A Data-Correlation Model of Aerodynamic Heating Based on Globally Optimal Learning Method

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Abstract. Aerodynamic heating is a critical problem to consider in hypersonic flight. It involves many factors, and most of them affect the result nonlinearly, which makes it difficult to get a proper model from experimental data. Even worse, it is hard to gather enough data for distilling a model since aerodynamic heating experiments are costly. Machine learning (ML) methods are possible candidates for its data modeling. However, general ML needs more data for modeling. Therefore, a ML strategy that can capture strong nonlinear relations with small-size dataset is desirable. In this work, a special ML strategy that aims at modeling data collected from hypersonic aerodynamic heating experiments is established. The strategy is based on the randomized neural network (RNN) whose basic model framework is a single-hidden layer feedforward neural network (SLFN). A global optimization (GO) technique, low dimensional simplex evolution (LDSE), is introduced to improve its correlation performance. The modified algorithm is referred to as LDSE enhanced RNN for short, in which the weights and biases in the hidden layer are globally optimized, rather than randomly generated. Theoretically, the LDSE enhanced RNN has the hierarchically global optimality. Meanwhile, the LDSE enhanced RNN has been applied to model a real word aerodynamic heating database of blunt-body. Study shows that the LDSE enhanced RNN has a good capability to balance the complexity and accuracy of a nonlinear regression model, and the model can give a reliable estimation of the aerodynamic heating.

Keywords: Aerodynamic heating · Machine learning · Randomized neural network · Global optimization

1 Introduction

Aerodynamic heating, is a typical physical phenomenon in hypersonic flow [1–3] with strong nonlinearity. When an aircraft flies in hypersonic speed, the strong compression by shock wave and shearing by viscosity will increase the temperature of gas around the aircraft steeply. This causes a huge amount of thermal transmission (the very high level of feat flux). The high temperature changes the physicochemical properties of gas,

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such as the vibrational excitation, dissociation, even ionization. The radiation becomes more significant in the very high temperature gas, as well. Besides, the shock wave interaction, transition or other factors in specific conditions will also severely influence the aerodynamic heating. The heat flux is seriously dangerous for flight security, so, estimating aerodynamic heating as exactly as possible plays an important role in hypersonic aircraft design, but it is nearly impossible to theoretical analysis those problems with considering all factors simultaneously. The computational fluid dynamics (CFD) technique provides a feasible option to simulating hypersonic flows numerically and has been widely applied to analyze aerodynamic heating. However, numerical schemes, physical mathematical models of gas, and the mesh quality of computational domain always restrict the accuracy of the simulation of aerodynamic heating. Though CFD can provide abundant information of flowfield, those results are numerical approximations. In fact, there are still some physical phenomena that cannot be duplicated by CFD and even can not be expressed by mathematical formulas. As a result, experiments are irreplaceable in aerodynamic heating analysis.

Data-driven modeling plays an important role in natural science, either discovering physical laws or fitting empirical/semi-empirical models. A number of useful aerodynamic heating correlation models have been established from experiments data. Nowadays, increasing complexity of problems makes us to seek for more automated even intelligent tools that can assist us in analyzing data.

The development of machine learning has brought us much convenience. In general, two kinds of machine learning methods are commonly used for modeling physical data, the symbolic regression [4] with explicit analytical expressions and black-box models (like support vector regression, kriging model, or neural networks) with preset structures. Symbolic regression has been applied to extract explicit expressions of free form equations [5], discover governing equations of nonlinear dynamics [6], and reconstruct physical laws [7] from data. A symbolic regression method, adaptive space transformation [8], has successfully explored the invariant of hypersonic aerodynamic coefficients. A multi block building symbolic regression method has been applied to predict parameters of shockwave interactions [9]. However, for the data modeling in aerodynamic heating analysis, the application is not straight forward. Feature engineering is the first issue to consider. It is too complicated to determine attributes for constructing the symbolic function due to both the restrictions from algorithm and physical attributes themselves. Thus, the black-box model may be a better choice and especially the neural networks because of its preset structure.

In recent years, more and more researches have exploited the applications of deep learning in fluid dynamics [10]. For instance, Reference [11] embed the Galilean invariance of stress tensor to the deep multilayer neural networks and trained the model on datasets from direct numerical simulation of turbulent flow to improve Reynolds stress model, Reference [12] introduced physical equations into the deep neural networks framework and reconstructed the flow fields by this model, Reference [13] used an encoder-decoder model based on convolutional neural networks and dealt with temporal evolution by traditional numerical scheme.

