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Nonlinear Design-Space Dimensionality Reduction in Shape Optimization

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ABSTRACT

Many design variables are often required for the optimization design of the whole hull, thus numerous new sample hulls need to be calculated. The dimensionality reduction of design space is essential for the optimization of whole ship design, which can save the consumption of calculation resources. In this paper, a nonlinear dimensionality reduction method called Auto Encoder (AE) based on the neural network is used to optimize the total resistance of the DTMB hull under Fr=0.18 in calm water. Firstly, based on the radius basis function modification method in in-house hull form optimization software—OPTShip-SJTU, a series of hull forms can be obtained under the high-dimensional design space. Then the neural network model is established and trained based on these hull forms. And the low dimensionality space information can be gotten after training. The new hull forms are gotten by the trained neural network. And then the viscous solver naoe-FOAM-SJTU is applied to calculate the resistance of new hull forms. The Kriging theory is used to construct the surrogate model, and the single-objective genetic algorithm is applied to get the lowest total drag hull based on the Kriging surrogate model. Finally, it shows the nonlinear dimensionality reduction method has the capacity for dimensionality reduction in hull form optimization. And we also can obtain optimization results under reduced-dimensionality design space compared with initial high design space.

KEY WORDS: CFD; nonlinear dimensionality reduction; AE; OPTShip-SJTU; total drag optimization;

INTRODUCTION

Simulation-based design optimization (SBDO) becomes the main technique for the design optimization process(Lin, 2018; Liu, 2018a; Nazemian, 2021) in recent years. And the gradient-free methods are also widely used in many fields(Liu, 2020; Park, 2015). Although the gradient-free methods have a wide range, it faces huge time-consuming and curse-of-dimensionality when the design variables increase. Design space dimensionality reduction is an effective measure to solve this problem (D'Agostino, 2017; Reddy, 2020). SBDO consists of three main elements as shown in Fig. 1: (1) hull form deformation tools; (2) the hydrodynamic performance evaluation; (3) high-efficiency optimization algorithms. The dimensionality reduction is applied in pre-processing of hull form modification. The types of dimensionality methods are divided into linear dimensionality (Cunningham, 2015) and non-linear dimensionality method(DeMers, 1993). The difference is whether the linear conversion is used in the dimensionality reduction process.

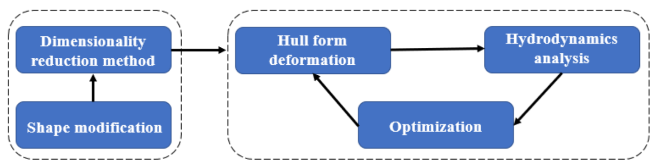

Fig. 1The flowchart of hull form optimization based on dimensionality reduction

In the past few years, many scholars focus on the dimensionality reduction application in hull form optimization. In the aspect of linear dimensionality reduction, Liu (2021) used a linear dimensionality reduction method called principal components analysis (PCA) to decrease the number of design variables and achieved multi-physics field learning based on proper orthogonal decomposition. Diez (2015) suppose the Karhunen–Loève expansion (KLE) method in dimensionality reduction and conduct an off-line dimensionality reduction method for single- and multi-disciplinary shape optimization based on the Karhunen–Loève expansion technique, which is also a linear dimensionality reduction method(Diez, 2016). D'Agostino (2020) used an off-line dimensionality reduction method based on the Karhunen–Loève expansion to optimize a DTMB model. Khan (2021) combined geometry- and physics-informed principal component analysis and the active subspace method in shape optimization. In an aspect of the non-linear dimensionality method, D'Agostino (2017) compared several non-linear dimensionality reduction methods. The dimensionality reduction methods are Kernel Principle Analysis (KPAC), Local Principle Analysis (LPA), and Deep Auto Encoder (DAE). They concluded that the Deep Autoencoder showed the best performance overall. Serani (2016) optimized the calm-water drag of DMTB by reducing the dimensionality of the design spaces, and the deformation methods are free form deformation, radial basis function, and global modification function. The dimensionality reduction methods are KLE, LPCA, KPCA, and DAE.

