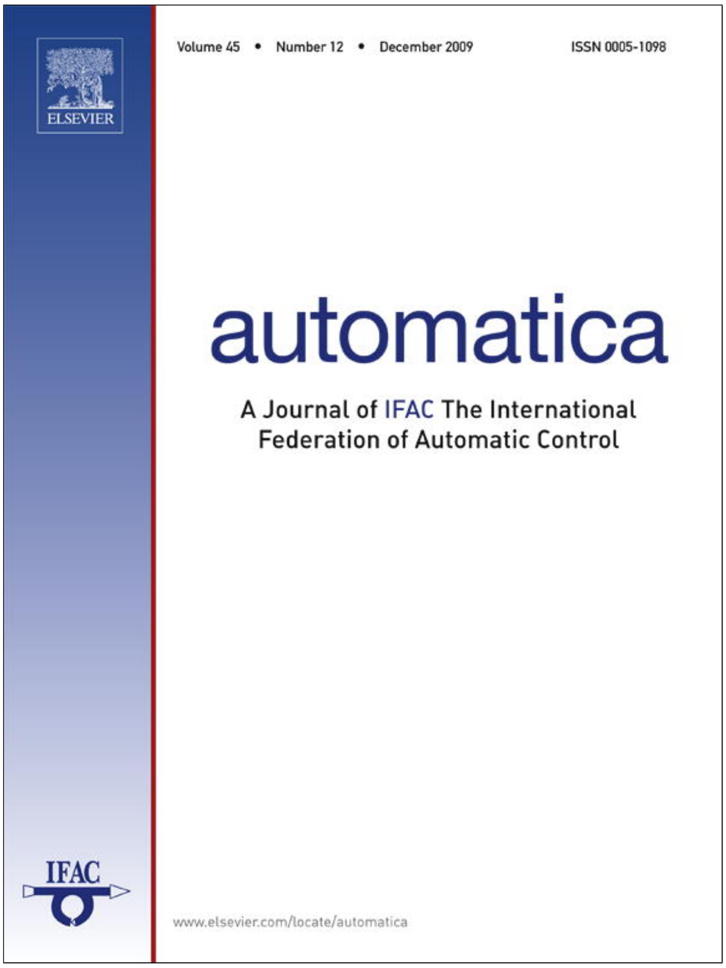
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Brief paper

A new approach to linear regression with multivariate splines ☆

C.C. de Visser *, Q.P. Chu, J.A. Mulder

Control and Simulation Division, Faculty of Aerospace Engineering, Delft University of Technology, P.O. Box 5058, 2600GB Delft, The Netherlands

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ABSTRACT

A new methodology for creating highly accurate, static nonlinear maps from scattered, multivariate data is presented. This new methodology uses the B-form polynomials of multivariate simplex splines in a new linear regression scheme. This allows the use of standard parameter estimation techniques for estimating the B-coefficients of the multivariate simplex splines. We present a generalized least squares estimator for the B-coefficients, and show how the estimated B-coefficient variances lead to a new model quality assessment measure in the form of the B-coefficient variance surface. The new modeling methodology is demonstrated on a nonlinear scattered bivariate dataset.

1. Introduction

The creation of accurate static nonlinear maps from scattered, multivariate data is a non-trivial problem in many fields of science and engineering. Many methods exist for creating such maps such as neural networks, polynomial neural networks, kernel methods, and multivariate splines. Multivariate splines have as advantage over other methods that they consist of ordinary multivariate polynomials. Multivariate splines have, until recently, been limited to approximating data on rectangular grids. Anderson et al. showed in Anderson, Cox, and Mason (1993) that multivariate tensor product splines are incapable of approximating scattered multivariate data. Recently, Awanou et al. presented a new type of multivariate spline, the multivariate simplex spline, which is capable of approximating scattered multivariate datasets (Awanou, Lai, & Wenston, 2005). The scheme for creating the multivariate simplex splines from scattered data as presented in Awanou et al. (2005), however, does not allow the use of standard parameter estimation techniques for estimating the parameters of the multivariate simplex splines and their variances.

The objective of this paper is to present a new methodology for creating accurate static nonlinear maps from scattered, multivariate data. This new methodology is based on a new linear regression scheme for multivariate simplex splines. This new linear regression scheme enables the use of standard parameter estimation techniques for estimating the parameters of the multivariate simplex splines. In this paper a generalized least squares estimator for the parameters of the multivariate simplex splines is introduced. The linear regression scheme allows the estimation of the variances in these parameters which, together with their spatial location, facilitates the definition of a spatial parameter variance structure. This structure aids the localization of model deficiencies and may complement the process of model structure selection.

2. Preliminaries on multivariate simplex splines

This section serves as a brief introduction on the theory of the multivariate simplex spline. For a more complete and in-depth coverage of the matter, we would like to refer to the work of Lai and Schumaker (2007).

2.1. The simplex and barycentric coordinates

The basis polynomials of the simplex spline are defined on simplices. A simplex is a geometric structure that provides a minimal, non-degenerate span of n-dimensional space. For example, the 2-simplex is the triangle and the 3-simplex the tetrahedron. A simplex is defined as follows. Let V be a set of $n+1$ unique, non-degenerate, points in n-dimensional space:

$$V := \{v_0, v_1, \ldots, v_n\} \in \mathbf{R}^n. \quad (1)$$

Then the convex hull of V is the n-simplex t:

$$t := \langle V \rangle . \quad (2)$$

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* Corresponding author.
E-mail addresses: c.c.devisser@tudelft.nl (C.C. de Visser), q.p.chu@tudelft.nl (Q.P. Chu), j.a.mulder@tudelft.nl (J.A. Mulder).

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The simplex has its own local coordinate system in the form of the barycentric coordinate system. The principle of barycentric coordinates is the following; every point $x = (x_1, x_2, \ldots, x_n)$ inside or outside an n-simplex t, with t as in (2), can be described in terms of a unique weighted vector sum of the vertices of t. The barycentric coordinate $b(x) = (b_0, b_1, \ldots, b_n)$ of x with respect to simplex t are these vertex weights:

$$x = \sum_{i=0}^{n} b_i v_{p_i}, \qquad \sum_{i=0}^{n} b_i = 1 \tag{3}$$

with p_i sorted vertex indices, i.e. $p_i < p_{i+1}$.

