

4.3. Curvature approximation for triangulated three-dimensional graphs of trivariate functions

The graph of a trivariate function $f(x, y, z)$, f in class C^m , $m \geq 2$, mapping an open set $U \subset \mathbb{R}^3$ into \mathbb{R} can be interpreted as a regular parametric three-dimensional surface in four-dimensional space (see Definition 4.1.) using the parametrization $x(u, v, w) = u$, $y(u, v, w) = v$, $z(u, v, w) = w$, and $W(u, v, w) = f(u, v, w)$,

$$\mathbf{x}(\mathbf{u}) = (u, v, w, f(u, v, w))^T, \quad (u, v, w) \in D \subset \mathbb{R}^3. \quad (4.33.)$$

For this particular hypersurface, one easily derives the formulae

$$\begin{aligned} \mathbf{x}_u &= (1, 0, 0, f_u)^T, & \mathbf{x}_v &= (0, 1, 0, f_v)^T, & \mathbf{x}_w &= (0, 0, 1, f_w)^T, \\ \mathbf{x}_{uu} &= (0, 0, 0, f_{uu})^T, & \mathbf{x}_{uv} &= (0, 0, 0, f_{uv})^T, & \mathbf{x}_{uw} &= (0, 0, 0, f_{uw})^T, \\ \mathbf{x}_{vv} &= (0, 0, 0, f_{vv})^T, & \mathbf{x}_{vw} &= (0, 0, 0, f_{vw})^T, & \mathbf{x}_{ww} &= (0, 0, 0, f_{ww})^T, \quad \text{and} \\ \mathbf{n}(\mathbf{u}) &= \frac{\text{cross product } (\mathbf{x}_u, \mathbf{x}_v, \mathbf{x}_w)}{\| \text{cross product } (\mathbf{x}_u, \mathbf{x}_v, \mathbf{x}_w) \|} = \frac{(-f_u, -f_v, -f_w, 1)^T}{\sqrt{1 + f_u^2 + f_v^2 + f_w^2}} \end{aligned} \quad (4.34.)$$

(for the n-dimensional cross product see [Weld '90]).

Definition 4.10. The three-dimensional **tangent space** at a point $\mathbf{x}_0 = \mathbf{x}(\mathbf{u}_0)$ on a regular parametric three-dimensional surface in four-dimensional space is defined as the set of all points \mathbf{y} in \mathbb{R}^4 satisfying the equation

$$\mathbf{y} = \mathbf{x}_0 + a\mathbf{x}_u(\mathbf{u}_0) + b\mathbf{x}_v(\mathbf{u}_0) + c\mathbf{x}_w(\mathbf{u}_0), \quad a, b, c \in \mathbb{R}. \quad (4.35.)$$

The Gauss-Weingarten map for this special graph interpreted as a three-dimensional hypersurface in four-dimensional space is given by

$$\begin{aligned}
 -A &= - \begin{pmatrix} a_{1,1} & a_{1,2} & a_{1,3} \\ a_{2,1} & a_{2,2} & a_{2,3} \\ a_{3,1} & a_{3,2} & a_{3,3} \end{pmatrix} \\
 &= \frac{1}{l} \begin{pmatrix} f_{uu} & f_{uv} & f_{uw} \\ f_{uv} & f_{vv} & f_{vw} \\ f_{uw} & f_{vw} & f_{ww} \end{pmatrix} \begin{pmatrix} 1 + f_u^2 & f_u f_v & f_u f_w \\ f_u f_v & 1 + f_v^2 & f_v f_w \\ f_u f_w & f_v f_w & 1 + f_w^2 \end{pmatrix}^{-1}, \tag{4.36.}
 \end{aligned}$$

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

Definition 4.11. The three (real) eigenvalues κ_1 , κ_2 , and κ_3 of the matrix $-A$ from equation (4.36.) are called the **principal curvatures** of the three-dimensional graph of the trivariate function $f(x, y, z)$. Therefore, the principal curvatures are the (real) roots of the characteristic polynomial of $-A$, the cubic polynomial

$$\begin{aligned}
 &\kappa^3 + (a_{1,1} + a_{2,2} + a_{3,3}) \kappa^2 + (a_{1,1}a_{2,2} + a_{1,1}a_{3,3} + a_{2,2}a_{3,3} - a_{1,2}a_{2,1} - a_{1,3}a_{3,1} - a_{2,3}a_{3,2}) \kappa \\
 &+ (a_{1,1}a_{2,2}a_{3,3} + a_{1,2}a_{2,3}a_{3,1} + a_{1,3}a_{2,1}a_{3,2} - a_{1,1}a_{2,3}a_{3,2} - a_{1,2}a_{2,1}a_{3,3} - a_{1,3}a_{2,2}a_{3,1}). \tag{4.37.}
 \end{aligned}$$