In this paper, for reducing the computational burden and improving optimization efficiency, we use a non-linear dimensionality based on a neural network to conduct dimensionality reduction at the pre-processing of optimization. We optimize the total resistance of a baseline model DTMB 5415 under Fr=0.18 in calm water. The in-house OPTShip-SJTU is applied to conduct this optimization. The radius basis function deformation method is applied to modify the hull form based on the initial hull form. Before hydrodynamic performance evaluation, the neural network called autoencoder is applied to achieve dimensionality reduction. Naoe-FOAM-SJTU is used to calculate the resistance of the new hull forms obtained from the low dimensionality. The Kriging model is established based on the difference hull form hydrodynamic performances. The single-objective genetic algorithm is applied to search for the lowest total drag hull form.

METHODS

Radial Basis Function Deformation

There are many hull form deformation techniques, including the Shifting method, Radial Basis Function method (RBF), Global Modification Function method (GMF), and Free Form Deformation (FFD). In this paper, we use the RBF deformation method to modify the hull form. The distance between an arbitrary point $\boldsymbol{X}$ and center point $\boldsymbol{X_i}$ can be written as follow:

$$\phi\left(\left\|\mathbf{x}-\mathbf{x}_i\right\|\right), \qquad i=1,2,\cdots,n \tag{1}$$

The interpolate function used in modifying the hull form is defined as:

$$s\left(\mathbf{x}\right)=\sum_{j=1}^{N}\lambda_j\phi\left(\left\|\mathbf{x}-\mathbf{x}_j\right\|\right)+p\left(\mathbf{x}\right) \tag{2}$$

Wheres $\boldsymbol{X}$ denotes the displacement function, which is the movement displacement of control points on the hull form. $\boldsymbol{N}$ is the number of control points. $X_j=(x_j,y,z_j)$ denotes the center of each radial basis function. Basis function φ is the distance function about Euclidean distance. The Compact Support Radial Basis Function (CSRBF) is selected as the basis function (Buhmann, 2001):

$$\phi\left(\left\|X\right\|\right)=\begin{cases}\left\{\left(1-\left\|X\right\|\right)^4\left(4\left\|X\right\|+1\right)\right. & 0\le\left\|X\right\|\le 1\\ 0 & \left\|X\right\|>1\end{cases} \tag{3}$$

$p(\mathbf{X})$ is the low order polynomial of the affine transformation, which can be described as:

$$p\left(\mathbf{X}\right)=c_1+c_2x+c_3y+c_4z \tag{4}$$

The movement distance of control points is known, thus

$$s\left(X_j\right)=f_j \quad , \quad j=1,2,\ldots,N \tag{5}$$

For calculating the unknown coefficient, an attached condition is added, shown as follow:

$$\sum_{j=1}^{N}\lambda_j p\left(X_j\right)=0 \quad , \quad j=1,2,\ldots,N \tag{6}$$

According to the above, we can summarize follow equations:

$$\begin{pmatrix} f\\ 0\end{pmatrix}=\begin{pmatrix}\boldsymbol{M} & \boldsymbol{q}\\ \boldsymbol{q}^T & \boldsymbol{0}\end{pmatrix}\begin{pmatrix}\boldsymbol{\lambda}\\ \boldsymbol{c}\end{pmatrix} \tag{7}$$

where

$$\boldsymbol{\lambda}=[\lambda_1,\lambda_2,\cdots\lambda_n]^T \tag{8}$$

$$\boldsymbol{c}=[c_1,c_2,c_3,c_4]^T \tag{9}$$

$$\boldsymbol{f}=[f_1,f_2,f_3,f_4]^T \tag{10}$$

$$M_{i,j}=\phi\left(\left\|\boldsymbol{X}_i-\boldsymbol{X}_j\right\|\right), \qquad i,j=1,2,\cdots,n \tag{11}$$

$$q=\begin{bmatrix} x_1 & x_2 & \cdots & x_n\\ y_1 & y_2 & \cdots & y_n\\ z_1 & z_2 & \cdots & z_n\\ 1 & 1 & \cdots & 1\end{bmatrix}^T \tag{12}$$

We can get the coefficients by solving these functions. By substituting coordinates of all mesh nodes into the interpolation function, the displacement of corresponding grid nodes can be obtained, and all grid nodes can be relocated accordingly. A box mesh deformation is selected as the example using radial basis function. The deformation effect is shown in Fig. 2