2.2. Triangulations of simplices

A triangulation $\mathcal{T}$ is a special partitioning of a domain into a set of J non-overlapping simplices.

$$\mathcal{T} := \bigcup_{i=1}^{J} t_i, \qquad t_i \cap t_j \in \left\{\emptyset, \tilde{t}\right\}, \quad \forall t_i, t_j \in \mathcal{T} \tag{4}$$

with the edge simplex $\tilde{t}$ a k-simplex with $0 \le k \le n-1$.

One of the most commonly used triangulation methods is the Delaunay triangulation. Fig. 1 shows a simple Delaunay triangulation consisting of three simplices (triangles).

2.3. Spline spaces

A spline space is the space of all spline functions s of a given degree d and continuity order C^r on a given triangulation $\mathcal{T}$. Such spline spaces have been studied extensively, see e.g. Lai (1990), Lai and Schumaker (1998) and Lai and Schumaker (2007). We use the definition of the spline space from Lai and Schumaker (2007):

$$S_d^r(\mathcal{T}) := \{s \in C^r(\mathcal{T}) : s|_t \in \mathbb{P}_d, \ \forall t \in \mathcal{T}\} \tag{5}$$

with $\mathbb{P}_d$ the space of polynomials of degree d. For example, $S_3^1(\mathcal{T})$ is the space of all cubic spline functions with continuity order C^1 defined on the triangulation $\mathcal{T}$.

2.4. The B-form of the multivariate simplex spline

The simplex spline is a B-spline in the sense that it can be expressed in the well known B-form, see de Boor (1987). The B-form follows from the multinomial theorem:

$$(b_0 + b_1 + \cdots + b_n)^d = \sum_{\kappa_0+\kappa_1+\cdots+\kappa_n=d} \frac{d!}{\kappa_0!\kappa_1!\cdots\kappa_n!} \prod_{i=0}^{n} b_i^{\kappa_i}. \tag{6}$$

Introducing the multi-index κ:

$$\kappa := (\kappa_0, \kappa_1, \ldots, \kappa_n) \in \mathbf{N}^{n+1}. \tag{7}$$

The 1-norm of the multi-index is:

$$|\kappa| = \kappa_0 + \kappa_1 + \cdots + \kappa_n = d, \quad d \ge 0. \tag{8}$$

The factorial of the multi-index is defined as:

$$\kappa! = \kappa_0!\kappa_1!\cdots\kappa_n!. \tag{9}$$

Lai and Schumaker (2007) introduced a very useful *lexicographical* sorting order on the elements of the multi-index:

$$\begin{aligned}&\kappa_{d,0,0\cdots0} > \kappa_{d-1,1,0\cdots0} > \kappa_{d-1,0,1,0\cdots0} > \cdots \\ &\qquad > \kappa_{0\cdots0,1,d-1} > \kappa_{0\cdots0,0,d}.\end{aligned} \tag{10}$$

The total number of valid permutations of κ is $\hat{d}$:

$$\hat{d} = \frac{(d+n)!}{n!d!} \tag{11}$$

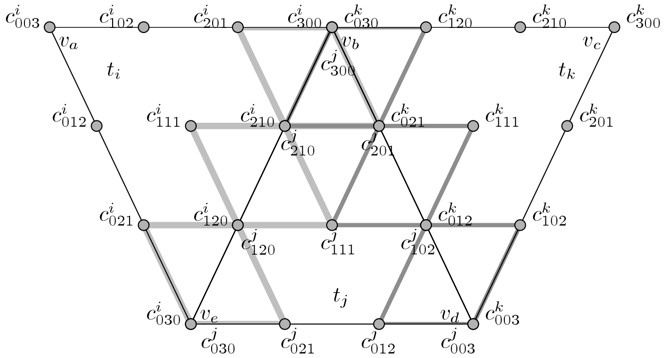

Fig. 1. B-net for third degree basis function on 3 simplices together with C^1 continuity structure (bold lines).

with the multi-index the multinomial equation (6) can be simplified into:

$$(b_0 + b_1 + \cdots + b_n)^d = \sum_{|\kappa|=d} \frac{d!}{\kappa!} b^{\kappa}. \tag{12}$$

The *basis function* $B_\kappa^d(b)$ of the multivariate spline can now be defined as follows:

$$B_\kappa^d(b) := \frac{d!}{\kappa!} b^{\kappa}. \tag{13}$$

de Boor proved (de Boor, 1987) that $\left\{B_\kappa^d(b), \ \kappa \in \mathbf{N}^{n+1}, \ |\kappa| = d\right\}$ is a stable basis for the space of polynomials of degree d. This means that any polynomial $p(b)$ of degree d can be written as a linear combination of B_κ^d 's as follows:

$$p(b) = \sum_{|\kappa|=d} c_\kappa B_\kappa^d(b). \tag{14}$$

This is the B-form of the multivariate simplex spline. In (14), c_κ is a vector of coefficients called control coefficients, or more commonly, *B-coefficients*. The B-coefficients uniquely determine the shape of the polynomial in the B-form. The total number of B-coefficients and basis functions for a dth degree polynomial on an n-dimensional simplex is equal to $\hat{d}$, the total number of valid permutations of κ. The B-form can be evaluated using either the *de Casteljau* algorithm (Hu, Han, & Lai, 2007), or directly by simply expanding the B-form (14), which we found to be more efficient computationally.

2.5. The B-coefficient net

The B-coefficients are strongly structured in what is called the B-coefficient net, or *B-net* for short. The B-net has a well known spatial representation that provides insight into the structure of B-form polynomials, see e.g. Farin (1986), Lai (1997) and Lai and Schumaker (2007). The B-net is also very useful in the visualization of the structure of continuity between simplices. Fig. 1 shows the spatial representation of the B-net corresponding with a third degree basis function (i.e. $d = 3$) defined on a triangulation consisting of the three simplices t_i, t_j and t_k.