Unfortunately, the cost, the performance of testing facilities, and the precision of measuring instruments [14] handicap the data acquisition. This means the aerodynamic heating dataset or database available usually includes only a small number of sample data. In other words, the quantity of aerodynamic heating experimental dataset is too small to train deep learning models, in which the number of parameters could be far more than that of samples in dataset. The hypersonic flow always contains too much unpredictable noise, which increases the uncertainty of collected data. Our purpose is training a low complexity model covering the complicated nonlinear relations via inadequate data with high uncertainty.

Randomized neural network (RNN) is an important path for training a neural network model without gradient based iterations. The implementations of these methods can be traced back to 1990s [15]. As a typical branch in those method, keeping the randomly generated parameters of the hidden layer and analytically determining the weights of output layer by Moore-Penrose Generalized Inverse, is the simplest way to implement RNN. Reference [16] has provide an alternative model framework called random vector functional link neural network (RVFL) which has a data stream directly linking input layer with output layer. However, practice indicates that the randomness of parameters of the hidden layer negatively influence the performance and robustness of the model. There have been many works focusing on improving RNN or RVFL. Reference [17] has given a review on those modifications and discussed different non-iterative learning method with closed-form solution. In our work, the basic frame work of single-hidden layer feedforward neural network is kept and a global optimization (GO) algorithm is introduced to improve the model's correlation performance.

In this work, we apply our modified method to model a database that has been generated through testing a 70 deg sphere-cone blunt-body in high-enthalpy carbon-dioxide flow with 16 deg angel of attack in an expansion tunnel [18]. We compare the performance among the SLFN model trained via backpropagation, RNN, and our method, respectively. Study shows that our method can acquire the best performance stably in acceptable training cost.

The rest of this paper is arranged as follows. In Sect. 2, we will briefly describe the RNN and the GO technique on improving RNN. In Sect. 3, we will show the details of feature engineering, model training and discussions. Finally, there will be the conclusion.

2 Introduction of Algorithm

2.1 Brief Review of Randomized Neural Network

This part shows the simplest form of randomized neural network (RNN) without any constrains like regularizations.

Giving a set of samples $\left\{\left(\mathbf{x}_j, y_j^*\right)|\mathbf{x}_j \in \mathbb{R}^n, y_j^* \in \mathbb{R}, j = 1, 2, \ldots, N_s\right\}$, the approximation of the jth sample point's target y_j^* by a single-hidden layer feedforward neural network (SLFN) with N_h hidden neurons, and activation function f_{act}, is expressed as

$$y_j = \sum\nolimits_{i=1}^{N_h} \beta_i f_{act}\left(w_i \cdot x_j + b_i\right) \tag{1}$$

where $\mathbf{w}_i \in \mathbb{R}^n$ and $b_i \in \mathbb{R}$ are the weighs vector and bias of the ith input neuron respectively, $\beta_i \in \mathbb{R}$ is the weight of the ith output neuron, and $y_i \in \mathbb{R}$ is the predicted value of jth sample point.

Using $\mathbf{y} = \left[y_{j\in N_s}\right] \in \mathbb{R}^{N^s}$ to represent model predictions vector and $\mathbf{y^*} = \left[y^*_{j\in N_s}\right] \in \mathbb{R}^{N^s}$ to represent the sample observations vector, the f_{loss} loss based on the principle of norm least square can be wrote as follows.

$$f_{loss} = \left\|\mathbf{y} - \mathbf{y}_2^*\right\| \tag{2}$$

According to non-iterative strategies, the learning progress is

$$\min_{\boldsymbol{\beta}} f_{loss} \tag{3}$$

Where $\boldsymbol{\beta} = \left[\beta_{i\in N^h}\right] \in \mathbb{R}^{N^h}$ is the output weights vector.

