



## An Improved N-dimensional NURBs-based Metamodel

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### A B S T R A C T

Non uniform rational b-splines (NURBs) have proved to be very promising for metamodeling in engineering problems, because they have unique properties such as local modification scheme, strong convex hull property, and infinitely differentiability, etc. Since NURBs are defined by control points, knot vector, and weights associated with control points, the precision of NURBs is influenced by all of the parameters. In order to improve the accuracy and calculation efficiency, an enhanced method of building NURBs metamodel is presented. Some improvements are made in certain aspects, such as: improving the data normalization method and the calculating method of weight coefficient. Compared with the existing methods, this method can calculate the weight coefficient of each control point more quickly, because it avoids the inverse operation of correlation matrix, which may cause singular. Several classic numerical examples show that the presented method is effective for building approximate model with higher accuracy than existing NURBs metamodel.

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## 1. INTRODUCTION

Computationally-expensive problems are often found in engineering designs [1, 2]. For example, simulation and analysis processes are expensive to run and often considered black-box functions [3]. Metamodel is a widely used strategy to approximate expensive analyses or simulation processes. In the last two decades, metamodeling techniques have been successfully applied to engineering designs especially for modeling and optimization.

Polynomial regression or interpolation based on classical design of experiments is called the initial response surface model or metamodel. Besides the commonly used polynomial functions, other types of models include radial basis functions (RBF) [4], Kriging [5] based on stochastic model, support vector regression (SVR) [6] model. Neural Networks [7] have also been applied in generating the response surfaces for system approximation. Each model has its adaptability. Therefore, there is no conclusion about which model is definitely superior to the others [8]. However, insights have been gained through a number of studies [9, 10]. In

general, the Kriging models are found more accurate for nonlinear problems, but it is difficult to obtain and use because a global optimization process should be applied to identify the maximum likelihood estimators. The RBF model seems to reach a tradeoff of accurate and efficiency between Kriging and polynomials. Tested SVR can achieve high accuracy over all other metamodeling techniques, but the reasons of theoretical foundation is not clear for why it can outperforms others. Recently, Wang [8] reviewed the applications of metamodeling techniques in the context of engineering design and optimization, and especially made surveys of metamodeling for high dimensional problems [3, 11]. It can be seen from the recent reviews that in order to reach acceptable accuracy, the metamodeling cost grows exponentially with the dimension of corresponding problems. Due to the computational challenge for modeling and optimization of high dimensional problems, these traditional approaches appear inadequate to model problems with large variables. Therefore, high dimensional model representation (HDMR) has drawn more and more attention in engineering. The theoretical foundation is an integrable function which can be decomposed into summands of different dimensions. Therefore, the

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HDMRs have a characteristic which expands a d-dimensional function into summands of different functions of less than d-dimensions. The details and research progress about HDMR are surveyed in [11]. Friedman [12] proposed the multivariate adaptive regression splines (MARS) [13] and fast MARS model, which take the tensor product of spline function as the basis function. Instead of truncated power basis functions, the multivariate adaptive regression B-spline (BMARS) [14] algorithm uses the B-splines as basis function, which will have superior numerical properties than truncated power basis functions. MARS and BMARS have shown their ability for high dimensional and lager data interpolation problems. Because B-spline basis functions have characteristics of local support and smooth connection, they are suitable for incremental construction of large data. Turner proposed a NURBS-based metamodel and extended it to model N-dimension problems [15]. Non Uniform Rational B-splines (NURBs) are proved to be very promising for metamodeling in engineering problems, because they have unique properties such as local modification scheme, strong convex hull property, and infinitely differentiability, etc. Since NURBs are defined by control points, knot vector, and weights associated with control points, the precision of NURBs is influenced by all of the parameters. This paper illustrates an improved N-dimensional NURBs-based metamodel compared with [15]. This method can calculate the weight coefficient of each control point more quickly, because it adopts a new method of calculating the correlation vector and correlation matrix. It avoids the inverse operation of correlation matrix which may cause singular.

The present paper is organized as follows. Section 2 introduces foundation of NURBs approximation. Section 3 proposes the improved N-dimensional NURBs-based metamodel, which adopts a more reasonable method to calculate the weight of NURBs. Section 4 studies the behavior of the proposed method through several numerical tests. Conclusions are drawn in Section 5.