There exists a direct relationship between the multi-index of a B-coefficient and its spatial location in barycentric coordinates $b(c_\kappa)$ with respect to a simplex:

$$b(c_\kappa) = \frac{\kappa}{d}, \quad |\kappa| = d. \tag{15}$$

2.6. Continuity between simplices

A spline function is, per definition, a piecewise defined polynomial function with C^r continuity between its pieces. Continuity between the polynomial pieces of the simplex spline are enforced by continuity conditions which are defined for every facet shared by two neighboring simplices. Let two neighboring n-simplices t_i and t_j, differing by only the vertex w, be defined as follows:

$$t_i = \langle v_0, v_1, \ldots, v_{n-1}, w \rangle, \qquad t_j = \langle v_0, v_1, \ldots, v_{n-1}, v_n \rangle. \quad (16)$$

Then t_i and t_j meet along the facet $\tilde{t}$ given by:

$$\tilde{t} = t_i \cap t_j = \langle v_0, v_1, \ldots, v_{n-1} \rangle. \quad (17)$$

Clearly, $\tilde{t}$ is an (n-1)-simplex. As de Boor observed in de Boor (1987) the facet simplex $\tilde{t}$ is indirectly defined by either one of the vertices v_n and w. This is an important observation, because it simplifies the implementation of the algorithm for formulating the continuity conditions. We use the formulation for the continuity conditions from Awanou et al. (2005) and Lai and Schumaker (2007):

$$c^{t_i}_{(\kappa_0,\ldots,\kappa_{n-1},m)} = \sum_{|\gamma|=m} c^{t_j}_{(\kappa_0,\ldots,\kappa_{n-1},0)+\gamma} B^m_\gamma(w), \quad 0 \le m \le r \quad (18)$$

with $\gamma = (\gamma_0, \gamma_1, \ldots, \gamma_n)$ a multi-index independent of κ. In Fig. 1 the graphical interpretation of the C^1 continuity structure for a third degree B-net on three simplices is shown. This graphical interpretation is well known in the literature, see e.g. Farin (1986) and Lai (1997). It is easy to check that the formulation from (18) is valid only for the continuity between simplices t_i and t_j in Fig. 1 while it fails to describe the correct continuity structure between t_j and t_k. In general, for a globally indexed B-net (such as the B-net in Fig. 1), the location of the constant in the multi-index (i.e. the m and 0) is equal to the location of the single non-zero value in the multi-index of B-coefficients located at the out-of-edge vertices w and v_n, respectively. For example, the correct continuity structure for t_j and t_k in Fig. 1 is obtained by reformulating (18) into

$$c^{t_j}_{(\kappa_0,m,\kappa_2)} = \sum_{|\gamma|=m} c^{t_k}_{(0,\kappa_1,\kappa_2)+\gamma} B^m_\gamma(v_e), \quad 0 \le m \le r.$$

For C^r continuity there are a total of R continuity conditions per edge:

$$R = \sum_{m=0}^{r} \frac{(d-m+n-1)!}{(n-1)!(d-m)!}. \quad (19)$$

Eventually we want all continuity conditions for all edges formulated in the following matrix form:

$$\mathbf{H}\mathbf{c} = 0 \quad (20)$$

where matrix $\mathbf{H}$ is the so-called smoothness matrix. Each row in $\mathbf{H}$ contains a single continuity condition (18) which is equated to zero. The vector $\mathbf{c}$ is the *global* vector of B-coefficients. Vector $\mathbf{c}$ is constructed as follows:

$$\mathbf{c} = \left[\mathbf{c}^{t_j}\right]_{j=1}^{J} \in \mathbf{R}^{J\cdot\hat{d}\times 1} \quad (21)$$

with $\mathbf{c}^{t_j}$ the per-simplex vector of lexicographically sorted B-coefficients:

$$\mathbf{c}^{t_j} = [c^{t_j}_\kappa]_{|\kappa|=d} \in \mathbf{R}^{\hat{d}\times 1}. \quad (22)$$

With C^r continuity between simplices we have $\mathbf{H} \in \mathbf{R}^{(E\cdot R)\times(J\cdot\hat{d})}$, with E the total number of edges in a triangulation and R and $\hat{d}$ as in (19) and (11) respectively. In general we have $rank(\mathbf{H}) \le (E \cdot R)$ but only for the simplest of triangulations will $\mathbf{H}$ be of full rank. As Lai and Schumaker observed in Lai and Schumaker (2007), the rank deficiency of $\mathbf{H}$ is caused by the fact that there are redundant continuity equations for triangulations with an interior vertex. For our purposes, we require $\mathbf{H}$ to be of full rank, that is, when $\mathbf{H} \in \mathbf{R}^{R^*\times J\cdot\hat{d}}$ with $R^* \le E \cdot R$ we have:

$$\text{rank}\, \mathbf{H} = R^*. \quad (23)$$

Our algorithm for constructing $\mathbf{H}$ therefore detects and removes any redundant continuity equations.

3. A linear regression scheme using B-form polynomials

In this section we present the new linear regression scheme for multivariate simplex splines. This regression scheme allows the use of the B-form basis polynomials of the multivariate simplex spline as regressors in a standard linear regression framework. We present a generalized least squares parameter estimator for the B-coefficients of the multivariate simplex spline, as well as a method for estimating B-coefficient variances.