Replacing $\mathbf{y}$ in Eq. 2 by merging Eq. 1 for all samples and representing $\mathbf{y^*}$ by $\mathbf{T}$, we obtain another form of Eq. 3

$$\min_{\boldsymbol{\beta}} \|H\boldsymbol{\beta} - T\| \Leftrightarrow H\boldsymbol{\beta} - T = 0 \tag{4}$$

where $\mathbf{H} = \mathbf{H}\left(\boldsymbol{w}_{i=1,\ldots,N_h}, b_{i=1,\ldots,N_h}, \boldsymbol{x}_{i=1,\ldots,N_h}\right)$ is called the hidden layer output, and is expressed as follow.

$$H = \begin{bmatrix} f_{act}(w_1 \cdot x_1 + b_1) & \cdots & f_{act}\left(w_{N_h} \cdot x_1 + b_1\right) \\ \vdots & \ddots & \vdots \\ f_{act}\left(w_1 \cdot x_{N_s} + b_1\right) & \cdots & f_{act}\left(w_{N_h} \cdot x_{N_s} + b_1\right) \end{bmatrix}$$

It is clearly that training SLFN by RNN is equivalent to solving an equation set. And the solution of Eq. 4 is

$$\hat{\beta} = \mathbf{H}^{\dagger}\mathbf{T} \tag{5}$$

where $\mathbf{H}^{\dagger}$ denotes the Moore-Penrose Generalized Inverse of matrix $\mathbf{H}$.

Therefore, the RNN analytical determines output weights, and if the $\mathbf{H}^{\dagger}$ is unique, the $\hat{\beta}$ will be unique too, which ensures the global optimality of output layer weights.

2.2 Global Optimization Techniques for Improving RNN

In RNN, the hidden layer parameters are randomly generated. The randomness has a negative influence on the robustness and performance of the model. It is necessary to optimize the hidden layer parameters via efficient methods for modeling aerodynamic heating experimental data.

Global optimization (GO) algorithms are widely used in solving operation research problems. The hidden layer parameters of neural networks can be flattened and concatenated in a vector, and then learned by GO. Though both the duration of training process and the cost of computing resource are insupportable when use those algorithms to training large scale neural networks, GO can achieve rapid convergence on the solution space of SLFN's input layer weights and biases with low complexity. Though, GO prolongs the process of RNN training SLFN, this cost is insignificant comparing with aerodynamic heating experiments or numerical simulations.

There has been a series of results about the theory and applications of GO improving RNN in traditional machine learning territory. Different GO algorithms have been employed in different research, and in this paper, the GO applied is low dimensional simplex evolution (LDSE) [19], a lightweight improved differential evolution algorithm.

The procedure of these methods can be briefly described as follows.

1. Initialization: Input dataset, hyperparameters, and convergence criteria;
2. Beginning: Randomly generate hidden layer parameters (HPs);
3. Optimization: Call LDSE to evolve HPs with RNN strategy determining the corresponding output layer weights to minimize the loss;
4. Finalization: Check the criteria, export the best weights at convergence.

A simple comparison of different training methods is listed in Table 1.

Table 1. Comparison of three algorithms for data modeling

Item	BP	RNN	GO enhanced RNN
Model complexity	Usually high	Low	Low
Learning duration	Uncertain,	Very fast	Medium (10–20 s in this work)
Number of iterations	$\mathbf{o}(10^2)$	None	$\mathbf{O}(10^2)$
Hidden layers para	Local optimum	Random	Global optimum
Output layers para	Local optimum	Global optimum	Global optimum

From the above procedure, we can see that GO enhanced RNN has two levels, RNN and GO. The basic RNN strategy ensures the best coefficients of nonlinear function basis for arbitrary single affine transformation searched by GO. That is, GO enhanced RNN has the hierarchical global optimality. Though LDSE optimized input layer parameters replace the randomized parameters in RNN, LDSE enhanced RNN is still a rational path to abbreviate our method.

3 Results and Discussion

From literatures about global optimization (GO) algorithm improving randomized neural networks (RNN), we find that the performance indicators (i.e. convergence, efficiency, and reliability) of different modified methods have no significant difference. That is, no one could dominate others. Therefore, the testing of our method on benchmark datasets is omitted in this paper. The low dimensional simplex evolution embedded globally optimal learning method for a single-hidden layer feedforward neural network in this work is specifically designed for aerodynamic heating data modeling.

