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A surrogate model based on NURBS entities for engineering problems

B. Vuillod^{1,2}, M. Zani², L. Hallo¹, E. Panettieri² and M. Montemurro²

¹French Atomic Energy Commission, Le Barp, France
²Université de Bordeaux, Arts et Métiers Institute of Technology, CNRS, INRA, Bordeaux INP, HESAM Université, I2M UMR, Talence, France

Abstract

Surrogate models are increasingly used in many sectors due to their ability to reproduce structural/system responses starting from numerical or experimental results. The main goal of a surrogate model is to preserve the same accuracy as the original model (within a certain interval) by considerably reducing the computational cost and, possibly, the required resources.

Among the methods available in the literature, the one proposed in this article is based on Non-Uniform Rational Basis Spline (NURBS) entities. In this context, these entities appear promising, as they are continuous, versatile, able to adapt to Multiple-Input-Multiple-Output problems, and can be modified locally without impacting the precision of the metamodel elsewhere in the definition domain, i.e., possess capabilities for local support. Conversely, the *off-line* tasks that allows generating the NURBS-based surrogate model can be relatively heavy. In this paper, we propose an optimisation strategy for reducing the amount of data required to drive the NURBS metamodel while still maintaining a good accuracy level.

Keywords: metamodel, gradient-based optimisation, fitting, NURBS hyper-surfaces, multiple-input-multiple-output, resources gain

1 Introduction

Despite the increase in computing power and resources over the past two decades, solving complex numerical problems with real-time processing or optimisation requirements still remains intractable. For this reason, much research effort has been focused on metamodelling techniques (also known as surrogate modelling techniques), which allow the computational burden to be reduced while maintaining a good level of accuracy for the problem at hand [1].

A metamodelling process consists of defining an approximation of a high-fidelity model requiring less resources to be executed than the original model. More precisely, a metamodel is used to map input variables into output responses even when the relationship between the two are not well defined or computationally expensive to evaluate [2]. Depending on the problem, the term resources can have different meanings. For example, surrogate models can be employed to reduce the number of data to stock as in image reduction [3], while a metamodel generated for optimisation purposes aims to reduce the computational cost to evaluate the outputs for a given sets of inputs [4, 5]. Several techniques have been developed for metamodelling all requiring a systematic approach composed of a calibration step, a training of the model parameters, and evaluation of the accuracy of the metamodel [2].

Among the existing metamodelling techniques [1, 2, 5-7], this study relies on the utilisation of M-D Non-Uniform Rational Basis Spline (NURBS) hyper-surfaces, defined over a N-D parametric domain to approximate a given set of data points called Target Points (TPs). NURBS entities offer many intrinsic advantages [1] compared to the other metamodelling techniques, and their use as surrogate model has been widely discussed in [1,8,9].

This work aims to generalise the metamodelling strategy based on NURBS hypersurfaces proposed by Audoux et al., [1]. Particularly, in [1], the strategy has been coupled to a hybrid optimisation algorithm composed of the union of a special Genetic Algorithm (GA) [10] and a general purposes gradient-based algorithm, i.e., the activeset method [11], to optimise all the integer and continuous parameters involved in the definition of the NURBS hyper-surfaces. The GA developed in [10] is used to optimise both integer variables, i.e., degrees and number of Control Points (CPs), and continuous variables, i.e., the inner components of the knot vectors and the weights, of the NURBS entity. The CPs coordinates are derived through an analytical formula (and the associated algorithm) discussed in [1]. Afterwords, only the weights and the inner components are optimised by using a gradient-based algorithm. However, in [1], the gradient of both the cost function and of the constraint functions were calculated by finite differences; accordingly, the computational cost of the second step remains too high.

To go beyond the aforementioned limits, the analytical expression of the gradient of the NURBS-based metamodel with respect to weights and knot vector components is proposed in this work to speed up the second step of the optimisation process discussed in [1]. The effectiveness of the proposed approach is illustrated through meaningful benchmarks taken from the literature.