3.1. Linear regression with polynomials in the B-form

Consider the pair of observations $(x(i), y(i))$ related as follows:

$$y(i) = f(x(i)) + r(i), \quad i = 1, 2, \ldots, N \quad (24)$$

with f an unknown function and with $r(i)$ a residual term. We now introduce a regression model structure for approximating f that is equivalent to a linear combination of B-form polynomials (14) of degree d, defined on a triangulation consisting of J simplices:

$$y(i) = \sum_{j=1}^{J} \sum_{|\kappa|=d} c^{t_j}_\kappa B^d_\kappa(b(i)) + r(i) \quad (25)$$

with $b(i)$ the barycentric coordinate of $x(i)$ with respect to the simplex t_j as in (3). The model structure in (25) is an entirely valid linear regression structure, but it would not lead to a meaningful approximation scheme because all data points $x(i)$ contribute to the approximation on a simplex t_j regardless of whether they are inside or outside t_j. In order to obtain a per-simplex interpolation scheme, a simplex membership operator $\delta_{jk(i)}$ is introduced:

$$\delta_{jk(i)} = \begin{cases} 1, & \text{if } j = k(i) \\ 0, & \text{if } j \ne k(i) \end{cases} \quad (26)$$

with $k(i)$ an index function that produces the index of the simplex which contains the data point $x(i)$, i.e., $x(i) \in t_{k(i)}, \forall i$. The membership operator (26) is now applied to the regression model (25), which leads to our multivariate simplex spline based linear regression model:

$$y(i) = \sum_{j=1}^{J} \left(\delta_{jk(i)} \sum_{|\kappa|=d} c^{t_j}_\kappa B^d_\kappa(b(i)) \right) + r(i). \quad (27)$$

This expression can be restated in a matrix form that includes all measurements. For this purpose we first have to define a vector formulation of the B-form from (14). First, let $\mathbf{B}^d_{t_j}$ be the vector of lexicographically sorted basis polynomial terms for the simplex t_j:

$$\mathbf{B}^d_{t_j}(i) = [B^{d,t_j}_\kappa(b(i))]_{|\kappa|=d} \in \mathbf{R}^{1\times\hat{d}} \quad (28)$$

where the simplex identifier t_j was added to the definition of the basis function for clarity. With (22) and (28) the per-simplex B-form in vector formulation is:

$$p(b(i)) = \mathbf{B}^d_{t_j}(i) \cdot \mathbf{c}^{t_j}. \quad (29)$$

We introduce the per-simplex $\hat{d} \times \hat{d}$ diagonal data membership matrix for observation i as follows:

$$\mathbf{D}_{t_j}(i) = \left[(\delta_{j,k(i)})_{q,q}\right]_{q=1}^{\hat{d}} \in \mathbf{R}^{\hat{d}\times\hat{d}}. \quad (30)$$

The full-triangulation basis function vector for a single observation is:

$$\mathbf{B}^d(i) = \left[\begin{array}{cccc} \mathbf{B}^d_{t_1}(i) & \mathbf{B}^d_{t_2}(i) & \cdots & \mathbf{B}^d_{t_J}(i) \end{array}\right] \in \mathbf{R}^{1\times J\cdot\hat{d}}. \quad (31)$$

The block diagonal full-triangulation data membership matrix $\mathbf{D}(i)$ for a single observation is a matrix with $\mathbf{D}_{t_j}(i)$ blocks on the main diagonal:

$$\mathbf{D}(i) = \left[\left(\mathbf{D}_{t_j}(i)\right)_{j,j}\right]_{j=1}^{J} \in \mathbf{R}^{(J\cdot\hat{d})\times(J\cdot\hat{d})}. \quad (32)$$

Using (21), (31) and (32) the B-form of the multivariate simplex spline for the complete triangulation in vector form becomes:

$$P(b(i)) = \mathbf{B}^d(i) \cdot \mathbf{D}(i) \cdot \mathbf{c}. \tag{33}$$

Now let $\mathbf{X}(i)$ be a single row in the full-triangulation regression matrix for all observations $\mathbf{X} \in \mathbf{R}^{N \times J \cdot \hat{d}}$ as follows:

$$\mathbf{X}(i) = \mathbf{B}^d(i) \cdot \mathbf{D}(i) \in \mathbf{R}^{1 \times J \cdot \hat{d}}. \tag{34}$$

For a single observation on y we then have:

$$y(i) = \mathbf{X}(i)\mathbf{c} + r(i) \tag{35}$$

which, for all observations, leads to the well known formulation:

$$\mathbf{Y} = \mathbf{X}\mathbf{c} + \mathbf{r} \in \mathbf{R}^{N \times 1}. \tag{36}$$

3.2. A generalized least squares estimator for the B-coefficients

Equation (36) can be solved using many different methods, depending on the assumptions made on the nature of the residual term $\mathbf{r}$. We will introduce a generalized least squares (GLS) estimator for (36), which implies the following assumptions on the residual $\mathbf{r}$:

$$E(\mathbf{r}) = 0, \quad Cov(\mathbf{r}) = \boldsymbol{\Sigma} \tag{37}$$

with $\boldsymbol{\Sigma} \in \mathbf{R}^{N \times N}$ the residual covariance matrix, which is both non-singular and positive definite. The well known (see e.g. Kariya and Kurata (2004)) GLS cost function is:

$$J_{GLS}(\mathbf{c}) = \frac{1}{2}(\mathbf{Y} - \mathbf{X}\mathbf{c})^{\top} \boldsymbol{\Sigma}^{-1}(\mathbf{Y} - \mathbf{X}\mathbf{c}). \tag{38}$$

Up to this point we have not discussed how continuity between simplices is achieved in the frame of the new regression scheme. As explained in Section 2.6, the continuity conditions are contained in the smoothness matrix $\mathbf{H}$ from (20). The continuity conditions act as constraints on B-coefficients located in the continuity structure of a triangulation. Therefore, the complete optimization problem can be stated as an equality constrained GLS problem (ECGLS) as follows:

$$\min_{\mathbf{c}} J_{GLS}(\mathbf{c}), \text{ subject to } \mathbf{H}\mathbf{c} = 0. \tag{39}$$