## 2. NURBS MATHEMATICS

The rational basis function of NURBs curve is:

$$R_{i,k}(t) = \frac{\omega_i N_{i,k}(t)}{\sum_{j=0}^n \omega_j N_{j,k}(t)} \quad (1)$$

The equation of NURBs curve can be defined as:

$$C(t) = \sum_{i=0}^n P_i R_{i,k}(t) = \frac{\sum_{i=0}^n P_i \omega_i N_{i,k}(t)}{\sum_{i=0}^n \omega_i N_{i,k}(t)} \quad (2)$$

where,  $k$  is the order.  $t$  is normalized parameter of design variable,  $t \in [0, 1]$ .  $P$  is a vector defining the  $n$  control points,  $w_i$  is a positive scalar defining the weight of the  $i^{th}$  control point, and  $N_{i,k}(t)$  is the B-spline basis function given as a parametric function of  $t$ . The B-spline basis function is defined by the following recursive function:

$$\begin{cases} N_{i,0}(t) = \begin{cases} 1, & \text{if } u_i \leq t < u_{i+1} \\ 0, & \text{otherwise} \end{cases} \\ N_{i,k}(t) = \frac{t - u_i}{u_{i+k} - u_i} N_{i,k-1}(t) + \frac{u_{i+k+1} - t}{u_{i+k+1} - u_{i+1}} N_{i+1,k-1}(t) \\ 0/0 = 0 \end{cases}, \quad k > 0 \quad (3)$$

where,  $U = [u_0, u_1, \dots, u_{n+k+1}]$  is knot vector which is calculated by Cox-de Boor recursion formula. Based on the tensor product theory, the N-dimensional NURBs function can be define as:

$$R(t_1, t_2, \dots, t_n) = \frac{\sum_{i_1=0}^{n_1} \sum_{i_2=0}^{n_2} \dots \sum_{i_N=0}^{n_N} \omega_{i_1, i_2, \dots, i_N} P_{i_1, i_2, \dots, i_N} N_{i_1, k}(t_1) N_{i_2, k}(t_2) \dots N_{i_N, k}(t_N)}{\sum_{i_1=0}^{n_1} \sum_{i_2=0}^{n_2} \dots \sum_{i_N=0}^{n_N} \omega_{i_1, i_2, \dots, i_N} N_{i_1, k}(t_1) N_{i_2, k}(t_2) \dots N_{i_N, k}(t_N)} \quad (4)$$

Research shows that models higher than quadratic produce little benefit, while diluting the local influence of control points [15]. Therefore, it can meet the precision requirement for  $k=2$ . Based on formula (4), in order to build a NURBs-based metamodel based on a given dataset  $D(X)$  ( $X$  is n-dimension variable vector), the main tasks are estimating control point weights, establishing knot vectors, and determining dependent control point coordinates.

## 3. IMPROVED N-DIMENSIONAL NURBS-BASED METAMODEL

Turner [15] proposed an N-dimension NURBS-based metamodel called HyPer Model. The main aspects of constructing NURBs metamodel are discussed in detail, such as the data normalization, determining weights of control point, knot vectors and dependent control point coordinates. As we know, just as NURBs curve or surface, the modeling accuracy is largely depends on the weights of control points. One of the main contributions of [15] is establishing a method to estimating control point weights. The weights in [15] are determined by a correlation matrix and its inverse. However, the inverse operation of correlation matrix may cause calculating difficulties when it is singular. Based on HyPer Model, we studied a new method to estimate weights of control point and enhance the accuracy of NURBs metamodel.

**3. 1. Estimating Control Point Weights** For a NURBs curve defined by (2), the most significant properties related to the weights are:

(1) The curve will be pull toward (or push away from) control point  $P_i$  if increasing or decreasing) the value of weight  $w_i$ . When the value of  $w_i$  becomes infinity, the curve passes through control point  $P_i$  and when  $w_i$  is zero, control point  $P_i$  has no impact on the curve.

(2) Local approximation. If a control point  $P_i$  is moved or its weight  $w_i$  is changed, it will affect only that portion of the curve on the interval  $t \in [u_i, u_{i+k+1})$ .