The paper is organised as follows. Section 2 gives an overview of the fundamentals of the NURBS geometric entities, whilst Section 3 focuses on the generation of the metamodel based on NURBS entities as a solution of an optimisation problem where the goal is to approximate a generic set of data points. Section 4 shows the application of the method through two test cases. Lastly, Section 5 ends the paper with conclusions and prospects.

In this paper upper-case bold letters and symbols are used to indicate matrices, while lower-case bold letters and symbols indicate column vectors.

2 Non-Uniform Rational Basis Spline Entities

NURBS entities are a generalisation of basis spline (B-spline) entities, which generalise the Bézier ones [12]. Originally employed in Computer-Aided Design (CAD) software in the 1990s as curves and surfaces, these entities are now used in several domains such as topology optimisation [13, 14], shape optimisation [15], anisotropy field optimisation for variable-stiffness composites [16], and surrogate model generation [1].

In this work, NURBS hyper-surfaces are used as surrogate models. These geometrical entities are considered as a general vector-valued functions $\mathbb{R}^N \to \mathbb{R}^M$ where N and M are respectively the input and output space dimensions. The goal is to fit a dataset of $N_{\text{TP}} = \prod_{k=1}^{N} (r_k + 1)$ TPs \mathbf{Q} of dimension M (i.e., each TP is defined in \mathbb{R}^M), coming from experiments or numerical simulations results.

Formally speaking, NURBS are able to approximate the behaviour of a model $\mathcal{M}: \mathbb{R}^N \to \mathbb{R}^M$. Their general parametric explicit form reads:

$$\mathbf{H}(\zeta_1,\cdots,\zeta_N) = \frac{\sum_{i_1=0}^{n_1}\cdots\sum_{i_2=0}^{n_2}N_{i_1,p_1}(\zeta_1)\dots N_{i_N,p_N}(\zeta_N)\omega_{i_1,\cdots,i_N}\mathbf{P}_{i_1,\cdots,i_N}}{\sum_{j_1=0}^{n_1}\cdots\sum_{j_2=0}^{n_2}N_{j_1,p_1}(\zeta_1)\dots N_{j_N,p_N}(\zeta_N)\omega_{j_1,\cdots,j_N}}, \quad (1)$$

with **H** the NURBS hyper-surface evaluated at the normalised coordinates $(\zeta_1, \dots, \zeta_N)$ and $\mathbf{P}_{i_1,\dots,i_N}$ the *M*-D array of CPs containing $N_{\text{CP}} = \prod_{k=1}^N (n_k + 1)$ CPs having *M* coordinates (i.e., the single CP is defined in \mathbb{R}^M). For each CP, one can also introduce its respective weight $\omega_{i_1,\dots,i_N} > 0$. Finally, N_{i_k,p_k} are the Bernstein's polynomials equations of degree p_k , evaluated recursively with the following Cox and De Boor algorithm [12]:

$$\begin{cases} N_{i_k,0}(\zeta_k) = \begin{cases} 1, \text{ if } v_{i_k} < \zeta_k < v_{i_{k+1}}, \\ 0, \text{ ortherwise,} \end{cases} \\ N_{i_k,q_k}(\zeta_k) = \frac{\zeta_k - v_{i_k}}{v_{i_k+q_k} - v_{i_k}} N_{i_k,q_k-1}(\zeta_k) + \frac{v_{i_k+q_k+1} - \zeta_k}{v_{i_k+q_k+1} - v_{i_k+1}} N_{i_k+1,q_k-1}(\zeta_k), \end{cases}$$
(2)

with $q_k = 1, ..., p_k$, ζ_k the dimensionless parameter along the parametric direction k and v_{i_k} the i_k -th component (knot) of the non-periodic and non-uniform knot-vector of length $m_k + 1$:

$$\mathbf{v}_{k}^{\mathrm{T}} = \{\underbrace{0, \cdots, 0}_{p_{k}+1}, v_{p_{k}+1}, \cdots, v_{m_{k}-p_{k}-1}, \underbrace{1, \cdots, 1}_{p_{k}+1}\}, \text{ with } m_{k} = n_{k} + p_{k} + 1.$$
(3)

In the rest of this paper, the knots $v_{i_k} \neq [0, 1]$ are called non-trivial knots, or inner knots, to distinguish them from the trivial ones $v_{i_k} = [0, 1]$. The knot-vector allows to define the range of variation of basis functions that are non-zero between $p_k + 1$ successive knots. Moreover, the trivial knots force the NURBS entities to pass exactly through the TPs defined on the boundary of the manifold. For more information on the fundamental properties of NURBS entities, the interested reader is referred to [12].