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

$$H = \frac{1}{3} (\kappa_1 + \kappa_2 + \kappa_3), \quad K = \kappa_1 \kappa_2 \kappa_3. \tag{4.38.}$$

Figure 4.9. shows the mean (left) and the Gaussian curvature (right) in three planes intersecting the three-dimensional domain of a trivariate function using the visualization technique described in chapter 2.3. (slicing). Curvature changes in f 's graph can clearly be recognized, giving rise to the use of these particular curvature measures as indicators for the smoothness of trivariate functions.

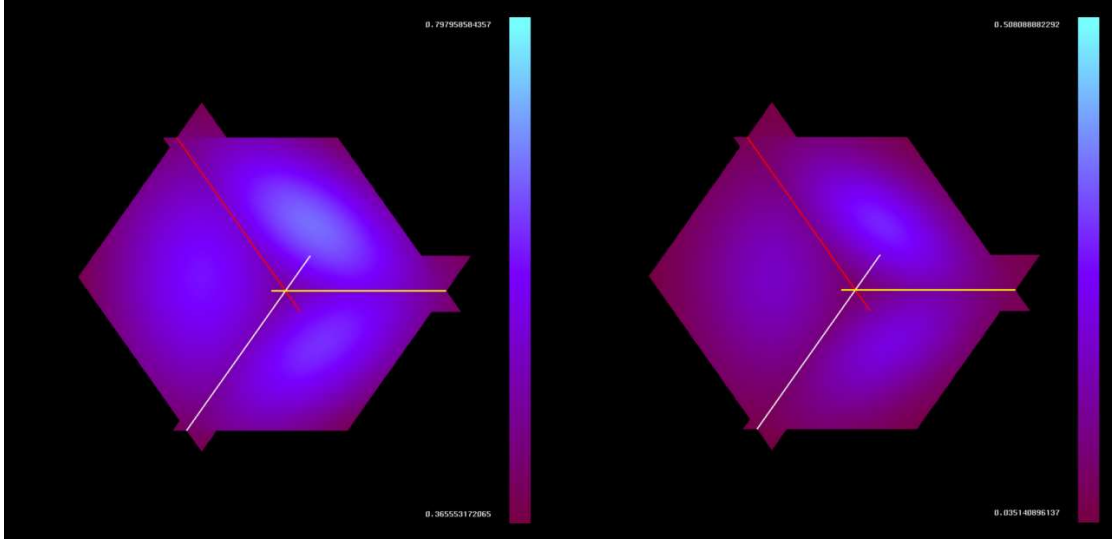


Fig. 4.9. Mean and Gaussian curvature of the graph of $f(x, y, z) = .4 (x^2 + y^2 + z^2)$, $x, y, z \in [-1, 1]$.

The properties of three-dimensional surfaces stated in the following theorems are needed for the curvature approximation method to be deduced subsequently.

Theorem 4.4. *Each regular parametric three-dimensional surface $\mathbf{x}(\mathbf{u})$ of class m , $m \geq 2$, can locally be represented in the explicit form $W = W(x, y, z)$, where W is an at least C^2 function. Choosing a surface point \mathbf{x}_0 as origin of a local coordinate system and the W -axis in the same direction as the surface normal \mathbf{n}_0 at \mathbf{x}_0 , the Taylor series for W considering only the terms up to degree 2 is given by*

$$W(x, y, z) = \frac{1}{2} (c_{2,0,0}x^2 + 2c_{1,1,0}xy + 2c_{1,0,1}xz + c_{0,2,0}y^2 + 2c_{0,1,1}yz + c_{0,0,2}z^2), \quad (4.39.)$$

choosing any 3 unit vectors in the xyz -tangent space determining a right-handed orthonormal coordinate system. Changing the orientation of these 3 unit vectors appropriately yields the equation of the so-called **osculating paraboloid** at \mathbf{x}_0 ,

$$W(x, y, z) = \frac{1}{2} (c_{2,0,0}^* x^2 + c_{0,2,0}^* y^2 + c_{0,0,2}^* z^2)$$

such that the three principal curvatures at \mathbf{x}_0 coincide with the coefficients of this paraboloid, $\kappa_1 = c_{2,0,0}^*$, $\kappa_2 = c_{0,2,0}^*$, and $\kappa_3 = c_{0,0,2}^*$.