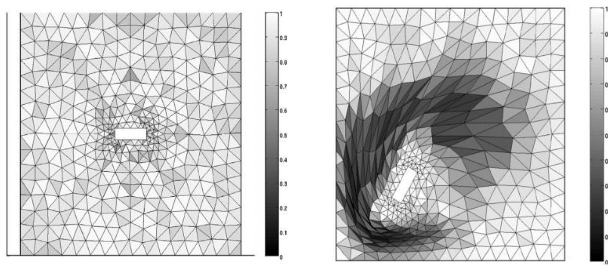

Fig. 2 The diagram of RBF deformation

Non-linear Dimensionality Reduction Method

To achieve the design space dimensionality reduction, the neural network is applied. The architecture of neural work contains three parts in general: input layer, hidden layers, and output layer. Each layer contains some neurons, a 4 layers neural network is selected as example, shown in Fig. 3. The mapping relationships between the input layer and output layer can be gotten by training the neural network parameters.

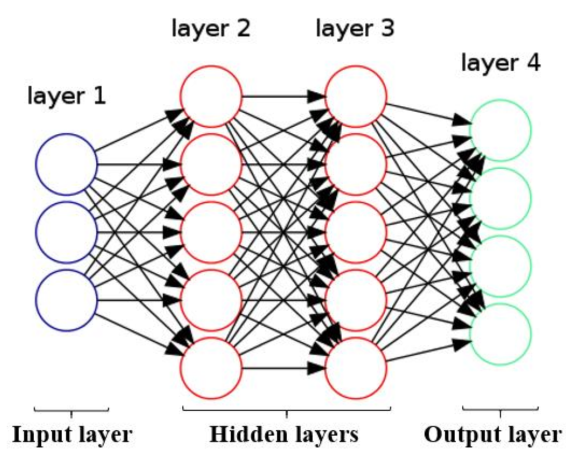

Fig. 3 The architecture of neural network (4 layers neural network)

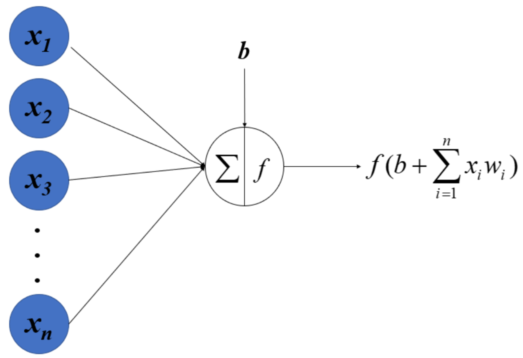

Fig. 4 Example of a neuron

Fig. 4 demonstrates a mathematical formula for a neuron in a neural network. f is a activation function, and the input of this function is weighted summation——($\mathrm{b}+\sum_{i=1}^{n} x_i w_i$), b is bias. The bias is also a weight. There are 2 broad categories of activation, linear and non-linear, like Rectified Linear Units (ReLU), Tanh, Sigmoid activation, and so on. 3 layers trained neural network function can be expressed by the following formula:

$$Q_i=\sum_{i=1}^{J} W_{ij} a(\sum_{k=1}^{K} W_{jk} f(b_{1k}+\sum_{n=1}^{N} x_n w_{kn})+b_{2j})+b_{3i} \tag{13}$$

Where O_i is the output variable; x_n is the input variable; W_{kn}, W_{jk}, W_{ij} are the weights of neurons in each layer; b_{1k}, b_{2j}, b_{3i} are the threshold value of each layer of neurons; i, j, k are the number of neurons in the input layer, the hidden layer, and the output layer in the neural network.

The autoencoder is a structurally symmetrical neural network. It contents two parts, encoder, and decoder, shown in Fig. 5. The encoder maps the raw data to the compressed data (low dimensionality). The decoder maps the compressed data to the initial high dimensionality. The flowchart can be described as following functions:

$$\boldsymbol{l}=E(\boldsymbol{H}_{(1)}\boldsymbol{h}) \tag{14}$$

$$\tilde{\boldsymbol{h}}=D(\boldsymbol{H}_{(2)}\boldsymbol{l}) \tag{15}$$

Where $\boldsymbol{h}$ is the high dimensionality input data, $\boldsymbol{H}$ is a relative weight matrix of an artificial neural network. $\boldsymbol{l}$ is the low dimensionality data. $\tilde{\boldsymbol{h}}$ is the reconstruction data. To verify the neural network model is stable and the low dimensionality can express the initial high dimensionality data information, mean square error (MSE) between the initial input data and reconstruction data is selected as the optimization objective. The neural network parameter $\boldsymbol{H}$ is evaluated by minimizing the MSE. The formula is shown as Eq. (4).

$$MSE=\frac{1}{S}\sum_{k=1}^{S}\|\boldsymbol{h}-\tilde{\boldsymbol{h}}\|^2 \tag{16}$$

The dimensionality number of low dimensionality space is lower than the number of design variables. It means the number of middle layer neurons is lower than the number of design variables. For hull form optimization, the number of sampling points varies exponentially with the number of design variables. After dimensionality reduction, the number of sampling points descends greatly and the time-consuming spending in calculation sampling points hydrodynamic performance decreases.

