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Curvature approximation of 3D manifolds in 4D space

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Abstract

A method for the approximation of the three principal curvatures at points on a discretized, triangulated 3D manifold in 4D space (referred to as 3-surface) is presented. The approximation scheme is based on the fact that a parametric 3-surface can locally be approximated by the graph of a trivariate function. Using a local coordinate system, a least square polynomial approximation is constructed for the estimation of the principal curvatures at each 3-surface point. Curvature is extremely useful for the analysis of qualitative characteristics of surfaces. The technique presented is an example of extending existing surface interrogation methods to multivariate data. Such a generalization is valuable for scientific visualization.

Keywords: Approximation; Curvature; Differentiable manifold; Gauss–Weingarten map; Least square approximation; Scattered data; Triangulation

1. Introduction

The theory of parametric surfaces can be generalized to parametric 3D manifolds (3-manifolds) in 4D space, which are referred to as 3-surfaces in the following. The notation

$$\boldsymbol{x}(\boldsymbol{u}) = (x(u,v,w), y(u,v,w), z(u,v,w), \alpha(u,v,w)) \tag{1}$$

is used for 3-surfaces. The graph of a trivariate function f is a special 3-surface, since its parametrization is given by

$$\boldsymbol{x}(\boldsymbol{u}) = (u,v,w,f(u,v,w)). \tag{2}$$

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A 3-surface can locally be approximated by the graph of a trivariate function. This fact is used for the approximation of the three principal curvatures at points $(x_i, y_i, z_i, \alpha_i)$ on a discretized, triangulated 3-surface.

Curvature is essential for understanding qualitative properties of curves, surfaces, and 3-surfaces (see (Farin, 1992)). Quality interrogation of parametric surfaces used in car body and ship hull design makes extensive use of curvature plots. The curvature of a 3-surface is rendered in its 3D parameter space by slicing in u-, v-, and w-directions and coloring the slicing planes according to curvature. Other visualization techniques for 3D data are discussed in (Hagen et al., 1993) and (Nielson and Hamann, 1990). Curvature plots are also used for the analysis of bivariate/trivariate scattered data interpolants (see (Nielson et al., 1991)).

This paper presents a method for the approximation of principal curvatures at 3-surface points. Normal vectors must be known at each 3-surface point for the approximation. Based on the triangulation and the normal vectors, local least square approximants are constructed. These are differentiated, and their graphs' curvatures are used as curvature estimates at the 3-surface points. The estimation of a normal vector at a point on a triangulated 3-surface is based on averaging the normals of tetrahedra sharing that point. This is analogous to the approximation of a normal at a point in a triangular surface mesh by averaging the normals of triangles surrounding the point. Normal vectors at points on the graph of a trivariate function f are given by the function's gradient. The gradient approximation schemes discussed in (Stead, 1984) for bivariate data can be generalized to trivariate data. A gradient estimation scheme that works particularly well for structured, rectilinear data is described in (Zucker and Hummel, 1981).

The method presented in this paper can be used for the analysis of multivariate data. Analysis tools for multivariate data are becoming increasingly important, in particular in computational fluid dynamics (CFD) and the finite element method (FEM). Sophisticated analysis and visualization techniques for vector and tensor fields have recently been developed (see (Helman and Hesselink, 1990) and (Delmarcelle and Hesselink, 1992)). Another application for curvature estimation is the area of scattered data interpolation. Future interpolation methods might utilize curvature input following the trend in geometric modeling of curves and surfaces ("geometric continuity," see (Farin, 1992)).

The concepts of differential geometry and vector calculus used in this paper can be found in (Auslander and MacKenzie, 1977; Chuang and Hoffmann, 1990; do Carmo, 1976; Farin, 1992; Marsden and Tromba, 1988; O'Neill, 1969). A comprehensive work on differential geometry is (Spivak, 1970). Data reduction schemes, which relate the significance of data points to curvature, are described in (Hamann, 1994) and (Hamann and Chen, 1994a, b).

2. Curvature of graphs of trivariate functions

As mentioned in the introduction, a parametric 3-surface can locally be approximated by the graph of a trivariate function. Therefore, the curvature properties of a 3-surface can be investigated by analyzing graphs of local trivariate approximants. The curvature properties of such graphs are reviewed in this section.

The graph of a trivariate function $f(u,v,w)$, f in class C^m, $m \geqslant 2$, mapping an open set $\mathcal{S} \subset \mathbb{R}^3$ into $\mathbb{R}$ can be viewed as a regular parametric 3-surface using the parametrization

$$\boldsymbol{x}(\boldsymbol{u}) = (u,v,w,f(u,v,w)), \quad (u,v,w) \in \mathcal{S} \subset \mathbb{R}^3. \tag{3}$$