Proof. See [Strubecker '58,'59] or [Spivak '70].

Theorem 4.5. *Let f be the trivariate polynomial*

$$f(x, y, z) = \sum_{\substack{i+j+k \leq n \\ i, j, k \geq 0}} c_{i,j,k} x^i y^j z^k, \quad (4.40.)$$

where a point in space has coordinates x , y , and z with respect to a coordinate system given by an origin \mathbf{o} and three orthonormal basis vectors \mathbf{d}_1 , \mathbf{d}_2 , and \mathbf{d}_3 ; changing the orientation of the orthonormal basis vectors changes the representation of the trivariate polynomial, but not its graph.

Proof. Analogous to the proof of Theorem 4.2.

As for the two-dimensional case, the principal curvature approximation technique requires a localization of a three-dimensional triangulation.

Definition 4.12. Given a three-dimensional triangulation (also referred to as a tetrahedrization) in three- or four-dimensional space, the **platelet** \mathcal{P}_i associated with a point \mathbf{x}_i in the triangulation is the set of all tetrahedra (determined by the index-quadruples (j_1, j_2, j_3, j_4) specifying their vertices) sharing \mathbf{x}_i as a common

vertex,

$$\mathcal{P}_i = \bigcup \{(j_1, j_2, j_3, j_4) \mid i = j_1 \vee i = j_2 \vee i = j_3 \vee i = j_4\}. \quad (4.41.)$$

The vertices constituting \mathcal{P}_i are referred to as **platelet points**.

The sequence of computations for principal curvature approximation in the two-dimensional case, described in chapter 4.2., can easily be extended to the three-dimensional case. The following steps must be executed.

- (i) Determine the platelet points associated with \mathbf{x}_i .
- (ii) Compute the tangent space P passing through \mathbf{x}_i and having \mathbf{n}_i (the normal at \mathbf{x}_i) as its normal.
- (iii) Define an orthonormal coordinate system in P with \mathbf{x}_i as its origin and three arbitrary unit vectors in P .
- (iv) Compute the distances of all platelet points from the tangent space P .
- (v) Project all platelet points onto the tangent space P , and represent their projections with respect to the local coordinate system in P .
- (vi) Interpret the projections in P as abscissae values and the distances of the original platelet points from P as ordinate values.
- (vii) Construct a trivariate polynomial f approximating these ordinate values.
- (viii) Compute the principal curvatures of f 's graph at \mathbf{x}_i .

Some steps are now explained in more detail. Let $\{ \mathbf{y}_j = (x_j, y_j, z_j, W_j)^T \mid j = 0 \dots n_i \}$ be the set of all platelet points associated with the point \mathbf{x}_i such that $\mathbf{y}_0 = \mathbf{x}_i$, and let $\mathbf{n} = (n^x, n^y, n^z, n^W)^T$ be the outward unit normal vector at \mathbf{y}_0 . The implicit equation for the tangent space P is given by

$$\begin{aligned} \mathbf{n} \cdot (\mathbf{x} - \mathbf{y}_0) &= n^x(x - x_0) + n^y(y - y_0) + n^z(z - z_0) + n^W(W - W_0) \\ &= n^x x + n^y y + n^z z + n^W W - (n^x x_0 + n^y y_0 + n^z z_0 + n^W W_0) \\ &= Ax + By + Cz + DW + E = 0. \end{aligned} \quad (4.42.)$$

Clearly, the four vectors

$$\mathbf{n} = \frac{(-f_u, -f_v, -f_w, 1)^T}{\sqrt{1 + f_u^2 + f_v^2 + f_w^2}},$$

$$\mathbf{a}_1 = (1, 0, 0, 0)^T, \quad \mathbf{a}_2 = (0, 1, 0, 0)^T, \quad \text{and} \quad \mathbf{a}_3 = (0, 0, 1, 0)^T$$

are linearly independent and therefore form a basis for \mathbb{R}^4 . Obviously, \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_3 are not necessarily perpendicular to the normal \mathbf{n} . Using Gram-Schmidt orthogonalization yields an orthonormal basis for \mathbb{R}^4 consisting of the basis vectors \mathbf{n} , \mathbf{b}_1 , \mathbf{b}_2 , and \mathbf{b}_3 , where \mathbf{b}_1 , \mathbf{b}_2 , and \mathbf{b}_3 are computed as