Using Lagrange multipliers this optimization problem can be formulated as a Karush–Kuhn–Tucker (KKT) system:

$$\begin{bmatrix} \mathbf{X}^{\top}\boldsymbol{\Sigma}^{-1}\mathbf{X} & \mathbf{H}^{\top} \\ \mathbf{H} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \boldsymbol{\nu} \end{bmatrix} = \begin{bmatrix} \mathbf{X}^{\top}\boldsymbol{\Sigma}^{-1}\mathbf{Y} \\ 0 \end{bmatrix} \tag{40}$$

with ν vector of Lagrange multipliers. The coefficient matrix in (40) is the KKT matrix. The solution of the KKT system is:

$$\begin{bmatrix} \hat{\mathbf{c}} \\ \hat{\boldsymbol{\nu}} \end{bmatrix} = \begin{bmatrix} \mathbf{C}_1 & \mathbf{C}_2 \\ \mathbf{C}_3 & \mathbf{C}_4 \end{bmatrix} \cdot \begin{bmatrix} \mathbf{X}^{\top}\boldsymbol{\Sigma}^{-1}\mathbf{Y} \\ 0 \end{bmatrix} \tag{41}$$

with $\hat{\mathbf{c}}$ and $\hat{\boldsymbol{\nu}}$ estimators for $\mathbf{c}$ and $\boldsymbol{\nu}$ respectively. Rao showed in Radhakrishna Rao (2002) that the matrix in (41) is equal to the pseudoinverse of the KKT matrix:

$$\begin{bmatrix} \mathbf{C}_1 & \mathbf{C}_2 \\ \mathbf{C}_3 & \mathbf{C}_4 \end{bmatrix} = \begin{bmatrix} \mathbf{X}^{\top}\boldsymbol{\Sigma}^{-1}\mathbf{X} & \mathbf{H}^{\top} \\ \mathbf{H} & 0 \end{bmatrix}^{+}. \tag{42}$$

Note that the sizes of the submatrices $\mathbf{C}_1, \mathbf{C}_2$ and $\mathbf{C}_3$ in (42) are equal to the sizes of $\mathbf{X}^{\top}\boldsymbol{\Sigma}^{-1}\mathbf{X}$, $\mathbf{H}^{\top}$ and $\mathbf{H}$ respectively.

3.3. A rank requirement for the KKT matrix

For our purposes we require the KKT matrix in (40) to be non-singular, which is the case when the dispersion matrix $\mathbf{Q} = \mathbf{X}^{\top}\boldsymbol{\Sigma}^{-1}\mathbf{X} \in \mathbf{R}^{J \cdot \hat{d} \times J \cdot \hat{d}}$ is positive definite on the kernel of the smoothness matrix $\mathbf{H}$:

$$\mathbf{H}\mathbf{c} = 0, \ \mathbf{c} \neq 0 \Longrightarrow \mathbf{c}^{\top}\mathbf{Q}\mathbf{c} > 0. \tag{43}$$

This statement holds if $\mathbf{Q}$ and $\mathbf{H}$ are both of full rank. The proof of (43) for the general KKT matrix is well known in the literature, see e.g. Boyd and Vandenberghe (2004). In Section 2.6 we stated that $\mathbf{H}$ is of full rank when no redundant continuity conditions are present. The following theorem will prove that the rank of $\mathbf{Q}$ is dependent on the volume and configuration of the data.

Theorem 1. *The dispersion matrix* $\mathbf{Q}$ *is non-singular when every simplex in a triangulation* $\mathcal{T}$ *contains a minimum of* $\hat{d}$ *non-coplanar data points, with* $\hat{d}$ *as in* (11).

Proof. The proof requires that the data content of every individual simplex is considered separately. We therefore first re-order the rows in $\mathbf{X}$ and $\boldsymbol{\Sigma}^{-1}$ such that they are in block diagonal form. This operation does not alter the rank of $\mathbf{Q}$. We denote the per-simplex blocks $\mathbf{X}_j$, and $\boldsymbol{\Sigma}_j^{-1}$ with $j = 0, 1, \ldots, J$. The number of data points in the simplex t_j is N_j. The rank of $\mathbf{Q}$ is now simply the sum of the ranks of the diagonal sub-blocks:

$$\operatorname{rank} \mathbf{Q} = \sum_{j=0}^{J} \operatorname{rank} \mathbf{X}_j^{\top}\boldsymbol{\Sigma}_j^{-1}\mathbf{X}_j. \tag{44}$$

For $\mathbf{Q}$ to be of full rank, we must have for every set of blocks:

$$\operatorname{rank} \mathbf{X}_j^{\top}\boldsymbol{\Sigma}_j^{-1}\mathbf{X}_j = \hat{d} \tag{45}$$

we make use of a nested form of the rank statement from Horn and Johnson (1985):

$$\begin{aligned} &\operatorname{rank} \mathbf{X}_j^{\top} + \operatorname{rank} \boldsymbol{\Sigma}_j^{-1}\mathbf{X}_j - N_j \leq \operatorname{rank} \mathbf{X}_j^{\top}\boldsymbol{\Sigma}_j^{-1}\mathbf{X}_j \\ &\quad \leq \min\{\operatorname{rank} \mathbf{X}_j^{\top}, \operatorname{rank} \boldsymbol{\Sigma}_j^{-1}\mathbf{X}_j\} \end{aligned} \tag{46}$$

where the rank of $\boldsymbol{\Sigma}_j^{-1}\mathbf{X}_j$ is given by:

$$\begin{aligned} &\operatorname{rank} \boldsymbol{\Sigma}_j^{-1} + \operatorname{rank} \mathbf{X}_j - N_j \leq \operatorname{rank} \boldsymbol{\Sigma}_j^{-1}\mathbf{X}_j \\ &\quad \leq \min\{\operatorname{rank} \boldsymbol{\Sigma}_j^{-1}, \operatorname{rank} \mathbf{X}_j\}. \end{aligned} \tag{47}$$

Because Σ is invertible, its rank is equal to the total number of data points N_j in simplex t_j. The rank of $\mathbf{X}_j$ is:

$$\operatorname{rank} \mathbf{X}_j = \min\{N_j, \hat{d}\}. \tag{48}$$

When $N_j < \hat{d}$, i.e. when there are less than $\hat{d}$ non-coplanar data points in simplex t_j, we get $\operatorname{rank} \mathbf{X}_j = N_j$ with which the inequalities in (47) reduce to the following equality:

$$\operatorname{rank} \boldsymbol{\Sigma}_j^{-1}\mathbf{X}_j = N_j. \tag{49}$$

Using this result in (46), and eliminating the inequalities we get:

$$\operatorname{rank} \mathbf{X}_j^{\top}\boldsymbol{\Sigma}_j^{-1}\mathbf{X}_j = N_j < \hat{d}. \tag{50}$$