The partial derivatives of this 3-surface are

$$\begin{pmatrix} \boldsymbol{x}_u & \boldsymbol{x}_v & \boldsymbol{x}_w \\ \boldsymbol{x}_{uu} & \boldsymbol{x}_{uv} & \boldsymbol{x}_{uw} \\ & \boldsymbol{x}_{vv} & \boldsymbol{x}_{vw} \\ & & \boldsymbol{x}_{ww} \end{pmatrix} = \begin{pmatrix} (1,0,0,f_u) & (0,1,0,f_v) & (0,0,1,f_w) \\ (0,0,0,f_{uu}) & (0,0,0,f_{uv}) & (0,0,0,f_{uw}) \\ & (0,0,0,f_{vv}) & (0,0,0,f_{vw}) \\ & & (0,0,0,f_{ww}) \end{pmatrix}, \tag{4}$$

and the 3-surface normal $\boldsymbol{n}(\boldsymbol{u})$ at $\boldsymbol{x}(\boldsymbol{u})$ is given by

$$\boldsymbol{n}(\boldsymbol{u}) = \frac{\text{cross product}\,(\boldsymbol{x}_u, \boldsymbol{x}_v, \boldsymbol{x}_w)}{\|\text{cross product}\,(\boldsymbol{x}_u, \boldsymbol{x}_v, \boldsymbol{x}_w)\|} = \frac{(-f_u, -f_v, -f_w, 1)}{\sqrt{1 + {f_u}^2 + {f_v}^2 + {f_w}^2}}. \tag{5}$$

Remark. The components of the normal vector $\boldsymbol{n} = (n^x, n^y, n^z, n^\alpha)$ of a 3-surface are defined by the determinant of the 4×4 matrix containing its first derivative vectors. Thus, the normal vector of the graph of a trivariate function is given by

$$n^x I + n^y J + n^z K + n^\alpha L = \begin{vmatrix} 1 & 0 & 0 & I \\ 0 & 1 & 0 & J \\ 0 & 0 & 1 & K \\ f_u & f_v & f_w & L \end{vmatrix}. \tag{6}$$

Definition 1. The *tangent space* at a point $\boldsymbol{x}_0 = \boldsymbol{x}(\boldsymbol{u}_0)$ on a regular 3-surface $\boldsymbol{x}(\boldsymbol{u})$ is the set of all points $\boldsymbol{y}$ in $\mathbb{R}^4$ satisfying the equation

$$\boldsymbol{y} = \boldsymbol{x}_0 + a\boldsymbol{x}_u(\boldsymbol{u}_0) + b\boldsymbol{x}_v(\boldsymbol{u}_0) + c\boldsymbol{x}_w(\boldsymbol{u}_0), \quad a,b,c \in \mathbb{R}. \tag{7}$$

The Gauss–Weingarten map (see (do Carmo, 1976)) for the graph of a trivariate function is given by

$$\begin{aligned} -A &= - \begin{pmatrix} a_{1,1} & a_{1,2} & a_{1,3} \\ a_{2,1} & a_{2,2} & a_{2,3} \\ a_{3,1} & a_{3,2} & a_{3,3} \end{pmatrix} \\ &= \frac{1}{l} \begin{pmatrix} f_{uu} & f_{uv} & f_{uw} \\ f_{uv} & f_{vv} & f_{vw} \\ f_{uw} & f_{vw} & f_{ww} \end{pmatrix} \begin{pmatrix} 1+f_u^2 & f_u f_v & f_u f_w \\ f_u f_v & 1+f_v^2 & f_v f_w \\ f_u f_w & f_v f_w & 1+f_w^2 \end{pmatrix}^{-1}, \end{aligned} \tag{8}$$

where $l = \sqrt{1 + f_u^2 + f_v^2 + f_w^2}$.

Definition 2. The three (real) eigenvalues κ_1, κ_2, and κ_3 of $-A$ in (8) are called *principal curvatures* of the graph of the trivariate function $f(u,v,w)$. They are the roots of the characteristic polynomial of $-A$, the cubic polynomial

$$\det(-A-\kappa I)=\kappa^3+(a_{1,1}+a_{2,2}+a_{3,3})\kappa^2 + (a_{1,1}a_{2,2}+a_{1,1}a_{3,3}+a_{2,2}a_{3,3}-a_{1,2}a_{2,1}-a_{1,3}a_{3,1}-a_{2,3}a_{3,2})\kappa + a_{1,1}a_{2,2}a_{3,3}+a_{1,2}a_{2,3}a_{3,1}+a_{1,3}a_{2,1}a_{3,2} - a_{1,1}a_{2,3}a_{3,2}-a_{1,2}a_{2,1}a_{3,3}-a_{1,3}a_{2,2}a_{3,1}. \tag{9}$$

The average H of the principal curvatures is called *mean curvature*, and the product K is called *Gaussian curvature*,

$$H=\tfrac{1}{3}(\kappa_1+\kappa_2+\kappa_3), \qquad K=\kappa_1\kappa_2\kappa_3. \tag{10}$$

3. Curvature approximation of triangulated 3-surfaces

This section describes the curvature approximation scheme for 3-surfaces. The scheme is based on the construction of a local polynomial approximation to the given data. This approximation requires a triangulation of the data points and normal vector estimates at the 3-surface points. At each 3-surface point, a least square quadratic polynomial is computed, and the principal curvatures of the graph of this approximant are used as curvature estimates at that point. The following theorems are needed for the approximation.