When a trained neural network is established, the low dimensionality data information can be gotten. We can sample from the low dimensionality and get the new hull form utilizing the decoder neural network. After getting the hull forms from the lower dimensionality, we can get an optimal hull form from these hull forms. The flowchart is shown in Fig. 6.

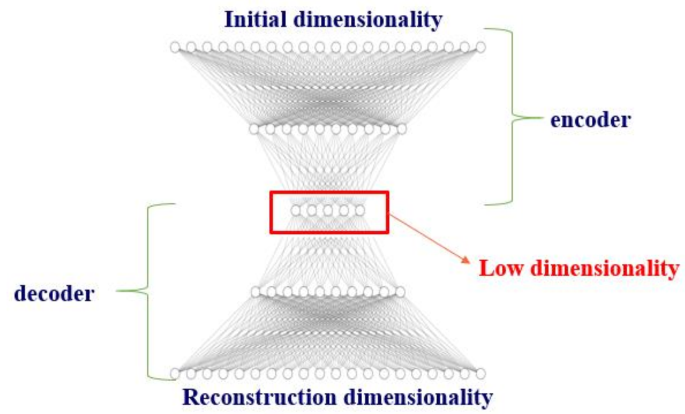

Fig. 5 The diagram of an autoencoder

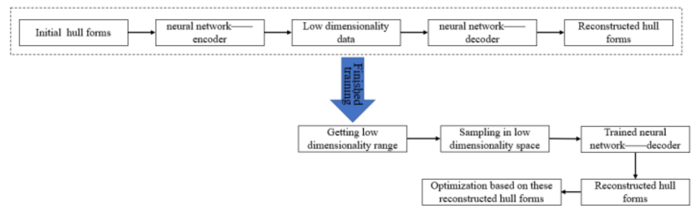

Fig. 6 Flowchart of dimensionality reduction for hull form optimization

Surrogate Model and Optimization Algorithm

Based on the hull forms and corresponding hydrodynamic performance data, the surrogate model can be used to fitting the reflection between the hull forms and hydrodynamic performances. the surrogate model is applied to establish the relationship between the hydrodynamic performance and the hull form deformation parameters. The surrogate models have the Kriging model (Liu, 2018b), Response surface methodology (RSM) (Kim, 2011), Support Vector Regression (SVR) (Smola, 2004), and neural network (Liu, 2020). In this paper, we use the Kriging model as the surrogate model. The Kriging model is presented firstly in 1951 by Krige (Krige, 1951). The Kriging model is a interpolate model, which is the linear weighted sum of sampling function values:

$$\hat{y}(\boldsymbol{x})=\sum_{i=1}^{n} w^{(i)} y^{(i)} \tag{17}$$

The $w^{(i)}$ is the weights. For calculating the weights, the stochastic process approach is used:

$$Y(\boldsymbol{x})=\beta_0+Z(\boldsymbol{x}) \tag{17}$$

The β is an unknown constant, denote the mathematical expectation of $Y(\boldsymbol{x})$. The $Z(\boldsymbol{x})$ satisfy normally distributed (0, σ^2), and non-zero covariance. By introducing a probabilistic approach, we can get any unknown function value. After establishing the Kriging surrogate model, we can use the optimization algorithm to search the lowest resistance hull form. The single-objective genetic algorithm is used in this paper. The algorithm is divided into 5 parts:

(1) Generating the initial population and encoder the value of each individual called genic encoder;
(2) Calculating the fitting value of each individual. The smaller the fitting value, the better individual;
(3) Selected the good performance individual as the next generation;
(4) The genic of each individual cross to create new individual;
(5) Changing the new individual genetic code randomly;
The flowchart of genetic algorithm is shown in Fig. 7. The iterations are

250 and the initial population is 60, the crossover fraction of genes swapped between individuals is set as 0.8, and the mutation rate is 0.2.