$$\mathbf{b}_1 = (\mathbf{a}_1 \cdot \mathbf{n}) \mathbf{n}, \quad \mathbf{b}_1 = \mathbf{a}_1 - \mathbf{b}_1, \quad \mathbf{b}_1 = \frac{\mathbf{b}_1}{\|\mathbf{b}_1\|},$$

$$\mathbf{b}_2 = (\mathbf{a}_2 \cdot \mathbf{n}) \mathbf{n} + (\mathbf{a}_2 \cdot \mathbf{b}_1) \mathbf{b}_1, \quad \mathbf{b}_2 = \mathbf{a}_2 - \mathbf{b}_2, \quad \mathbf{b}_2 = \frac{\mathbf{b}_2}{\|\mathbf{b}_2\|}, \quad \text{and}$$

$$\mathbf{b}_3 = (\mathbf{a}_3 \cdot \mathbf{n}) \mathbf{n} + (\mathbf{a}_3 \cdot \mathbf{b}_1) \mathbf{b}_1 + (\mathbf{a}_3 \cdot \mathbf{b}_2) \mathbf{b}_2, \quad \mathbf{b}_3 = \mathbf{a}_3 - \mathbf{b}_3, \quad \mathbf{b}_3 = \frac{\mathbf{b}_3}{\|\mathbf{b}_3\|},$$

$$\|\mathbf{b}_i\| = \sqrt{(\mathbf{b}_i \cdot \mathbf{b}_i)}, \quad i = 1, 2, 3.$$

The perpendicular signed distances d_j , $j = 0 \dots n_i$, of all platelet points \mathbf{y}_j from the tangent space P are

$$d_j = \text{dist}(\mathbf{y}_j, P) = \frac{Ax_j + By_j + Cz_j + DW_j + E}{\sqrt{A^2 + B^2 + C^2 + D^2}} = Ax_j + By_j + Cz_j + DW_j + E. \quad (4.43.)$$

Projecting all platelet points \mathbf{y}_j onto P yields the points \mathbf{y}_j^P , where

$$\mathbf{y}_j^P = \mathbf{y}_j - d_j \mathbf{n}. \quad (4.44.)$$

Again, \mathbf{y}_0 is seen as the origin, and \mathbf{b}_1 , \mathbf{b}_2 , and \mathbf{b}_3 are regarded as the three unit basis vectors of a local three-dimensional orthonormal coordinate system for the tangent space P . Each point \mathbf{y}_j^P in P is expressed in terms of that coordinate system. Computing the difference vectors \mathbf{d}_j as

$$\mathbf{d}_j = \mathbf{y}_j^P - \mathbf{y}_0, \quad j = 0 \dots n_i,$$

and expressing them as linear combinations of the basis vectors \mathbf{b}_1 , \mathbf{b}_2 , and \mathbf{b}_3 in P , one obtains a new representation for \mathbf{d}_j ,

$$\mathbf{d}_j = (\mathbf{d}_j \cdot \mathbf{b}_1) \mathbf{b}_1 + (\mathbf{d}_j \cdot \mathbf{b}_2) \mathbf{b}_2 + (\mathbf{d}_j \cdot \mathbf{b}_3) \mathbf{b}_3, \quad (4.45.)$$

defining the local coordinates u_j , v_j , and w_j of the point \mathbf{y}_j^P in terms of the local coordinate system:

$$(u_j, v_j, w_j)^T = (\mathbf{d}_j \cdot \mathbf{b}_1, \mathbf{d}_j \cdot \mathbf{b}_2, \mathbf{d}_j \cdot \mathbf{b}_3)^T. \quad (4.46.)$$

The local coordinates u_j , v_j , and w_j define the abscissae values and the signed distances d_j the ordinate values (in direction of the normal \mathbf{n}) for a polynomial

$f(u, v, w)$ of degree two (see Theorem 4.4.) which is constructed by approximating these ordinate values. Forcing f to satisfy the conditions $f(0, 0, 0) = f_u(0, 0, 0) = f_v(0, 0, 0) = f_w(0, 0, 0) = 0$ the constraints

$$f(u_j, v_j, w_j) = \frac{1}{2} \left(c_{2,0,0}u_j^2 + 2c_{1,1,0}u_jv_j + 2c_{1,0,1}u_jw_j + c_{0,2,0}v_j^2 + 2c_{0,1,1}v_jw_j + c_{0,0,2}w_j^2 \right) = d_j,$$