Theorem 1. *Each regular parametric 3-surface $\boldsymbol{x}(\boldsymbol{u})$ of class m, $m \geqslant 2$, can locally be represented in explicit form $f=f(\hat{x},\hat{y},\hat{z})$, where f is at least C^2 continuous. Choosing a 3-surface point $\boldsymbol{x}_0$ as origin of a local coordinate system and the f-axis in the same direction as the surface normal $\boldsymbol{n}_0$ at $\boldsymbol{x}_0$, the Taylor series of f, considering terms up to degree two, is*

$$f(\hat{x},\hat{y},\hat{z})=\tfrac{1}{2}(c_{2,0,0}\hat{x}^2+2c_{1,1,0}\hat{x}\hat{y}+2c_{1,0,1}\hat{x}\hat{z} + c_{0,2,0}\hat{y}^2+2c_{0,1,1}\hat{y}\hat{z}+c_{0,0,2}\hat{z}^2). \tag{11}$$

Any three unit vectors in the tangent space at $\boldsymbol{x}_0$ determining a right-handed orthonormal coordinate system can be chosen. Changing the orientation of the three unit vectors appropriately yields the osculating paraboloid at $\boldsymbol{x}_0$,

$$f(\hat{x},\hat{y},\hat{z})=\tfrac{1}{2}(\bar{c}_{2,0,0}\hat{x}^2+\bar{c}_{0,2,0}\hat{y}^2+\bar{c}_{0,0,2}\hat{z}^2). \tag{12}$$

The principal curvatures at $\boldsymbol{x}_0$ are the coefficients of the osculating paraboloid, i.e., $\kappa_1=\bar{c}_{2,0,0}$, $\kappa_2=\bar{c}_{0,2,0}$, and $\kappa_3=\bar{c}_{0,0,2}$.

Proof. See (Spivak, 1970). □

Remark. In Theorems 1 and 2, the independent variables are denoted by $\hat{x}$, $\hat{y}$, and $\hat{z}$ in order to indicate their relation to the local coordinate system at $\boldsymbol{x}_0$.

Theorem 2. *Let f be the trivariate polynomial*

$$f(\hat{u},\hat{v},\hat{w})=\sum c_{i,j,k}\hat{u}^i\hat{v}^j\hat{w}^k, \quad i+j+k\leqslant n,\ i,j,k\geqslant 0, \tag{13}$$

where a point in 3D space has coordinates $\hat{u}$, $\hat{v}$, and $\hat{w}$ it with respect to a coordinate system given by an origin $\boldsymbol{o}$ *and three orthonormal basis vectors* $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, *and* $\boldsymbol{b}_3$. *Changing the orientation of the orthonormal basis vectors changes the representation of the trivariate polynomial, but not its graph* $\{(\hat{u}, \hat{v}, \hat{w}, f(\hat{u}, \hat{v}, \hat{w}))\}$.

Proof. See surface case treated in (Hamann, 1993). □

At each 3-surface point, the curvature approximation scheme considers a certain neighborhood of data in the triangulation, which is called platelet. This allows the localization of the approximation process.

Definition 3. Given a triangulation of a set of 3-surface points, the *platelet* $\mathcal{P}_i$ associated with the point $\boldsymbol{x}_i$ is the set of all tetrahedra (determined by their index-quadruples (j_1, j_2, j_3, j_4)) sharing $\boldsymbol{x}_i$ as a common vertex,

$$\mathcal{P}_i = \bigcup \{(j_1, j_2, j_3, j_4) \mid i = j_1 \ \vee \ i = j_2 \ \vee \ i = j_3 \ \vee \ i = j_4\}. \tag{14}$$

The vertices of $\mathcal{P}_i$ are called *platelet points*.

These are the steps required for the approximation of the three principal curvatures at a 3-surface point $\boldsymbol{x}_i$:

(i) Determine the platelet points associated with $\boldsymbol{x}_i$.
(ii) Approximate the outward normal $\boldsymbol{n}_i$ at $\boldsymbol{x}_i$.
(iii) Compute the tangent space $\mathcal{T}$ passing through $\boldsymbol{x}_i$ having normal $\boldsymbol{n}_i$.
(iv) Define a local coordinate system for $\mathcal{T}$ with $\boldsymbol{x}_i$ as origin and three orthonormal basis vectors in $\mathcal{T}$.
(v) Compute the distances of the platelet points from $\mathcal{T}$.
(vi) Project the platelet points onto the tangent space $\mathcal{T}$.
(vii) Represent the projections obtained in (vi) with respect to the local coordinate system constructed in (iv).
(viii) Interpret the projections of the platelet points in $\mathcal{T}$ as independent variables and their distances from $\mathcal{T}$ as function values.
(ix) Construct a polynomial f approximating the data derived in (viii).
(x) Compute the three principal curvatures of f's graph at $\boldsymbol{x}_i$.