3.1 Blunt-Body Aerodynamic Heating and Feature Engineering

In this part, the feature engineering of the aerodynamic heating dataset will be shown. The database from Reference [18] contains the initial states of experiments, measurements of heating, pressure, and the comparison between experiments and numerical simulations. The database from the reference in this work contains data from 20 groups of wind tunnel experiments arranged by their total enthalpy of free stream.

Initial states in a specific testing group are identical among each measuring point. The difference of each measuring point can only be distinguished by geometrical information. If input attributes of the dataset used for modeling are initial states and geometrical parameters, it means that the correlation model should capture the compression by the shock wave, the shearing by the viscosity, and some other physical factors. More complicated relations call for more complex model, which need more data for training. The number of samples in the database we selected cannot support such a brute-force strategy. Therefore, feature engineering is necessary before modeling.

Heat flux is related to the gradient of temperature. That is, local flowfield property affects the heat flux more significantly. Therefore, the main task of feature engineering is to extract information of local flowfield parameters at measuring points from initial inflow conditions.

In this work, the flowfield parameters at the outer edge of boundary layer are used for model inputs. The parameters near measuring points are determined by an inviscid computational fluid dynamics (CFD) simulation for each wind tunnel test. In fact, simulating the flowfield to duplicate the real-world conditions ties up with too many details and expends the enormous amount of computing resource that are meaningless for our feature engineering. Referring to the practice of some aerodynamic heating estimation methods, we use the finite volume method (FVM) converting initial inflow parameters to local flowfield at measuring points by solving Euler Equations (the detail settings of CFD presenting in Table 2, the geometry of the blunt-body showed in Fig. 1, and the mesh with computational domain illustrated in Fig. 2).

Table 2. CFD settings in our aerodynamic simulations

Item	Basic information	Extras
Governing equations	Compressible Euler equations	3D, thermal equilibrium gas model
Equation of State	Redlich-Kwong-Soave	
Numerical scheme	2^{nd} order TVD with HLLC	Centralized FVM
Time integration	Steady	Implicit iteration
Quantity of mesh	0.8 Million	Structure and unstructured at central line
Components of fluid	Only CO_2	Disassociation or ionization not considered
Boundary conditions	Far-field: hypersonic inflow Outflow: extrapolation by inner grid Wall: inviscid slip wall	Radiation not considered

Essentially, this feature engineer is that the inviscid flow at wall approximates the outer edge of boundary layer in real world. Meanwhile, solving Euler Equations can capture the effect of the shock wave, which has the mathematical discontinuity. That is, modeling aerodynamic heating through the information of flowfield at the outer edge of boundary layer can weaken the nonlinearity than modeling with the initial states of inflow with geometric parameters directly. This helps reduce the model complexity.

Due to the symmetry, the computational domain contains only a half of the windward surface of this geometrical model. The feature engineering of each group costs 0.5 ~ 1 h, which is far less than calculating aerodynamic heating by CFD.

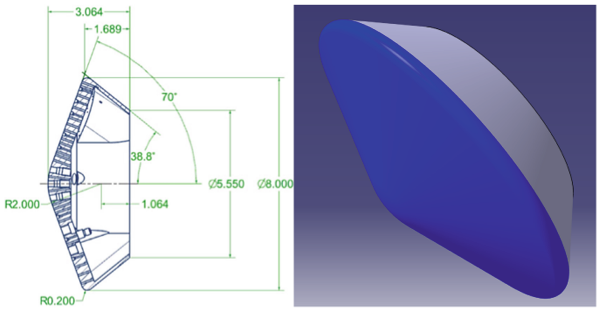

Fig. 1. Model geometry [18] (dimension in inch) (left) and 3D effect (right)

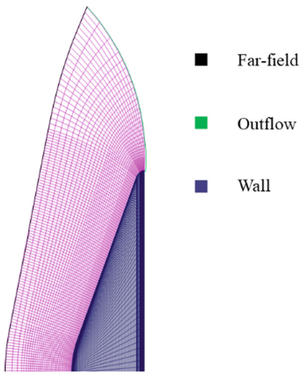

Fig. 2. Mesh and boundary condition of the computational domain

Experimental data have been used to test the reliability of numerical simulations. The comparison shows that our simulations agree well with the experimental data. The comparison is illustrated in Fig. 3.

The input attributes for data modeling are listed in the following Table 3.

The output is heat flux ($q_{wall} < W/m^2 >$). There are 504 measurement results (504 sample points) in total.