Therefore, the modeling accuracy is largely depends on the weights of control points. For control point  $P_i$ , the weight is determined by its neighborhood. The control point weights are estimated by [15] using a spatial correlation function with Equations (5) to (7).

$$w_{cp} = w_{min} + (w_{max} - w_{min})(\mathbf{r}^T \mathbf{R}^{-1} \mathbf{r}) \tag{5}$$

where,  $w_{cp}$  is the weight of the control point,  $w_{min}$  (set 0.1) is the minimum weight value,  $w_{max}$  (set 1) max is the maximum weight value.  $\mathbf{r}$  and  $\mathbf{R}$  are correlation vector and matrix derived from the spatial correlation function (SCF) [16].

$$R_{i,j} = R(t_i, t_j) = e^{-\theta |t_i - t_j|^p} \tag{6}$$

$$r_i = R(t_{cp}, t_i) = e^{-\theta |t_{cp} - t_i|^p} \tag{7}$$

where,  $t$  is the parametric coordinate of input variables.  $\mathbf{r}$  is derived from the spatial correlation function of the parametric control point location ( $t_{cp}$ ) and the location of the  $i^{th}$  nearby neighbor data points ( $t_i$ ).  $\mathbf{R}$  is derived from the spatial correlation function of the location of data point  $t_i$  and the location of data point  $t_j$ . In order to limit the computational cost of inversion,  $\mathbf{r}$  and  $\mathbf{R}$  are calculated based on the 10 nearest neighbors to each control point rather than the entire dataset [15].  $\theta$  defines the range of influence of the data ( $\theta > 0$ ), and  $p$  defines the smoothness of the model, which are discussed in detail in literature [15]. With the increase of samples, rows of the  $\mathbf{R}$  matrix become very similar. Therefore, it becomes a nearly singular matrix and it is difficult to get its inverse. The SCF of Equation (6) referred to as the Gaussian model is known to result in unstable kriging systems due to the behavior of the covariance model for short separation distances. Sasena [16] and Turner [15] have improved the model, the parameter  $p$  is limited to [0, 1.99] and [0, 2], respectively.

In fact, as Turner [15] presented, the more distance between a control point and its nearest neighboring data

points, with the less confidence is in the location of the control point. Thus, the control point weight should be reduced. Therefore, we try to use a simple method to determine the weight like inverse distance weighted interpolation, where, weights are usual inverse proportion to a power of distance and direct proportion to its slope. So, we define the weight as Equation (8). Multiple dimensions can be handled through a tensor product of the single dimension weights.

$$w_{cp} = w_{min} + (w_{max} - w_{min}) \frac{\sum r_i}{\sum R_{ij}} der(m_{cp}) \tag{8}$$

where,  $m$  is the normalized current metamodel, and  $der(m_{cp})$  represents the normalized derivative of the current metamodel at the current control point location ( $t_{cp}$ ).

**3. 2. Procedure of Building Nurbs-Based Metamodel**

The procedure of building NURBs-based metamodel is described as following based on literature [15].

Step 1. Random sampling. Anyrandom sampling method is available, such as the Latin hypercube sampling method.

Step 2. Data normalization. Chord length method is adopted to normalize the N dimensions data  $D(x^1, x^2, \dots, x^i, \dots, x^n)$ . It is worth mentioning that, the normalization method given by Turner [15] can not guarantee the normalized value belong to the interval [0, 1].

Step 3. Establishing initial model. Establish the initial model with control points at each corner and an open knot vector. Control point weights are calculated by the Equations (6) to (8).

Step 4. Identifying the location of maximum error. Compare this error to the user tolerance, and check the unused data set's correlation to the model data. Stop if the model has converged.

Step 5. Increasing control points and updating knot vector by the method as Turner [15].

Step 6. Calculating control point weights by the Equation (6) to (8).

Step 7. Calculating control point locations by Equation (4).

Step 8. Establishing the new NURBs metamodel, and go to Step 4.

**4. EXPERIMENTAL TRIALS**

Several classic numerical functions are selected for building their NURBs approximate models and compared with other methods by the following measure criteria.

**4. 1. Measure Criteria** The coefficient of determination ( $R^2$ ) of regression model, relative average absolute error (RAAE), and the maximum error are evaluated and compared.