Some of these steps are explained in further detail. Let $\{\boldsymbol{y}_j = (x_j, y_j, z_j, \alpha_j) \mid j = 0, \ldots, n_i\}$ be the set of platelet points associated with $\boldsymbol{x}_i$. All 3-surface tetrahedra in $\boldsymbol{x}_i$'s platelet must have the same orientation for the approximation of an outward (!) normal. Since the associated platelet in parameter space is given by the triples (u_j, v_j, w_j), $j = 0, \ldots, n_i$, implying a set of 3D domain tetrahedra, the boundary of the union of these domain tetrahedra is a set of triangles. If the vertices of all these triangles are ordered consistently (all clockwise/all counter-clockwise), the 3-surface platelet points on the 3-surface are ordered consistently as well (see (Edelsbrunner, 1987)).

An outward normal vector is computed for each 3-surface tetrahedron in $\boldsymbol{x}_i$'s platelet. Such an outward normal vector is defined by the cross product of the three vectors

$$(v_k^x, v_k^y, v_k^z, v_k^\alpha) = \boldsymbol{x}_i - \boldsymbol{y}_{j_k}, \quad j_k \in \{0, \ldots, n_i\} \setminus \{i\}, \ k = 1, 2, 3, \tag{15}$$

where k implies the order of the three 3-surface points of a boundary face in $\boldsymbol{x}_i$'s platelet. The components of the 3-surface tetrahedron's outward normal vector $(\hat{n}^x, \hat{n}^y, \hat{n}^z, \hat{n}^\alpha)$ are given by the determinant

$$\hat{n}^x I + \hat{n}^y J + \hat{n}^z K + \hat{n}^\alpha L = \begin{vmatrix} v_1^x & v_2^x & v_3^x & I \\ v_1^y & v_2^y & v_3^y & J \\ v_1^z & v_2^z & v_3^z & K \\ v_1^\alpha & v_2^\alpha & v_3^\alpha & L \end{vmatrix}. \tag{16}$$

Eventually, the outward unit normal vector $\boldsymbol{n}_i = (n^x, n^y, n^z, n^\alpha)$ at $\boldsymbol{x}_i$ is estimated by averaging the outward normal vectors of all 3-surface tetrahedra in $\boldsymbol{x}_i$'s platelet and normalizing the result.

The implicit linear equation for the tangent space $\mathcal{T}$ at $\boldsymbol{x}_i$ is

$$\begin{aligned} \boldsymbol{n}_i \cdot (\boldsymbol{x} - \boldsymbol{x}_i) &= n^x x + n^y y + n^z z + n^\alpha \alpha - (n^x x_i + n^y y_i + n^z z_i + n^\alpha \alpha_i) \\ &= Ax + By + Cz + D\alpha + E = 0. \end{aligned} \tag{17}$$

The four vectors

$$\begin{pmatrix} \boldsymbol{a}_1 \\ \boldsymbol{a}_2 \\ \boldsymbol{a}_3 \\ \boldsymbol{n}_i \end{pmatrix} = \begin{pmatrix} (1,0,0,0) \\ (0,1,0,0) \\ (0,0,1,0) \\ (-f_u, -f_v, -f_w, 1)/\sqrt{1 + f_u^2 + f_v^2 + f_w^2} \end{pmatrix} \tag{18}$$

are linearly independent and define a basis for $\mathbb{R}^4$. Obviously, $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, and $\boldsymbol{a}_3$ are not necessarily perpendicular to $\boldsymbol{n}_i$.

Gram–Schmidt orthogonalization is used for the construction of an orthonormal basis for $\mathbb{R}^4$ consisting of the basis vectors $\boldsymbol{n}_i$, $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, and $\boldsymbol{b}_3$, where $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, and $\boldsymbol{b}_3$ are computed sequentially as

$$\begin{aligned} \boldsymbol{b}_1 &= \frac{\boldsymbol{a}_1 - (\boldsymbol{a}_1 \cdot \boldsymbol{n}_i)\boldsymbol{n}_i}{\|\boldsymbol{a}_1 - (\boldsymbol{a}_1 \cdot \boldsymbol{n}_i)\boldsymbol{n}_i\|}, \\ \boldsymbol{b}_2 &= \frac{\boldsymbol{a}_2 - ((\boldsymbol{a}_2 \cdot \boldsymbol{n}_i)\boldsymbol{n}_i + (\boldsymbol{a}_2 \cdot \boldsymbol{b}_1)\boldsymbol{b}_1)}{\|\boldsymbol{a}_2 - ((\boldsymbol{a}_2 \cdot \boldsymbol{n}_i)\boldsymbol{n}_i + (\boldsymbol{a}_2 \cdot \boldsymbol{b}_1)\boldsymbol{b}_1)\|}, \quad \text{and} \\ \boldsymbol{b}_3 &= \frac{\boldsymbol{a}_3 - ((\boldsymbol{a}_3 \cdot \boldsymbol{n}_i)\boldsymbol{n}_i + (\boldsymbol{a}_3 \cdot \boldsymbol{b}_1)\boldsymbol{b}_1 + (\boldsymbol{a}_3 \cdot \boldsymbol{b}_2)\boldsymbol{b}_2)}{\|\boldsymbol{a}_3 - ((\boldsymbol{a}_3 \cdot \boldsymbol{n}_i)\boldsymbol{n}_i + (\boldsymbol{a}_3 \cdot \boldsymbol{b}_1)\boldsymbol{b}_1 + (\boldsymbol{a}_3 \cdot \boldsymbol{b}_2)\boldsymbol{b}_2)\|} \end{aligned} \tag{19}$$

("$\| \ \|$" denoting the Euclidean norm).

