows:

1. The commonly used feature combination ($d, w, u$ and $u_s$) for LDC prediction is derived from an unproved theoretical deduction. To verify it, a framework for feature engineering is carried out on an enhanced dataset. This dataset contains 8 possible features of LDC. Its consistency and reliability is improved through outliers cleaning by IQR and set dividing by SSKS. Feature selection with Feature Gradient selector and validation based on Tree-structured Parzen Estimator reveals that a novel feature set of $w, u, s, A$ shows superiority over other combinations in both performance and simplicity.

2. Based on the physical relationship between features, $d, w, u, s$ and $w, s, Q$ are mutations of the optimal solutions. However, those combinations lead to weaker predictive performance. The set of $d, w, u, s$ suffers from poor adaptability.
Those prevalent ML-techniques perform better on optimal set of $w, u, s, A$, which indicates that the combination of $w$ and $A$ are more informative and suitable for prediction of LDC than other combinations. As for set of $w, s, Q$, the information behind this set might be equal to the optimal set in physics. However, the connection of $u$ and $A$ reduces the feature freedom and limits the range of possible operations.

(3) For prediction problems, the increase in feature numbers has no direct propensity to enhance the model performance. On one hand, the enriching of features does provide more information for the learning of ML models. On the other hand, the amount of noise in the dataset is also increased. When the negative impact of feature increase surpasses the positive impact, the model performance will start to deteriorate. Hence, blind enrich in the dimension can hinder the improvement in prediction accuracy of models.

(4) For the prediction of $D_l$ in this paper, the support vector machine (SVM) is the optimal ML model. It achieves a good balance between training and testing. Decision Tree (DT) is not a suitable choice for prediction due to weak generalization ability.

(5) Single learning model outperforms ensemble learning model in the prediction of $D_l$. With lower complexity, single learning model is less likely to overfit and give biased results. Although its generalization ability is weaker, the overall performance is better than ensemble models due to the better balance between model complexity and the sample number. For a bigger dataset, the ensemble model might achieve better performance.

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