(1) The coefficient of determination ( $R^2$ ).

$$R^2 = 1 - \frac{\sum_{i=1}^m (f_i - \hat{f}_i)^2}{\sum_{i=1}^m (f_i - \bar{f}_i)^2} \tag{9}$$

where,  $m$  is the number of samples, and the  $f_i$  and  $\hat{f}_i$  are the true function value and predicted value calculated from the approximation model at the  $i^{\text{th}}$  testing point respectively, and  $\bar{f}_i$  is the average value of  $\hat{f}_i$ .  $R^2$  describes the proportion of variance of the dependent variable. The better of the approximation model, the values of  $R^2$  is closer to 1.

(2) Relative average absolute error (RAAE)

$$RAAE = \frac{\sum_{i=1}^n |f_i - \hat{f}_i|}{m \cdot STD} \tag{10}$$

where, STD is standard deviation, and the smaller the value of RAAE, the approximation model has better accuracy.

**4. 2. Numerical Tests** Some well-known benchmark functions are used to test for accuracy. All these functions are approximated with the presented enhanced NURBs (Mark as ENURBs) model and HyPer Model. In order to facilitate comparison, the metamodels are constructed through with same sampling size and sampling strategy (equidistant sampling).

**Test (1): Tangent function**

$$f = \tan x, \quad x \in [-4\pi/9, 4\pi/9] \tag{11}$$

The function is smooth and relatively easy to construct metamodel. Therefore, the accuracy of both HyPer Model and ENURBs are satisfactory. Figure 1 is the metamodel of Test (1) by ENURBs model. As shown from Table 1, although the Maximum error of HyPer Model is little than ENURBs, the values of RAAE and  $R^2$  of ENURBs are equal or better than the values of HyPer Model.

**Test (2): sinusoidal function**

$$f(x) = 10 - \sin(x) - e^{x/100}, \quad 0 \leq x \leq 10 \tag{12}$$

As shown in Table 2. The accuracy of both HyPer Model and ENURBs for Test (2) are satisfactory. In Figure 3, the horizontal axis represents the values of

samples and the longitudinal axis represents the difference of absolute error between HyPer Model and ENURBs, which is the absolute errors of HyPer Model subtracted the absolute errors of ENURBs. Therefore, if the difference scatter above the  $Z=0$ , it represents that the absolute error of HyPer Model is greater than ENURBs, and contrariwise, if the difference scatter below the  $Z=0$ , it represents that the absolute error of ENURBs is greater than HyPer Model.

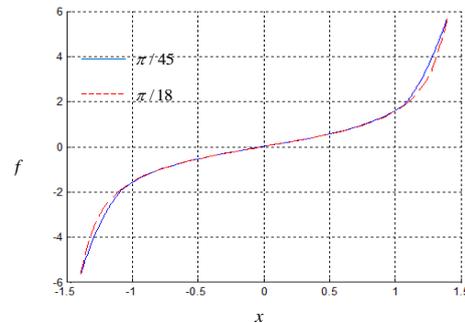
**Test (3): Six-hump camel-back (SC) function**

$$f(x_1, x_2) = 4x_1^2 - 2.1x_1^4 + \frac{1}{3}x_1^6 + x_1x_2 - 4x_2^2 + 4x_2^4 \tag{13}$$

It is shown from Table 3 that the values of RAAE and Maximum errors of ENURBs are less or equal to the values of HyPer Model. Therefore, the ENURBs has more accuracy than HyPer Model for this function.

**TABLE 1.** Comparison of the NURBs models for tangent function.

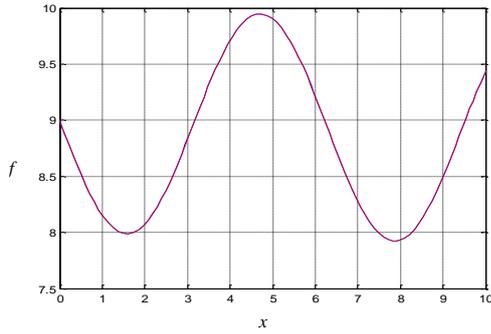
Sampling distance		$\pi / 45$	$\pi / 18$
$R^2$	HyPer Model	0.9993	0.9869
	ENURBs	0.9993	0.9871
RAAE	HyPer Model	0.0168	0.0786
	ENURBs	0.0166	0.0781
Maximum error	HyPer Model	0.1843	0.5906
	ENURBs	0.1882	0.6121