The perpendicular, signed distances d_j, $j = 0, \ldots, n_i$, of the platelet points $\boldsymbol{y}_j$ from the tangent space $\mathcal{T}$ are

$$d_j = Ax_j + By_j + Cz_j + D\alpha_j + E. \tag{20}$$

Projecting the platelet points $\boldsymbol{y}_j$ onto $\mathcal{T}$ yields the points $\boldsymbol{y}_j^{\mathcal{T}}$, where

$$\boldsymbol{y}_j^{\mathcal{T}} = \boldsymbol{y}_j - d_j \boldsymbol{n}_i. \tag{21}$$

Each point $y_j^{\mathcal{T}}$ in $\mathcal{T}$ is expressed with respect to the coordinate system given by the origin $\boldsymbol{x}_i$ and the basis vectors $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, and $\boldsymbol{b}_3$. Computing the difference vectors

$$\boldsymbol{d}_j = \boldsymbol{y}_j^{\mathcal{T}} - \boldsymbol{x}_i, \quad j = 0, \ldots, n_i, \tag{22}$$

and expressing $\boldsymbol{d}_j$ as linear combinations of the basis vectors $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, and $\boldsymbol{b}_3$ in $\mathcal{T}$, one obtains the required representation

$$\hat{\boldsymbol{d}}_j = (\boldsymbol{d}_j \cdot \boldsymbol{b}_1)\boldsymbol{b}_1 + (\boldsymbol{d}_j \cdot \boldsymbol{b}_2)\boldsymbol{b}_2 + (\boldsymbol{d}_j \cdot \boldsymbol{b}_3)\boldsymbol{b}_3. \tag{23}$$

Thus, the local coordinates of $\boldsymbol{y}_j^{\mathcal{T}}$ are

$$(u_j, v_j, w_j) = (\boldsymbol{d}_j \cdot \boldsymbol{b}_1, \boldsymbol{d}_j \cdot \boldsymbol{b}_2, \boldsymbol{d}_j \cdot \boldsymbol{b}_3). \tag{24}$$

The local coordinates u_j, v_j, and w_j are viewed as independent variables, and the signed distances d_j are viewed as function values (in direction of $\boldsymbol{n}_i$) of a polynomial $f(u, v, w)$ of degree two (see Theorem 1). The function f is defined by the interpolation conditions

$$\begin{aligned} f(u_j, v_j, w_j) = d_j = \tfrac{1}{2}(c_{2,0,0}u_j^2 + 2c_{1,1,0}u_jv_j + 2c_{1,0,1}u_jw_j \\ + c_{0,2,0}v_j^2 + 2c_{0,1,1}v_jw_j + c_{0,0,2}w_j^2), \end{aligned} \tag{25}$$

$j = 1, \ldots, n_i$. Alternatively, the interpolation conditions can be written in matrix form as

$$\begin{pmatrix} u_1^2 & 2u_1v_1 & 2u_1w_1 & v_1^2 & 2v_1w_1 & w_1^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ u_{n_i}^2 & 2u_{n_i}v_{n_i} & 2u_{n_i}w_{n_i} & v_{n_i}^2 & 2v_{n_i}w_{n_i} & w_{n_i}^2 \end{pmatrix} \begin{pmatrix} c_{2,0,0} \\ c_{1,1,0} \\ c_{1,0,1} \\ c_{0,2,0} \\ c_{0,1,1} \\ c_{0,0,2} \end{pmatrix} = U\boldsymbol{c} = \boldsymbol{d} = \begin{pmatrix} d_1 \\ \vdots \\ d_{n_i} \end{pmatrix}. \tag{26}$$

The normal equations of the implied least square approximation problem are

$$U^{\mathrm{T}}U\boldsymbol{c} = U^{\mathrm{T}}\boldsymbol{d}. \tag{27}$$

This 6×6 system is solved using Gaussian elimination. If the determinant of $U^{\mathrm{T}}U$ vanishes the set of platelet points is expanded by using additional points in the platelet's neighborhood.

A theorem from multidimensional differential geometry ensures that the three principal curvatures at a point on the graph of a trivariate function are always real.