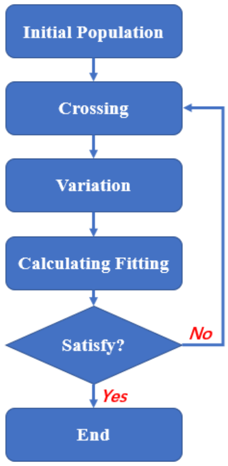

Fig. 7 The flowchart of genetic algorithm

APPLICATION

Design Space Construction and Hull Form Deformation

In this paper, a baseline model DTMB 5415 is selected as the optimization objective hull. The shape and main particulars of the hull are shown in Fig. 8 and Table 1.

Fig. 8 DTMB model

Table 1. the main particulars of DTMB

parameter	value
Length between perpendiculars/ m	5.719
Length of waterline/ m	5.726
Displacement volume of a hull/ m^3	0.554
Draft/ m	0.248
The maximum beam of waterline/ m	0.768

The optimization objective is total resistance. The optimization problem can be described as follows. For the low dimensionality space, the $\boldsymbol{x} \in R^l$. For the high dimensionality space, the $\boldsymbol{x} \in R^h$.The optimization is conducted in low dimensionality.

$$\begin{aligned} \text{minimize} \quad & R_t(\boldsymbol{x}) \\ \text{subject to} \quad & L_{pp}(\boldsymbol{x}) = L_{pp\_initial} \\ & \Delta B(\boldsymbol{x}) \le 0.01 B_0 \\ & |\Delta V(\boldsymbol{x})| \le 0.05 V_0 \\ & |\Delta S(\boldsymbol{x})| \le 0.05 S_0 \\ & -0.005 \le \boldsymbol{x} \le 0.005 \end{aligned}$$

28 mesh points are selected as the deformation design variables. the distribution of deformation points on the hull surface is shown in Fig. 9. The experimental design method called Optimized Latin Hypercube Sampling method (OLHS) is applied to obtain the sampling points. The ranges of 28 design variables are listed in Table 2. The distribution of design variables about X1 and X20 is shown in Fig. 10.

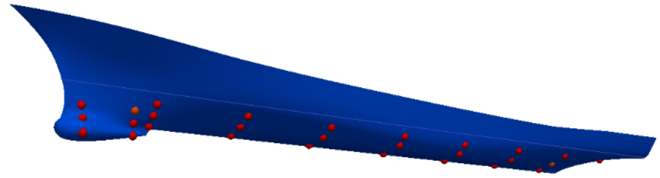

Fig. 9 The selected deformation points distribution

Table 2 the range of design variables

Design variables	Deformation direction	Value range
X_1	y	$-0.005 \le X_1 \le 0.005$
X_2	y	$-0.005 \le X_2 \le 0.005$
…	…	…
X_{28}	y	$-0.005 \le X_{28} \le 0.005$

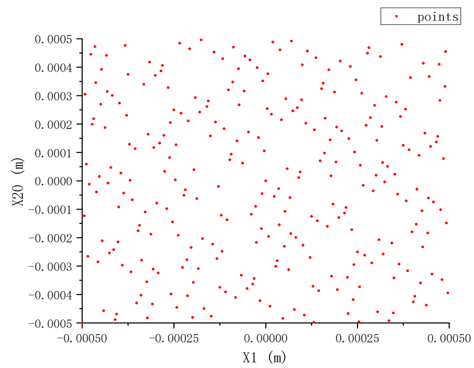

Fig. 10 The distribution of design variables about X_1 and X_{20}

After getting the sampling points, the RBF deformation based on the deformation module of OPTShip-SJTU is used to create different hull forms, see Fig. 11, the deformation effect of DTMB 5415 utilizing RBF Deformation method. 5600 hulls form are generated by the RBF deformation method to generate the hull form data set. Based on the hull form data set, the neural network achieves using several variables to express the hull form data set information, which is the dimensionality reduction.