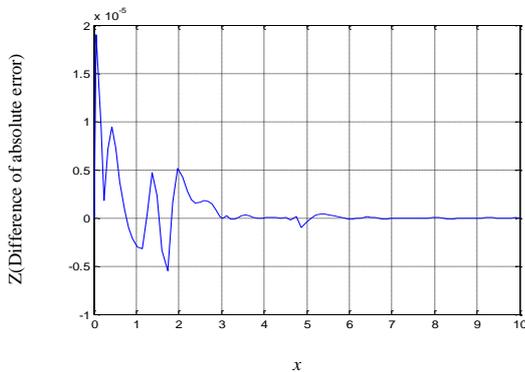
**Figure 1.** The metamodel of  $f = \tan x$  built by ENURBs model. The blue solid line and the red dotted line are built by sampling distance of  $\pi / 45$  and  $\pi / 18$ , respectively.

**TABLE 2.** Comparison of the NURBs models for sinusoidal function.

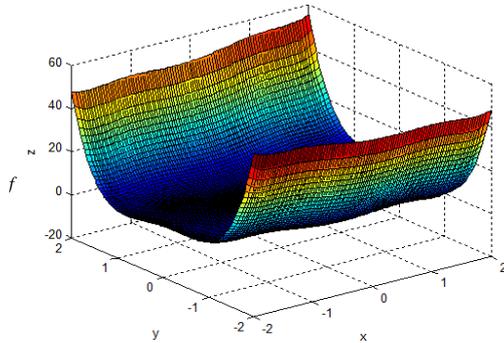
Sampling distance		0.1	0.5
$R^2$	HyPer Model	0.9999983	0.9999732
	ENURBs	0.9999983	0.9999732
RAAE	HyPer Model	0.0011257	0.0045287
	ENURBs	0.0011268	0.0045239
Maximum error	HyPer Model	0.0012496	0.0049921
	ENURBs	0.0012496	0.0049831



**Figure 2.** The metamodel of sinusoidal function built by ENURBs model with sampling distance of 0.1.



**Figure 3.** The difference of absolute error between HyPer Model and ENURBs for sinusoidal function.



**Figure 4.** The metamodel of SC function built by ENURBs model with sampling distance of 0.2.

**TABLE 3.** Comparison of the NURBs models for SC function.

Sampling distance		0.1	0.2
$R^2$	HyPer Model	1.0000	0.9995
	ENURBs	1.0000	0.9996
RAAE	HyPer Model	0.0039	0.0148
	ENURBs	0.0037	0.0139
Maximum error	HyPer Model	0.2055	0.7640
	ENURBs	0.2007	0.7479

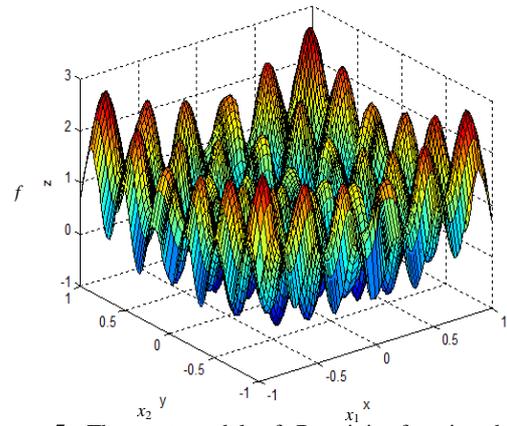
**Test (4):** Rastrigin function

$$f(x_1, x_2) = x_1^2 + x_2^2 - \cos 18x_1 - \cos 18x_2, x_{1,2} \in [-1, 1] \quad (14)$$

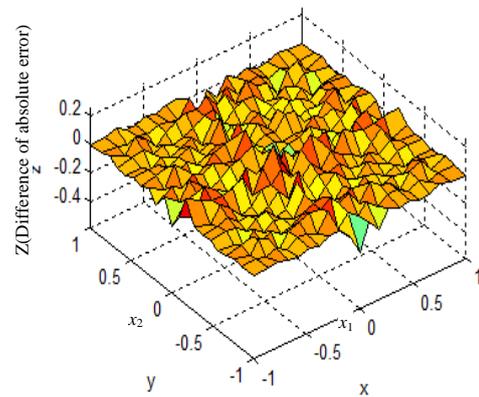
As shown in Table 4, the values of  $R^2$ , RAAE and Maximum errors of ENURBs are better than the values of HyPer Model. In Figure 6, the  $x_1, x_2$  represents the values of samples and the Z axis represents the difference of absolute error between HyPer Model and ENURBs.