Theorem 3. *The principal curvatures κ_1, κ_2, and κ_3 at any point on the graph $\{(u, v, w, f(u, v, w))\}$ of a trivariate function f of class m, $m \geqslant 2$, are real. They are the eigenvalues of the Gauss–Weingarten map associated with the graph.*

Proof. See (Spivak, 1970). □

Theorem 4. *The principal curvatures* κ_1, κ_2, *and* κ_3 *of the graph* $\{(u,v,w,f(u,v,w))\}$ *of the trivariate polynomial*

$$f(u,v,w)=\tfrac{1}{2}(c_{2,0,0}u^2+2c_{1,1,0}uv+2c_{1,0,1}uw + c_{0,2,0}v^2+2c_{0,1,1}vw+c_{0,0,2}w^2) \tag{28}$$

at the 3-surface point $(0,0,0,f(0,0,0))$ *are given by the three roots of the cubic polynomial*

$$\begin{aligned}\kappa^3 &- (c_{2,0,0}+c_{0,2,0}+c_{0,0,2})\kappa^2 \\ &+ (c_{2,0,0}c_{0,2,0}+c_{2,0,0}c_{0,0,2}+c_{0,2,0}c_{0,0,2}-c_{1,1,0}^2-c_{1,0,1}^2-c_{0,1,1}^2)\kappa \\ &- (c_{2,0,0}c_{0,2,0}c_{0,0,2}+2c_{1,1,0}c_{1,0,1}c_{0,1,1}-c_{2,0,0}c_{0,1,1}^2-c_{0,2,0}c_{1,0,1}^2-c_{0,0,2}c_{1,1,0}^2).\end{aligned} \tag{29}$$

Proof. According to Definition 2, the principal curvatures of f's graph are the eigenvalues of the matrix

$$-A=\frac{1}{l}\begin{pmatrix} f_{uu} & f_{uv} & f_{uw} \\ f_{uv} & f_{vv} & f_{vw} \\ f_{uw} & f_{vw} & f_{ww}\end{pmatrix}\begin{pmatrix} 1+f_u^2 & f_uf_v & f_uf_w \\ f_uf_v & 1+f_v^2 & f_vf_w \\ f_uf_w & f_vf_w & 1+f_w^2\end{pmatrix}^{-1}, \tag{30}$$

where $l=\sqrt{1+f_u^2+f_v^2+f_w^2}$. Evaluating $-A$ for $(u,v,w)=(0,0,0)$, one obtains the symmetric matrix

$$-A=\begin{pmatrix} c_{2,0,0} & c_{1,1,0} & c_{1,0,1} \\ c_{1,1,0} & c_{0,2,0} & c_{0,1,1} \\ c_{1,0,1} & c_{0,1,1} & c_{0,0,2}\end{pmatrix} \tag{31}$$

having the characteristic polynomial (29). □

The roots of the characteristic polynomial (29) are used as approximations of the three principal curvatures at $\boldsymbol{x}_i$.

Remark. It is known in linear algebra that all eigenvalues of a symmetric matrix are real. Therefore, the roots of the cubic characteristic polynomial (29) are real. The first root of (29) is computed using Newton's method, the other two roots are calculated after factorization.

4. Examples

The principal curvature approximation method has been tested for graphs of trivariate functions. In this case, the outward normal vectors are defined by the gradient, since the outward normal vector of the graph of a trivariate function is $\boldsymbol{n}=(-f_x,-f_y,-f_z,1)$. The exact gradients are used for all test functions.

Table 1
RMS errors of curvature approximation of graphs of trivariate functions; $x, y, z \in [-1, 1]$

Function	Curvature type	
	Mean curvature	Gaussian curvature
1. Quadratic polynomial: $0.4(x^2 + y^2 + z^2)$	0.0030	0.0026
2. Quadratic polynomial: $0.4(x^2 - y^2 - z^2)$	0.0011	0.0022
3. Cubic polynomial: $0.15(x^3 + 2x^2y - xz^2 + 2y^2)$	0.0025	0.0012
4. Exponential function: $e^{-0.5(x^2+y^2+z^2)}$	0.0063	0.0028
5. Trigonometric function: $0.1(\cos(\pi x) + \cos(\pi y) + \cos(\pi z))$	0.0033	0.0091

The exact mean curvature $H^{\text{ex}} = (\kappa_1^{\text{ex}} + \kappa_2^{\text{ex}} + \kappa_3^{\text{ex}})/3$ is compared with the average of the approximated principal curvatures $H^{\text{app}} = (\kappa_1^{\text{app}} + \kappa_2^{\text{app}} + \kappa_3^{\text{app}})/3$, and the exact Gaussian curvature $K^{\text{ex}} = \kappa_1^{\text{ex}}\kappa_2^{\text{ex}}\kappa_3^{\text{ex}}$ is compared with the product of the approximated principal curvatures $K^{\text{app}} = \kappa_1^{\text{app}}\kappa_2^{\text{app}}\kappa_3^{\text{app}}$.