3 A NURBS-based metamodel

The steps required to generate a metamodel based on NURBS hyper-surfaces, similar to other metamodelling strategies, care essentially two: the *off-line* part and the *on-line* part. The first one represents the learning phase during which a database, from experiments or numerical results, is built and used to generate the metamodel. Depending on its accuracy, which is based on the evaluation of an error estimator, it can be optimised. The second one corresponds to the use of the metamodel, which replaces the original high-fidelity model.

The flowchart in Fig. 1 presents the main steps of the *off-line* part. The global scalar parameters, i.e., r_k , n_k and p_k can be set following literature guidelines [1, 12, 15, 18]. However, the evaluation of N_{i_k,q_k} , ω_{i_1,\dots,i_N} and $\mathbf{P}_{i_1,\dots,i_N}$ is a quite challenging task. The Bernstein's polynomials $N_{i_k,q_k}(u_k)$, are evaluated recursively with the algorithm Eq. (2) at each dimensionless parameter u_k at which the NURBS hyper-surface is evaluated (the dimensionless coordinates u_k can be calculated directly from the input variables [19]). The inner components of the knot vector \mathbf{v}_k can be initialised as uniform or by considering the De Boor's algorithm [17] and then optimised later. Moreover, the weights ω_{i_1,\dots,i_N} can be initialised either by setting them equal to 1 or by considering empirical rules as discussed in [8].

Subsequently, it is necessary to compute the CPs coordinates, $\mathbf{P}_{i_1,\dots,i_N}$. They are calculated from the database via the resolution of a least-square by using a dedicated algorithm conceived for multi-dimensional hyper-surface fitting problems [1]. The goal of the least-squares problem is to determine the optimum value of the CPs coordinates by minimising the difference between **H** and **Q**, i.e.:

$$f_{\rm obj} = \sum_{i=1}^{M} \sum_{j=1}^{N_{\rm TP}} \left(H_i(\mathbf{u}_j) - Q_i) \right)^2.$$
(4)

Therefore, by differentiating the above expression with respect to the CPs coordi-

nates, one gets:

$$\begin{split} \min_{\mathbf{P}}(f_{\text{obj}}) &\Rightarrow \frac{\partial}{\partial \mathbf{P}} \left(\sum_{i=1}^{M} \sum_{j=1}^{N_{\text{TP}}} \left(H_i(\mathbf{u}_j) - Q_i \right) \right)^2 \right) = 0, \\ &\Rightarrow (\mathbf{N}^{\text{T}} \mathbf{N}) \mathbf{P} = \mathbf{N}^{\text{T}} \mathbf{Q}, \\ &\Rightarrow \mathbf{P} = (\mathbf{N}^{\text{T}} \mathbf{N})^{-1} \mathbf{N}^{\text{T}} \mathbf{Q}, \end{split}$$
(5)

where N is a multi-dimensional array containing all the Bernstein's polynomial evaluated at the dimensionless coordinates corresponding to the values of the input variables used to build the database of TPs. The calculation of the multi-dimensional array N and the determination of the CPs coordinates are anything but trivial and require dedicated algorithms. For more details on these aspects, the interested reader can refer to [1].



Figure 1: The main steps of the workflow needed to generate the metamodel based on NURBS entities.