This result proves that $\mathbf{Q}$ is singular when there are one or more simplices with less than $\hat{d}$ non-coplanar data points. When $N_j \geq \hat{d}$ we have $\operatorname{rank} \mathbf{X}_j = \hat{d}$ with which the inequalities in (47) reduce to:

$$\operatorname{rank} \boldsymbol{\Sigma}_j^{-1}\mathbf{X}_j = \hat{d}. \tag{51}$$

Substituting this result in (46) and eliminating the inequalities we get:

$$\operatorname{rank} \mathbf{X}_j^{\top}\boldsymbol{\Sigma}_j^{-1}\mathbf{X}_j = \hat{d} \tag{52}$$

which proves that $\mathbf{Q}$ is non-singular only if $N_j \geq \hat{d}$. □

3.4. Model quality assessment

The quality of multivariate spline based models created with the new linear regression scheme can be assessed in two different ways. First, the model residue $\mathbf{r}$ from (36) can be analyzed directly.

Second, the new linear regression scheme enables the use of a statistical model quality measure based on the B-coefficient covariance matrix. Rao showed in Radhakrishna Rao (2002) that if the pseudoinverse in (42) is equal to the true inverse, the GLS parameter covariance matrix of $\hat{\mathbf{c}}$ is equal to the $\mathbf{C_1}$ submatrix in (42). We proved earlier that the KKT matrix from (40) is invertible when sufficient data is present in every simplex, and when the smoothness matrix $\mathbf{H}$ is of full rank; in the following we will assume that both these conditions are met. In that case the GLS parameter covariance matrix is given by:

$$Cov(\hat{\mathbf{c}}) = \mathbf{C_1} \tag{53}$$

with B-coefficient variances equal to the main diagonal of $Cov(\hat{\mathbf{c}})$:

$$Var(\hat{\mathbf{c}}_q) = Cov(\hat{\mathbf{c}})_{q,q}, \quad q = 1, 2, \ldots, J \cdot \hat{d}. \tag{54}$$

The estimation of the B-coefficients and the B-coefficient covariance matrix requires the residual covariance matrix $\boldsymbol{\Sigma}$ to be known, which in general is not the case. Calculation of $\boldsymbol{\Sigma}$ is not trivial, and many different methods for constructing it are presented in the literature, see e.g Radhakrishna Rao (2002) and Kariya and Kurata (2004). We propose a two-stage method that considers only per-simplex correlations in the residual $\mathbf{r}$. In the first stage, it is assumed that $\boldsymbol{\Sigma} = \sigma\mathbf{I}$, in which case (40) reduces to an ordinary least squares problem. Under this assumption the estimator for the B-coefficients (41) is still unbiased, but less efficient, leading to inaccurate estimates for the B-coefficient variances. The residual vector $\mathbf{r}$ is then calculated with (36) using the estimated B-coefficients. With the residual vector, per-simplex residual covariance matrix blocks $\boldsymbol{\Sigma}_{t_j} \in \mathbf{R}^{N_j \times N_j}$ can now be estimated as follows:

$$\boldsymbol{\Sigma}_{t_j} = \frac{1}{N_j} \sum_{i=1-l}^{N_j-k} r_{t_j}(i-l) r_{t_j}(i-l+k), \quad k, l = 1, 2, \ldots, N_j. \tag{55}$$

The per-simplex residual covariance matrix blocks are then assembled into the full-triangulation, block diagonal, residual covariance matrix $\boldsymbol{\Sigma}$ as follows:

$$\boldsymbol{\Sigma} = \left[(\boldsymbol{\Sigma}_{t_j})_{j,j}\right]_{j=1}^{J} \in \mathbf{R}^{N \times N} \tag{56}$$

where it is assumed that every per-simplex residual covariance matrix block $\boldsymbol{\Sigma}_{t_j}$ is non-singular and positive definite. In the second stage of the estimation procedure, the B-coefficients are reestimated with (41) using the estimated $\boldsymbol{\Sigma}$ from (56). An estimate of the B-coefficient variances can then be obtained with (54).

4. Demonstration of the new modeling method

In this section the new modeling methodology is demonstrated with a simple bivariate data fitting experiment. In the experiment, bivariate simplex spline functions of varying polynomial degree and continuity order are used to approximate a nonlinear, scattered, bivariate dataset on a triangulation consisting of 3 simplices. The quality of the spline approximation is assessed using the residual and statistical analysis methods from Section 3. Finally, the system matrices for a first degree spline function with C^0 continuity are written out.

4.1. Demonstration setup

For the numerical experiment 1000 scattered data points $(x_1, x_2) \in \mathbf{R}^2$ on the interval [0, 1] were generated using a uniform random number generator. The data values were generated with a bivariate function $f(x_1, x_2)$ as follows:

$$f(x_1, x_2) = x_2^2 \sin(10x_1 + 10) + x_1 \cos(5x_2) + k(t_j) \cdot \nu \tag{57}$$

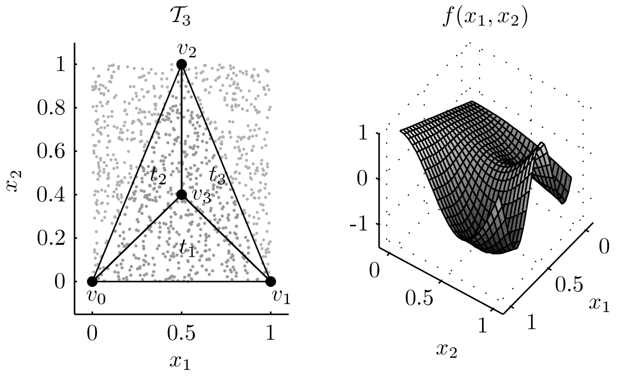

Fig. 2. Triangulation $\mathcal{T}_3$ and identification dataset (left) and data generating function $f(x_1, x_2)$ (right).

with $k(t_j) \cdot \nu$ a uniformly distributed white noise sequence of simplex-dependent magnitude $k(t_j)$. The linear regression model from (36) was used to model this dataset. A non-type-I/II triangulation $\mathcal{T}_3$ consisting of 3 simplices was assumed, see Fig. 2. The values for the noise magnitude were chosen to be $\{k(t_1), k(t_2), k(t_3)\} = \{0.2, 0.05, 0.02\}$. In this case it is clear that $Cov(\mathbf{r}) \neq \sigma\mathbf{I}$ which warrants the use of the GLS estimator from (41).