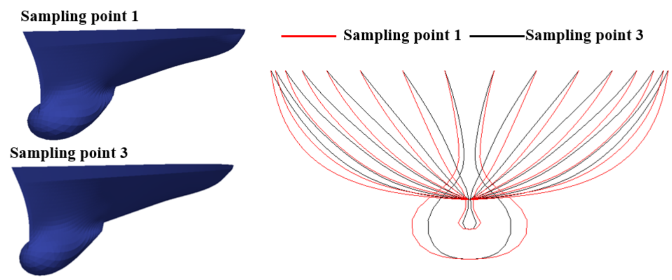

Fig. 11 The deformation diagram

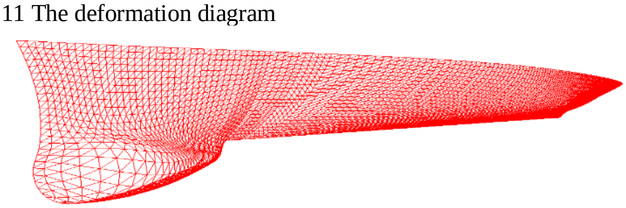

Fig. 12 The mesh points of DTMB

Dimensionality Reduction Model Establishment

The number of hull mesh is 5050, shown in Fig. 12. The example of a sampling hull mesh point coordinates is shown in Table 3. The mesh point coordinates are selected as the input and the output is also the mesh point coordinates, which means learning itself by this neural network. The autoencoder architecture is shown in Fig. 13.

Table 3 The example of a sampling hull mesh point coordinates

Number	x coordinate	y coordinate	z coordinate
1	-0.323991	-5.29415e-06	-0.0433653
2	0.3895	-7.46956e-06	-0.0512381
……	……	……	……
5049	-0.494027	0.00300887	-0.00447348
5050	-0.494111	0.00151207	-0.004544

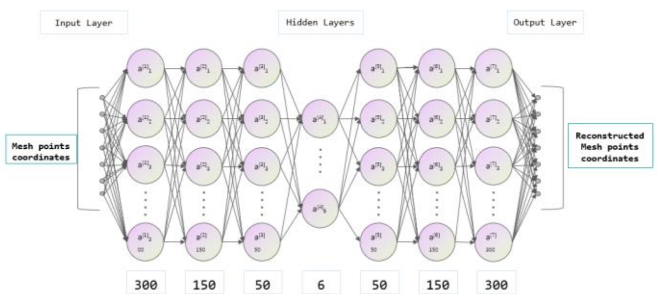

Fig. 13 The established neural network for dimensionality reduction

The neural network is established based on the open-source artificial intelligence platform TensorFlow. The number of middle layer neurons is 6, less than the initial 28 design variables. The total layer number is 7. The total number of neurons is 1006. The activation function is Relu. Adam is selected as the optimizer, the MSE is the optimization objective for training. 4480 hull forms are used to train the neural network model. 1120 hull forms are used to verify the neural network model. After 500 iterations, the MSE reaches about 0.03 and satisfies the requirement, shown in Fig. 14.

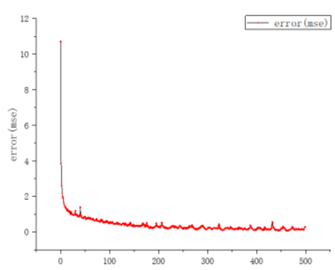

Fig. 14 The MSE trend during training

For evaluating the reconstruction error between the initial hull form and reconstruct hull form obtained from decoder neural network, sampling point 1 and sampling 2 are selected as the comparison to check the reconstruction error, see Fig. 15. The max error is 0.00038 and satisfies the requirement.

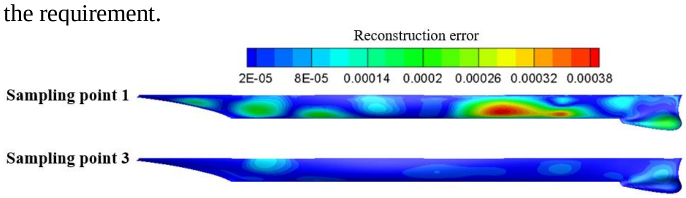

Fig. 15 The reconstruction error of sampling 1 and sampling 2

Low Dimensionality Sampling and Optimization

Based on the trained neural network, we can get low dimensionality information. According to the trained neural network, we can get the boundary of low dimensionality, see Table 4.

Table 4 The boundary of low dimensionality space

Low dimensionality design variables	range
X_1'	$-244.2 \leq X_1' \leq 161.1$
X_2'	$-0.005 \leq X_2' \leq 0.005$
X_3'	$-0.005 \leq X_3' \leq 0.005$
X_4'	$-0.005 \leq X_4' \leq 0.005$
X_5'	$-0.005 \leq X_5' \leq 0.005$
X_6'	$-0.005 \leq X_6' \leq 0.005$

After getting the boundary of low dimensionality space, the OLHS method is also applied to sample from the low dimensionality space. Fig. 16 shows the distribution of X_1' and X_6'.