After the determination of the optimum value of the CPs coordinates, the obtained objective function f_{obj} is checked by comparing it to the required accuracy, in terms of average relative error ε_{obj} , which is defined *a priori* by the user. If this convergence check is met, the metamodel based on B-spline hyper-surfaces can be used. Otherwise, two further steps are considered corresponding to just as many optimisation problems. The first optimisation aims to minimise the objective function f_{obj} with respect to the

coefficient β_{i_k} , used to compute the inner knots v_{i_k} of each knot vector \mathbf{v}_k according to the strategy presented in for surface fitting problems [15]. At each iteration of the optimisation process, the CPs coordinates are updated according to Eq. (5), where the array N is updated by computing the Bernstein's polynomial using the new optimised knot vector according to Eq. (2). The second gradient-based optimisation aims to minimise the objective function f_{obj} with respect to the weights $\boldsymbol{\omega}$. The details of the related algorithm work-flow are shown in Fig. 2, where ξ_i are the optimisation variables, i.e., β_k or $\boldsymbol{\omega}$. Each optimisation is performed by using the Sequential Least Squares Programming (SLSQP) algorithm and by considering only the following box constraints: $\beta_{i_k} \in [\beta_{lb}, \beta_{ub}]$, and $\boldsymbol{\omega} \in [\omega_{lb}, \omega_{ub}]$. It is noteworthy, that at the end of each optimisation, the value of the objective function of the optimised solution is compared with ε_{obj} to determine if the criterion on the required accuracy is satisfied.



Figure 2: Workflow of the gradient-based optimisation to determine the optimum value of the inner components of the knot vectors (updating the CPs) and of the weights.

The analytical expression of the gradient of the cost function with respect to knotvector components and weights has been obtained by generalising the approach presented in [15] and more details will be provided during the speech.

4 Numerical results

This section shows the effectiveness of the proposed metamodelling strategy through two test cases. The first test case deals with the approximation of a plane closed parametric curve, taken from [13]. The second benchmark focuses on approximating the maximum displacement of a thin plate under bending forces, by considering as input variables the thickness and the applied force.

4.1 Benchmark 1: The four-leaf clover

The four-leaf clover is a plane closed curve described by two outputs, x and y, as a function of the angle θ (the input variable), as follows:

$$\begin{cases} x(\theta) = \cos(\theta)\sin(2\theta), \\ y(\theta) = \sin(\theta)\cos(2\theta), \end{cases} \quad \theta \in [0, \ 2\pi].$$
(6)

The considered Single-Input-Multiple-Output (SIMO) system is characterised by N = 1 input and M = 2 outputs. The overall number of TPs is $N_{\text{TP}} = r_1 + 1 = 54$ and the degree of the Bernstein's polynomial is set as $p_1 = 2$. The design variables together with their bounds for the knot vector components and weights are summarised in Table ??.

n_1	p_1	m_1	$\beta_{\rm lb}$	$\beta_{ m lb}$	$\omega_{ m lb}$	$\omega_{ m lb}$
10, 15	2	13, 18	0	1	1	10

Table 1: Design variables and their bounds for the four-leaf clover problem.

Fig. 3 shows the results of the gradient-based optimisation of the NURBS curve by considering the inner components of the knot vector and the weights as design variables according to the algorithm illustrated in Fig. 1. The optimised solutions illustrated in Fig. 3 are obtained by considering two values of the number of CPs, i.e., $N_{\rm CP} = 11$ and $N_{\rm CP} = 16$.



Figure 3: Results of the gradient based optimisation for the approximation of the fourleaf clover curve. Plots (c) - (d) show the differences in the curve fitting for $n_1 = 10$ and $n_1 = 15$, i.e., respectively with $N_{\rm CP} = 11$ and $N_{\rm CP} = 16$.