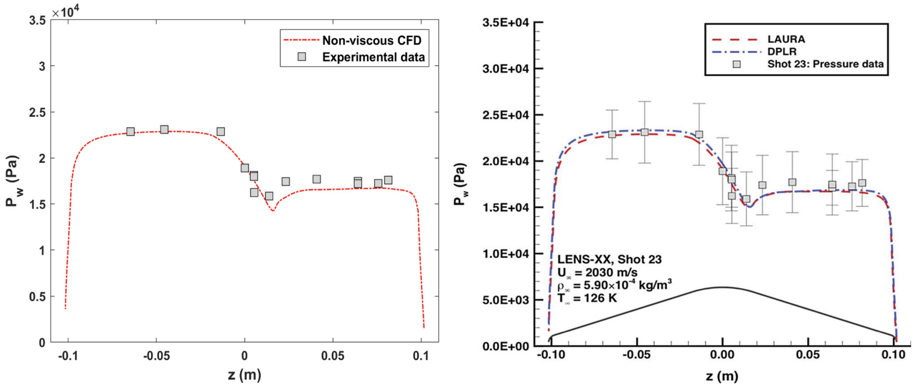

Fig. 3. An example of the comparison of pressures, simulations of inviscid flow (left) and figure from reference [18] (right)

Table 3. List of input attributes

Notation	Physical quantities
P_{edge}	Static pressure at boundary edge (Pa)
T_{edge}	Static temperature at boundary edge (K)
U_{edge}	Magnitude of velocity at boundary edge (m/s)
L_{stag}	Distance from stagnation point to measuring point along the surface (m)
A	Angle between free stream and local surface normal
Ma_{inf}	Mach number of free streams
Re_{inf}	Reynold number of free streams

3.2 Regression Analysis of Aerodynamic Heating Dataset

In this part, performance of three different data modeling algorithms, including backpropagation (BP), basic RNN, and LDSE enhanced RNN, are compared.

To improve the effect of training, all input attributes are linearly mapped to $[-1, 1]$. The target values, heat flux, are distributed in a wide range of order of magnitudes, that is, the linear mapping is executed for logarithmic target values.

The datasets are randomly split into training set and validation set and the loss function in LDSE enhanced RNN is defined as follows

$$f_{loss}^{LDSE-RNN} = (1 - \sigma_{train}) f_{loss}^{train} + \sigma_{train} f_{loss}^{validation} \tag{6}$$

where σ_{train} is the proportion of training set (range from 0 to 1).

The number of hidden neurons ranges from 10 to 100 with step 5 are tested by each training algorithm, which indicates the complexity of the target model. The coefficient of determination (R^2) is used to evaluate the goodness of fit of each model. For each complexity at a given number of hidden neurons, we averaged the performance of model of 20 times with different random seeds. The activation function is set to Tanh. The BP algorithm is called from Pytorch [20] using MSE loss and Adam optimizer. Each run takes iterates 20000 epochs iteration to gain the best R^2 value. The comparison results are shown in Fig. 4.

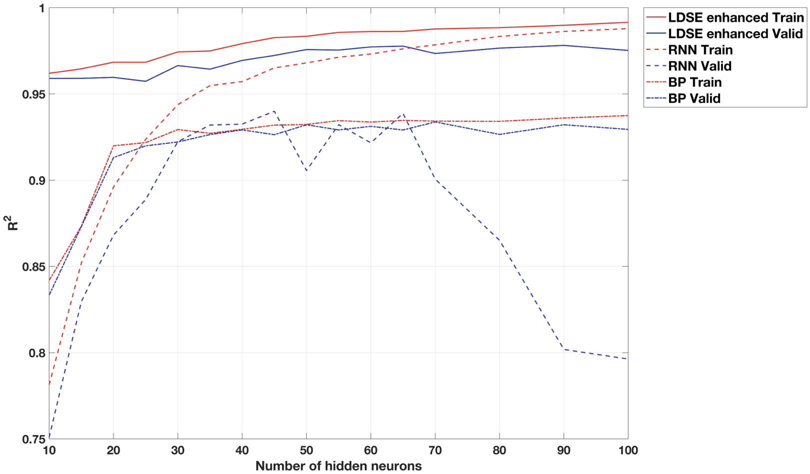

Fig. 4. Correlation performance of different data modeling algorithms with different number of hidden neurons

Figure 4 shows that the model trained by LDSE enhanced RNN has the best performance among these three strategies. Though BP do not tend to overfitting, its regression effect is mediocre. When the number of hidden neurons is over 65, the model trained by RNN is obviously overfitting. In this study, if the performance of models trained by LDSE enhanced RNN with different number of hidden neurons are similar, the lower complexity one will be selected to further study.