**TABLE 4.** Comparison of the NURBs models for Rastrigin function.

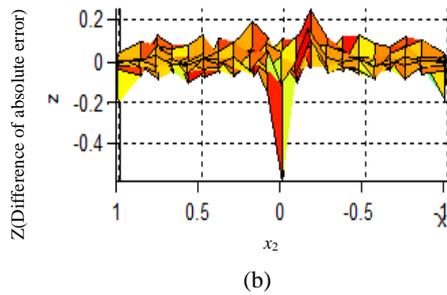
Sampling distance		0.1	0.2
$R^2$	HyPer Model	0.8937	0.8945
	ENURBs	0.9316	0.9268
RAAE	HyPer Model	0.2658	0.7423
	ENURBs	0.2090	0.7044
Maximum error	HyPer Model	1.1015	2.6577
	ENURBs	1.0715	2.4235



**Figure 5.** The metamodel of Rastrigin function built by ENURBs model with sampling distance of 0.2.



(a)



**Figure 6.** The difference of absolute error between HyPer Model and ENURBs for Rastrigin function. (a) and (b) are the Isometric view and  $X_2OZ$  direction projection respectively about the difference of absolute error between HyPer Model and ENURBs.

## 5. CONCLUSION

NURBs have unique advantages which make it suitable for constructing metamodel. Turner [15] proposed an N-dimension NURBS-based metamodel called HyPer Model, which is proved very effective. However, the accuracy of NURBs is influenced by many parameters. How to determine the reasonable parameter values is important. The accuracy of NURBs model largely depends on the weights of control points. The control point weights of HyPer Model are estimated based on spatial correlation function. However, with the increase of samples, rows of the correlation matrix, derived from the spatial correlation function, become very similar, resulting in a nearly singular matrix and making it difficult to get its inverse. We try to use a simple method to determine the weight like inverse distance weighted interpolation, where, weights are usually inversely proportional to a power of distance. Based on the modified weight calculation method and data normalization method, an improved N-dimension NURBS-based metamodel is studied. Compared with the existing method, this proposed method can calculate the weight coefficient of each control point more quickly, because it avoids the inverse operation of correlation matrix. Several classic numerical examples show that the presented method is effective for building approximate model with higher accuracy. In addition, the sampling method and sampling efficiency is not in the scope of this study, which is studied in-depth based on HyPer Model.

## 6. ACKNOWLEDGMENTS

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Metamodel

Weight Coefficient

منحنیهای غیر یکنواخت گویا (NURBS) برای متامدل در مسائل مهندسی بسیار امیدوار کننده هستند، چرا که آنها دارای خواص منحصر به فرد مانند طرح اصلاح شده محلی، خاصیت بدنه محدب قوی و مشتق پذیری بی نهایت و غیره می باشند. از آنجا که NURBS توسط نقاط کنترل، بردار گره، و وزن مرتبط با نقاط کنترل تعریف شده اند، دقت NURBS توسط تمام پارامترهای تحت تاثیر قرار می گیرد. به منظور بهبود دقت و محاسبه بهره وری، یک روش بهبود یافته از ساخت NURBS متامدل ارائه شده است. بعضی از اصلاحات در زمینه های خاصی ساخته شده اند: از قبیل بهبود روش نرمال سازی داده ها، تاریخ و محاسبه روش ضریب وزن. با مقایسه روش های موجود با یکدیگر، این روش می تواند ضریب وزن هر نقطه کنترل را با سرعت بیشتری محاسبه کند، به دلیل آن که از عملیات معکوس ماتریس همبستگی که ممکن است باعث منحصر به فرد بودنش شود، جلوگیری می کند. چندین مثال عددی کلاسیک نشان می دهد که روش ارائه شده برای ساخت و ساز مدل تقریبی با دقت بالاتر از متامدل NURBS موجود موثر است.

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