However, a number of CPs $N_{\rm CP} = 11$ is not sufficient to correctly approximate the curve, as shown in Fig. 3-(c). In fact, increasing the number of CPs to $N_{\rm CP} = 16$, results in an objective function value 100 times lower than the one. Nonetheless, the gain obtained in optimising the weights and the knot vector components has the same

	n_1	Initial B-spline	Optimised B-spline	Optimised NURBS	Gain [%]
$f_{\rm obj}$	10	$1.21 \cdot 10^{-1}$	$1.036 \cdot 10^{-1}$	$0.86 \cdot 10^{-1}$	28.9
$f_{\rm obj}$	15	$3.7\cdot10^{-3}$	$3.36 \cdot 10^{-3}$	$3.32 \cdot 10^{-3}$	10.1

Table 2: Results of the gradient based optimisation for the four-leaf clover curve fitting problem. The gain is evaluated comparing the initial B-spline with the optimised NURBS.

order of magnitude for both cases. This result confirms one of the guidelines provided by [18], which specifies to consider at least a ratio of number of CPs to number of TPs equal to 1/3 to have a good approximation.

4.2 Benchmark 2: The thin plate under bending force

The second test case belongs to the field of solid mechanics and it consists of study the out of plane displacement of a thin plate under bending force. The geometry and boundary conditions for the thin plate are illustrated in Fig. 4.



Figure 4: Geometries and boundary conditions for test case 2.

The metamodel aims at providing the displacement along the z axis of the node where the force is applied for different values of the thickness t and force F. The thickness t varies in the range [1, 10] mm, and the force F varies in the interval [150, 300] N. The metamodel is characterised by two inputs N = 2 and one output M = 1. The Finite Element (FE) model is made of 1250 SHELL181 elements with four nodes and six degrees of freedom per node. The number of elements has been chosen as a result of a convergence analysis (not reported here for the sake of brevity). The set of TPs (whose total number is $N_{\rm TP} = 400$), obtained through a nonlinear FE static analysis carried out via the ANSYS code, is represented by the displacement along the z axis of the node where the force is applied for different values of t and F. A bi-linear elastic perfectly plastic material model is considered in the non-linear static analysis whose properties are listed in [20]. The design variables together with their bounds for the knot vector components and weights are summarised in Table **?**:

Fig. 5 shows the displacement along z axis of the node where the force is applied for for different values of t and F.

Table 3: Design variables and bounds for the optimisation problem of benchmark 2.



Figure 5: Contour plot of the predicted displacements. Plots (a) and (b) present the behaviour of the metamodel for constant force and thickness, respectively.

As for test case 1, the efficiency of the gradient based optimisation method, is measured by evaluating the decreasing of the objective function as listed in Table ??. The results of this second test case show the effectiveness of applying the optimised

Initial B-splineOptimised B-splineOptimised NURBSGain [%]
$$f_{\rm obj}$$
 $8.7 \cdot 10^{-1}$ $4.173 \cdot 10^{-5}$ $4.166 \cdot 10^{-5}$ 99.99

Table 4: Results of the optimisation strategy for the thin plate under bending. The gain is evaluated comparing the initial B-spline with the optimised NURBS.

NURBS-based metamodel to a physical case. In this case, the ratio between the number of CPs and TPs is $N_{\rm CP}/N_{\rm TP} \approx 1/3$, which satisfies the minimum condition of [18]. However, the $N_{\rm CP}$ is not sufficient to approximate with good accuracy the initial database without the optimisation. Accordingly, after the optimisation, the error is greatly reduced and the final gain from the optimisation is almost 100 %. Finally, a good initialisation of the parameters combined with an intelligent optimisation makes

it possible to obtain promising first results for this type of optimised NURBS-based metamodel.

5 Concluding remarks

This paper presents an innovative metamodelling technique based on NURBS hypersurfaces. Thanks to its versatility, the proposed approach can be easily employed for problems of different complexity.

Moreover, when the number of CPs is sufficiently high, the optimisation of the knot vectors components and the weight not systematically required. However, when the database is poor in terms of data points amount, or if the number of CPs is reduced for storage reasons, the error criterion will be no longer satisfied. Accordingly, the optimisation of the inner components of the knot vectors and the weights associated to the CPs, should be performed to improve the solution accuracy.

Nonetheless, the gradient-based optimisation may introduce noise into the approximated results. Therefore, to overcome this limitation a smoothing term should be introduced in the expression of the objective function. Research is ongoing on this aspect.

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