All test functions $f(x, y, z)$, $x, y, z \in [-1, 1]$, are evaluated on a $26 \times 26 \times 26$ grid $(n = 25)$ with equidistant spacing, i.e.,

$$(x_i, y_j, z_k) = \left(\frac{2i-n}{n}, \frac{2j-n}{n}, \frac{2k-n}{n}\right), \quad i, j, k = 0, \ldots, n, \tag{32}$$

defining the set of points on their graphs, which is

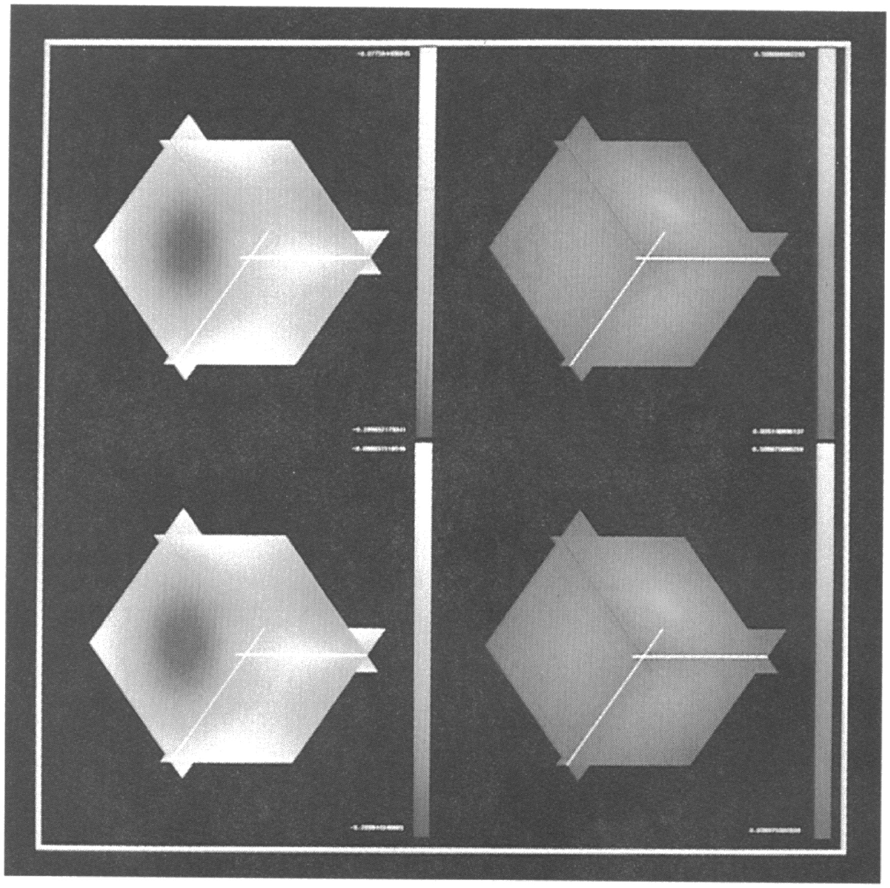
$$\{(x_i, y_j, z_k, f(x_i, y_j, z_k)) \mid i, j, k = 0, \ldots, n\}. \tag{33}$$

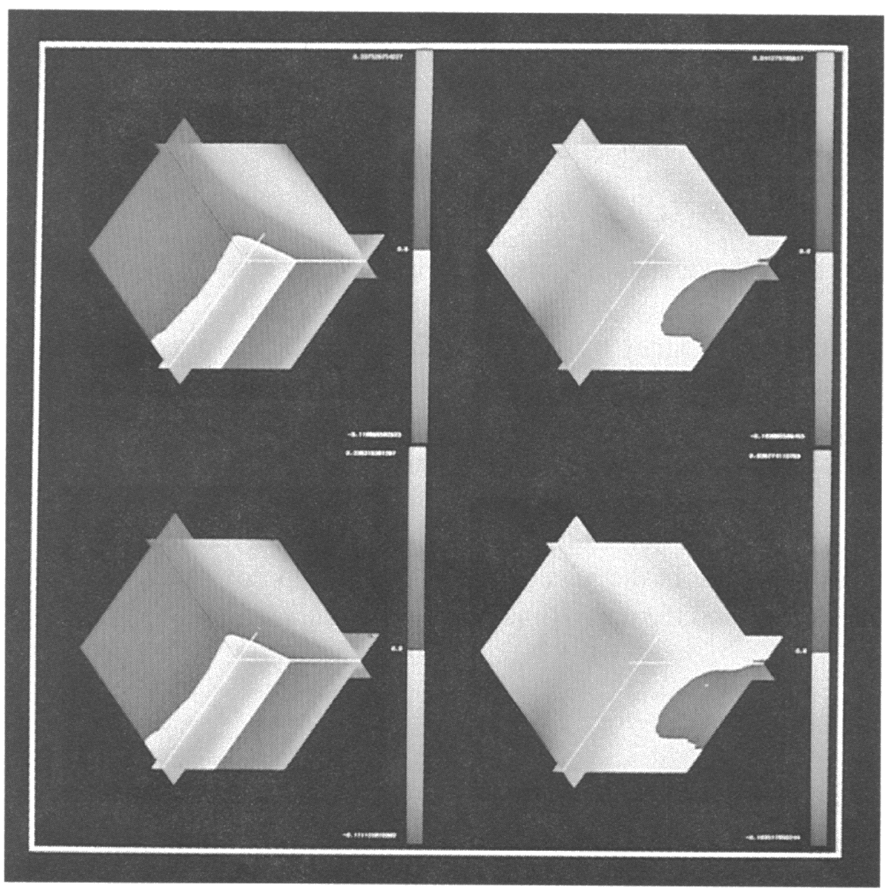
The triangulation of the domain is constructed by splitting each domain cuboid $C_{i,j,k}$ with vertices $\boldsymbol{x}_{i+I,j+J,k+K} = (x_{i+I,j+J,k+K}, y_{i+I,j+J,k+K}, z_{i+I,j+J,k+K})$, $I, J, K \in \{0, 1\}$, into six tetrahedra yielding a Delaunay triangulation. Table 1 lists the root-mean-square (RMS) errors for the approximation of mean and Gaussian curvature.