The single-hidden layer feedforward neural network has only one hyperparameter, the number of hidden neurons. It is easy to select the suitable model complexity, such as plotting a figure like Fig. 4.

The regression performance of the LDSE enhanced RNN trained model is demonstrated in Fig. 5.

An example of heat flux prediction from the LDSE enhanced RNN trained model is presented (see Fig. 6).

Figure 6 shows that the model's predictions agree well with results from Reference [18], considering the uncertainty intervals at each measurement point. The LDSE enhanced RNN trained model gives cogent predictions of both the order of magnitudes and the trend of distribution for heat flux.

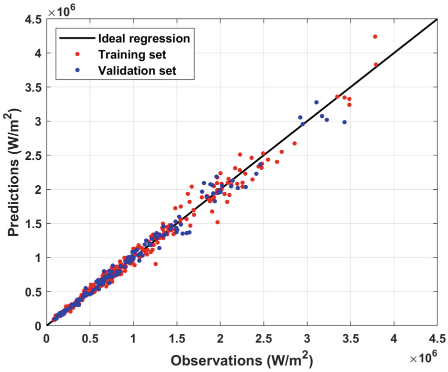

Fig. 5. Performance of the LDSE enhanced RNN trained model with 60 hidden neurons, random seed 2020 (R^2 on training set: 0.9868; R^2 on validation set: 0.9852)

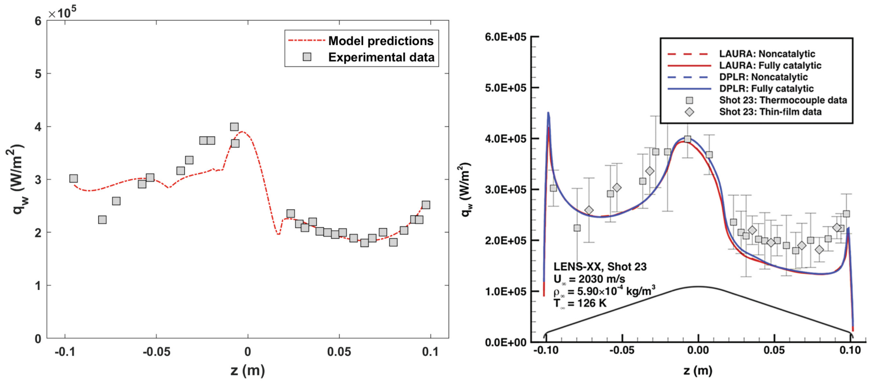

Fig. 6. An example of the comparison of heat flux and model predictions (left), and the figure from reference [18] (right)

4 Conclusion

A special globally optimal learning method combining low dimension simplex evolution (LDSE) and randomize neural network (RNN) has been proposed to model aerodynamic heating from experimental data. The modified method, named LDSE enhanced RNN, is still a kind of single-hidden layer feedforward neural network, and it has a hierarchical global optimality in theory.

Feature engineering of original aerodynamic heating data has also been carried out. Initial states of wind tunnel experiments are processed by computational fluid dynamics (CFD) technique. The numerical simulations of inviscid flow distill the flowfield of the outer edge of boundary layer corresponding to initial inflow conditions. Information of inviscid flow, geometrical parameters, and two parameters from initial states have been used as input attributes in dataset for training a model. The aerodynamic heating dataset contains a relatively small number of samples.

The performance of LDSE enhanced RNN on the aerodynamic heating dataset has been compared with RNN and back propagation (BP). Results show that LDSE enhanced RNN outperforms BP, and is more stable than RNN. The model generated by LDSE enhanced RNN can rapidly give the predictions, and the predicted heat flux agree well with the wind tunnel result. LDSE enhanced RNN has a good ability to balance the complexity and accuracy of model. It is a promising method for aerodynamic heating data modeling.

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