$j = 1 \dots n_i$, remain. In matrix representation, these constraints are

$$\begin{pmatrix} u_1^2 & 2u_1v_1 & 2u_1w_1 & v_1^2 & 2v_1w_1 & w_1^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ u_{n_i}^2 & 2u_{n_i}v_{n_i} & 2u_{n_i}w_{n_i} & v_{n_i}^2 & 2v_{n_i}w_{n_i} & w_{n_i}^2 \end{pmatrix} \begin{pmatrix} c_{2,0,0} \\ c_{1,1,0} \\ c_{1,0,1} \\ c_{0,2,0} \\ c_{0,1,1} \\ c_{0,0,2} \end{pmatrix} = U \mathbf{c} = \mathbf{d} = \begin{pmatrix} d_1 \\ \vdots \\ d_{n_i} \end{pmatrix}. \quad (4.47.)$$

Using the least squares approach, the resulting normal equations are

$$U^T U \mathbf{c} = U^T \mathbf{d}. \quad (4.48.)$$

This 6·6–system of linear equations can easily be solved using Gaussian elimination provided the determinant of $U^T U$ does not vanish.

A theorem in multi-dimensional differential geometry ensures that the three principal curvatures at a point on the graph of a trivariate function are always real.

Theorem 4.6. *The principal curvatures $\kappa_1, \kappa_2,$ and κ_3 at any point on the graph $(u, v, w, f(u, v, w))^T \in \mathbb{R}^4, u, v, w \in \mathbb{R}$, of a trivariate function f of class m ,*

$m \geq 2$, are real and are the eigenvalues of the Gauss-Weingarten map associated with its graph at a particular point.

Proof. See [Spivak '70] or [Weld '90].

Theorem 4.7. *The three principal curvatures κ_1, κ_2 , and κ_3 of the graph $(u, v, w, f(u, v, w))^T \subset \mathbb{R}^4$, $u, v, w \in \mathbb{R}$, of the trivariate polynomial*

$$f(u, v, w) = \frac{1}{2} \left(c_{2,0,0}u^2 + 2c_{1,1,0}uv + 2c_{1,0,1}uw + c_{0,2,0}v^2 + 2c_{0,1,1}vw + c_{0,0,2}w^2 \right) \quad (4.49.)$$

at the point $(0, 0, 0, f(0, 0, 0))^T$ are given by the three real roots of the cubic equation

$$\begin{aligned} & -\kappa^3 + (c_{2,0,0} + c_{0,2,0} + c_{0,0,2})\kappa^2 \\ & - (c_{2,0,0}c_{0,2,0} + c_{2,0,0}c_{0,0,2} + c_{0,2,0}c_{0,0,2} - c_{1,1,0}^2 - c_{1,0,1}^2 - c_{0,1,1}^2)\kappa \\ & + (c_{2,0,0}c_{0,2,0}c_{0,0,2} + 2c_{1,1,0}c_{1,0,1}c_{0,1,1} - c_{2,0,0}c_{0,1,1}^2 - c_{0,2,0}c_{1,0,1}^2 - c_{0,0,2}c_{1,1,0}^2) = 0. \end{aligned} \quad (4.50.)$$

Proof. According to Definition 4.11. and equation (4.36.) the principal curvatures of f 's graph are the eigenvalues of the matrix

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

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

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

having the characteristic polynomial in (4.50.).

q.e.d.

The roots of the characteristic polynomial in (4.50.) finally determine the approximations for the principal curvatures at the point \mathbf{x}_i .

Remark 4.3. It is well known in linear algebra that the eigenvalues of a symmetric matrix are all real (see [Lang '66]). Considering this fact, it is obvious that the three roots of the cubic characteristic polynomial appearing in Theorem 4.7. must also be real since the matrix $-A$ is symmetric.

Remark 4.4. The first root of the cubic polynomial in equation (4.50.) is computed using Newton's method. The other two roots are calculated after factorization of the cubic polynomial.

The principal curvature approximation technique is examined for graphs of six trivariate functions. The exact mean curvature $H^{ex} = \frac{1}{3} (\kappa_1^{ex} + \kappa_2^{ex} + \kappa_3^{ex})$ is compared with the average of the approximated principal curvatures $H^{app} = \frac{1}{3} (\kappa_1^{app} + \kappa_2^{app} + \kappa_3^{app})$ and the exact Gaussian curvature $K^{ex} = \kappa_1^{ex} \kappa_2^{ex} \kappa_3^{ex}$ with the product of the approximated principal curvatures $K^{app} = \kappa_1^{app} \kappa_2^{app} \kappa_3^{app}$.