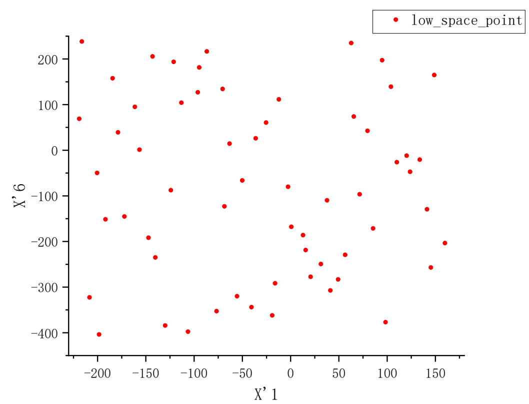

Fig. 16 The distribution of X_1' and X_6'

When the low dimensionality space samplings are gotten, the decoder is used to obtain the reconstructed hull form, the reconstruction effect can refer to Fig. 17. Benefit from the auto-encoder, only 60 cases need to be calculated by naoe-FOAM-SJTU to get the resistance of hull. If the dimensionality reduction is not used, 280 hull forms need to be calculated for optimization.

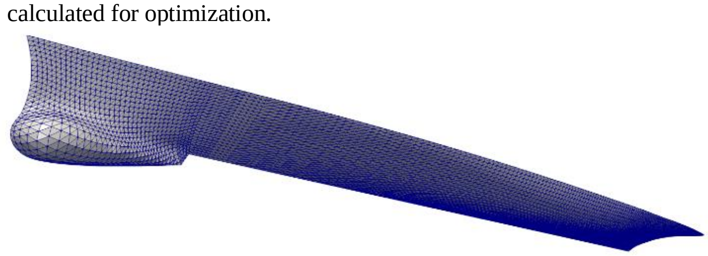

Fig. 17 The hull form sample 58 reconstructed from low dimensionality space

Based on the 60 hull form resistances, the Kriging model is established based on the Kriging theory. The single-objective genetic algorithm is used to obtain the optimal hull form. And the final optimization result can be summarized in Table 5. According to the optimization results, we can realize non-linear dimensionality reduction can also get the optimal hull form, and it can improve the optimization efficiency greatly at the same time.

Fig. 18 demonstrates the hull form line comparison between the initial hull form and optimal hull form.

Table 5 The optimization results

	$Rt/*10^{-3}$	Optimization effect
Initial hull form	3.97	19.31%
Optimal hull form (obtained from low dimensionality)	3.17	

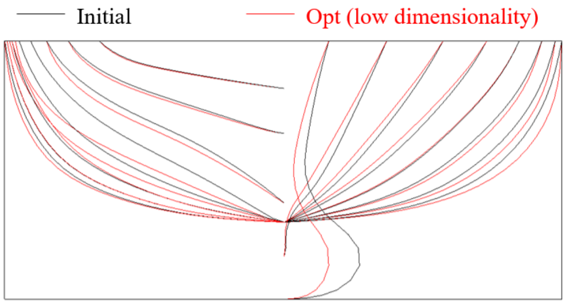

Fig. 18 The hull line comparison between the initial hull form and optimal hull forms

CONCLUSIONS

In this paper, the neural network called autoencoder is applied to conduct dimensionality reduction at pre-processing of hull form optimization. the baseline model DTMB is selected as the optimization hull. The resistance is the optimization objective at the Fr=0.18 under calm water condition. Results indicate the non-leaner dimensionality reduction method can be used for hull form optimization and improving the optimization efficiency. The optimal hull form still can be gotten under the low dimensionality space. Non-linear dimensionality method can achieve a lower dimensionality information extraction compared with linear dimensionality reduction. But the non-linear dimensionality method cannot describe the rule in low dimensionality. Some conclusions can be summarized as following points:

(1) the OPTShip-SJTU has the capacity for design space dimensionality reduction in hull form optimization.

(2) the application of a neural network can achieve a better dimensionality reduction effect.

(3) the resistance drops by 19.31%, and the hull form optimization efficiency has increased by about 79.6%.

(4) compared with other methods, the non-linear dimensionality method can obtain a better efficiency improvement and keep a good optimization result.

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