The curvature of a trivariate function's graph is rendered by slicing the function's domain with planes and representing curvature by color (see (Nielson and Hamann, 1990)). Exact and approximated curvatures are shown for the functions 2, 3, and 5 in Figs. 1–3. The exact mean curvature is shown in the upper-left corner of each figure, the exact Gaussian curvature in the upper-right corner, the approximated mean curvature in the lower-left corner, and the approximated Gaussian curvature in the lower-right corner.

5. Conclusions

A technique for approximating the three principal curvatures at points on a discretized, triangulated 3-surface has been developed. The test results confirm the quality of the





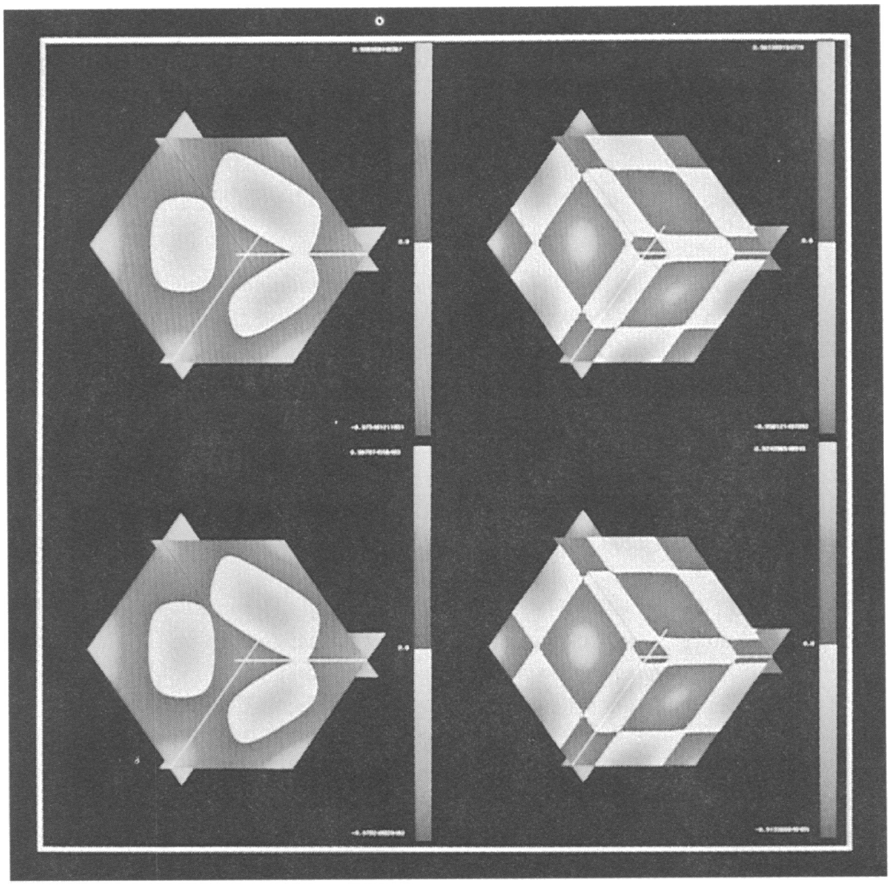


Fig. 1 (*opposite, top*). Exact and approximated mean and Gaussian curvature, $f(x, y, z) = 0.4(x^2 - y^2 - z^2)$, $x, y, z \in [-1, 1]$.

Fig. 2 (*opposite, bottom*). Exact and approximated mean and Gaussian curvature, $f(x, y, z) = 0.15(x^3 + 2x^2y - xz^2 + 2y^2)$, $x, y, z \in [-1, 1]$.

Fig. 3 (*above*). Exact and approximated mean and Gaussian curvature, $f(x, y, z) = 0.1(\cos(\pi x) + \cos(\pi y) + \cos(\pi z))$, $x, y, z \in [-1, 1]$.

approximation for graphs of trivariate functions. The curvature approximation technique is useful for the analysis of the "smoothness" of discrete 3-surfaces arising in CFD/FEM applications. The concept can be extended to n-manifolds (n-surfaces) in $(n+1)$D space. Future scattered data approximation methods for 3-surface data using curvature input will benefit from this scheme.

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