4.2. Demonstration results

A number of spline spaces were used to approximate the data. In Fig. 3 the general performance of these spline spaces is shown in the form of RMS of the residual $r(x_1, x_2)$. Also shown in Fig. 3 are the estimated mean B-coefficient variances. This figure clearly shows that increasing the degree of the spline spaces reduces the residual RMS, as expected. From Fig. 3 it is clear that the estimated B-coefficient variances depend heavily on the continuity order of the spline spaces.

In Fig. 4 the $s \in S_6^2(\mathcal{T}_3)$ spline approximation is shown together with the residual $r(x_1, x_2)$, which consists mostly of the added white noise. Fig. 5 shows the estimated B-coefficient variance structure for the $s \in S_6^2(\mathcal{T}_3)$ spline together with a simulated B-coefficient variance structure. The simulated B-coefficient variance structure was obtained by numerically calculating the variance in the estimated B-coefficients for 1000 noise realizations. Fig. 5 clearly shows a close correspondence between estimated and simulated B-coefficient variances. Note that the B-coefficient variances shown in Fig. 5 are lowest around the internal vertex.

4.3. First degree spline with 0th order continuity

We will now derive the regression matrix $\mathbf{X}$, the observation vector $\mathbf{Y}$ and the smoothness matrix $\mathbf{H}$ for the $s \in S_1^0(\mathcal{T}_3)$ spline function. In this case we have 3 B-coefficients per simplex which, according to (15), are located at the simplex vertices, see Fig. 6. The global B-coefficient vector $\mathbf{c}$ (21) is:

$$\mathbf{c} = [\; c_{100}^{t_1} \;\; c_{010}^{t_1} \;\; c_{001}^{t_1} \;\; c_{100}^{t_2} \;\; c_{010}^{t_2} \;\; c_{001}^{t_2} \;\; c_{100}^{t_3} \;\; c_{010}^{t_3} \;\; c_{001}^{t_3} \;]^\top.$$

Now let $x(i) = (x_1(i), x_2(i))$ be a single data point located inside simplex t_1, and let $b(i)$ be its barycentric coordinate with respect to t_1. The regression structure (33) for $y(i)$ then is:

$$\begin{aligned} y(i) &= \mathbf{B}^1(i) \cdot \mathbf{D}(i) \cdot \mathbf{c} \\ &= [\; \mathbf{B}_{t_1}^1(i) \;\; \mathbf{B}_{t_2}^1(i) \;\; \mathbf{B}_{t_3}^1(i) \;] \cdot \begin{bmatrix} I_{3\times3} & 0 \\ 0 & 0_{6\times6} \end{bmatrix} \cdot \mathbf{c} \\ &= [\; b_0(i) \;\; b_1(i) \;\; b_2(i) \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;] \cdot \mathbf{c}. \end{aligned}$$

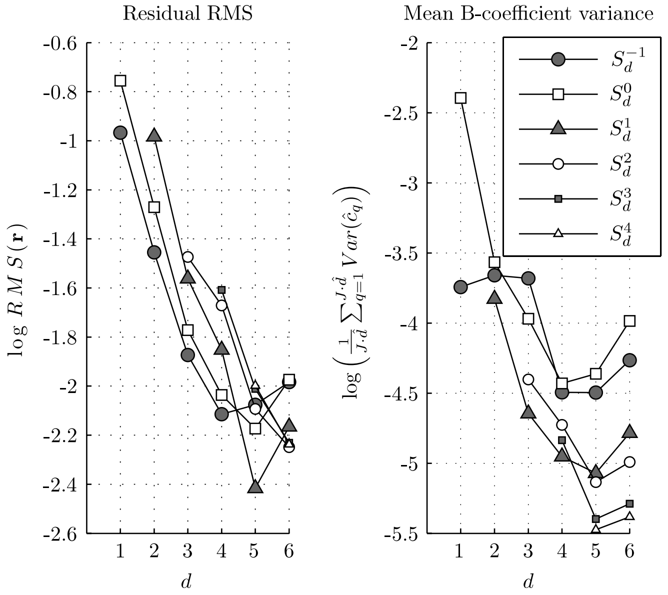

Fig. 3. RMS of the residual $r(x_1, x_2)$ (left) and mean B-coefficient variances (right) for the different spline spaces.

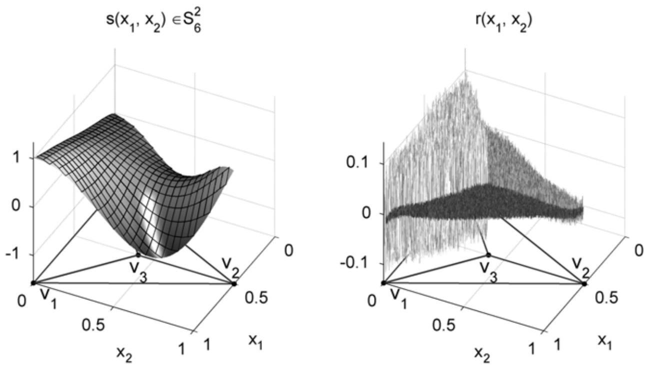

Fig. 4. Sixth degree spline function with C^2 continuity (left) and model error (right).

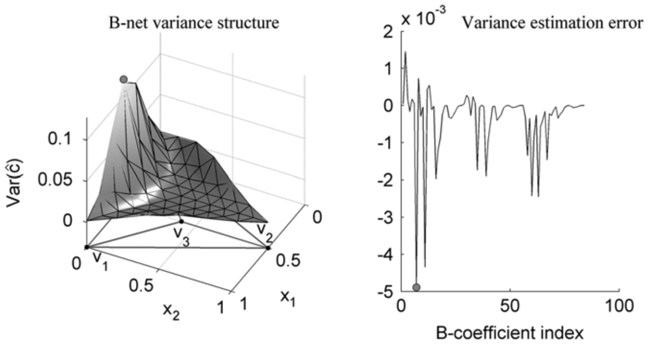

Fig. 5. Estimated (= solid) and simulated (= wireframe) B-coefficient variance structure (left) and the error in the variance estimation (right). The dot corresponds to the B-coefficient at which the largest error between estimated and simulated variance occurs.

The continuity conditions for the given triangulation are formulated using (18). For example, the continuity conditions of t_1 with respect to t_2 are:

$$c^{t_1}_{(\kappa_0,0,\kappa_2)} = \sum_{|\gamma|=0} c^{t_2}_{(\kappa_0,0,\kappa_2)} B^0_\gamma(v_2) = c^{t_2}_{(\kappa_0,0,\kappa_2)}.$$

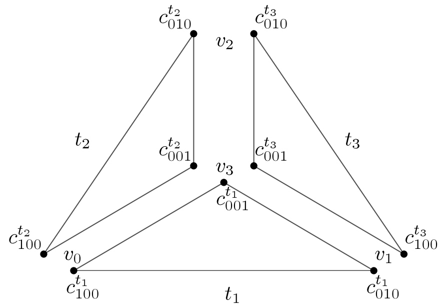

Fig. 6. Exploded view of the B-net for $s \in S^0_1(\mathcal{T}_3)$.

It can be checked that the complete, full rank smoothness matrix **H** for C^0 continuity for this example is:

$$\mathbf{H} = \begin{bmatrix} -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 1 & 0 \end{bmatrix}$$

where rows 1 and 2 are the continuity conditions for t_1 with respect to t_2, rows 3 and 4 the continuity conditions for t_1 with respect to t_3 and row 5 the single continuity condition for t_2 with respect to t_3. Note that the continuity condition $c^{t_2}_{001} = c^{t_3}_{001}$ was removed as it was redundant, causing **H** to be rank deficient.

5. Conclusions

In this paper, a new methodology for creating accurate static nonlinear maps from scattered multidimensional data is presented. This methodology uses B-form polynomials in barycentric coordinates inside an equality constrained linear regression scheme. The linear regression scheme requires a new vector formulation for the B-form of the multivariate simplex spline, which is derived in this paper. A generalized least squares estimator for the B-coefficients of the multivariate simplex splines is presented. The new linear regression scheme facilitates the estimation of the variances of the B-coefficients. These variances can be used, together with the spatial location of the B-coefficients, to define variance hypersurfaces.

A numerical demonstration experiment was conducted in which the new modeling methodology was applied in the approximation of a nonlinear, scattered dataset with simplex splines of varying degree and continuity order. The statistical model quality assessment method introduced in this paper was shown to complement the standard residual analysis. Furthermore, it was shown that increasing the continuity order of a spline function reduces B-coefficient variances, especially for B-coefficients located near internal vertices.

Finally, the practicality of the new methodology has been demonstrated in de Visser, Mulder, and Chu (2009), in which a highly nonlinear aerodynamic dataset is modeled with multivariate simplex splines inside a linear regression framework.

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C.C. de Visser received the B.Sc. and M.Sc. degrees from the Faculty of Aerospace Engineering of the Delft University of Technology in 2006 and 2007. From 2007 he has been a Ph.D. candidate at the Faculty of Aerospace Engineering, Delft University of Technology, Delft, The Netherlands. His research interests include nonlinear system identification, multivariate spline theory, flight dynamics, aerodynamics and fault tolerant control.

Q.P. Chu received his Ph.D. degree from the Faculty of Aerospace Engineering, Delft University of Technology, The Netherlands, in 1987. Currently, he is an Associate Professor at the Faculty of Aerospace Engineering, Delft University of Technology, responsible for aerospace guidance, navigation and control education, and research activities. He has (co)authored more than 150 journal and conference papers ranging from adaptive control, nonlinear control, robust control and intelligent control to nonlinear state estimation, system identification and nonlinear optimization for aerospace vehicles. Dr. Chu was the designer of the attitude control system for the third Dutch satellite Sloshsat launched in Feb. 2005 and is a member of the American Institute of Aeronautics and Astronautics (AIAA).

J.A. Mulder graduated with honors as engineer-pilot from the faculty of Aerospace Engineering of the Delft University of Technology, The Netherlands, in 1968. He received his Ph.D. degree on aerodynamic model identification in 1986 with honors and was next appointed Full Professor in 1989 as chair of the Control and Simulation Division in the Faculty of Aerospace Engineering. He is the founding Scientific Director of the Institute for research in Simulation, Motion and Navigation Technologies (SIMONA) and of the institute for Aerospace Software and Technologies (ASTI) of Delft University of Technology. He has (co)authored more than 200 conference and journal papers on subjects ranging from human–machine interface design and cybernetics to identification, estimation and advanced flight control. Prof. Mulder has served in numerous ministerial advisory committees, as advisor to the board of the National Aerospace Laboratory (NLR) and the Radiobiological Institute of the Netherlands Organization for Applied Scientific Research (TNO). He was a member of the AGARD Flight Mechanics panel from 1982 to 1997. Presently he is member of the Aerospace Control & Guidance Systems Committee of the Society of Automotive Engineers (SAE), of the Society of Flight Test Engineers (SFTE) and senior member of the American Institute of Aeronautics and Astronautics (AIAA), of its Avionics Committee and Associate Editor of the AIAA Journal of Aerospace Computing, Information, and Communication and of the Journal of Micro Aerial Vehicles.