All trivariate test functions $f(x, y, z)$ are defined over $[-1, 1] \times [-1, 1] \times [-1, 1]$ and are evaluated on a $26 \cdot 26 \cdot 26$ -grid with equidistant spacing,

$$(x_i, y_j, z_k)^T = \left(-1 + \frac{i}{12.5}, -1 + \frac{j}{12.5}, -1 + \frac{k}{12.5} \right)^T, \quad i, j, k = 0 \dots 25,$$

determining the set of four-dimensional points on their graphs,

$$\left\{ (x_i, y_j, z_k, f(x_i, y_j, z_k)) \mid i, j, k = 0 \dots 25 \right\}.$$

The triangulation (tetrahedrization) for a function's graph is determined by splitting each domain cell C_i (see Definition 3.12.) specified by its eight indices in the tuple

$$((i, j, k), (i + 1, j, k), (i + 1, j + 1, k), (i, j + 1, k),$$

$$(i, j, k + 1), (i + 1, j, k + 1), (i + 1, j + 1, k + 1), (i, j + 1, k + 1))$$

into the six tetrahedra T_i^l , $l = 1 \dots 6$, mentioned in chapter 3.2. (splitting a cuboid into six tetrahedra).

Table 4.2. summarizes the test results for the approximation of the mean and the Gaussian curvature.

Tab. 4.2. RMS errors of curvature approximation for graphs of trivariate functions.

Function	H	K
1. Linear polynomial: .2 $(x + y + z)$.	0	0
2. Quadratic polynomial q_1 : .4 $(x^2 + y^2 + z^2)$.	.002950	.002597
3. Quadratic polynomial q_2 : .4 $(x^2 - y^2 - z^2)$.	.001115	.002216
4. Cubic polynomial: .15 $(x^3 + 2x^2y - xz^2 + 2y^2)$.	.002545	.001207
5. Exponential function: $e^{-\frac{1}{2}(x^2+y^2+z^2)}$.	.006349	.002802
6. Trigonometric function: .1 $(\cos(\pi x) + \cos(\pi y) + \cos(\pi z))$.	.003269	.009065

Curvature of a trivariate function's graph is rendered by slicing the function's domain with planes and representing the magnitude of the curvature by different colors (see slicing methods, chapter 2.3.). Exact and approximated curvatures are shown for the functions 3, 4, and 6. In each figure, the exact mean and Gaussian curvatures are shown at the top, the corresponding approximated curvatures at the bottom. Figure 4.10. shows the exact and the approximated mean and Gaussian curvatures for the graph of function 3, Figure 4.11. for the graph of function 4, and Figure 4.12. for function 6.

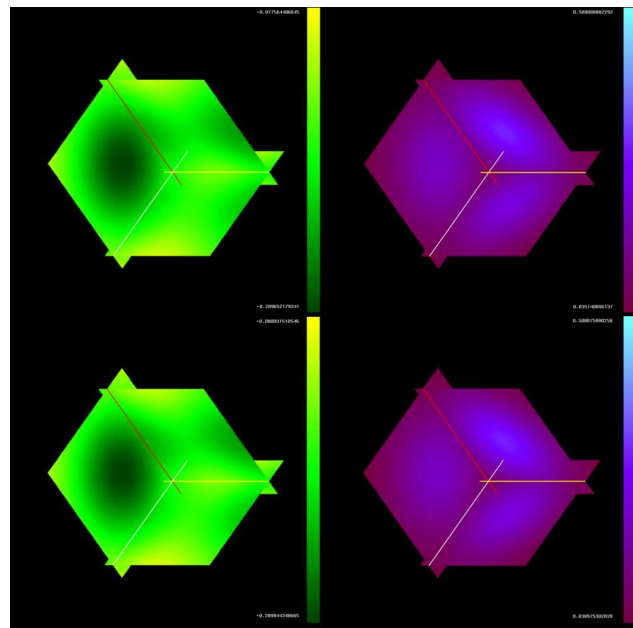


Fig. 4.10. Exact and approximated mean and Gaussian curvatures of the graph of $f(x, y, z) = .4 (x^2 - y^2 - z^2)$, $x, y, z \in [-1, 1]$.

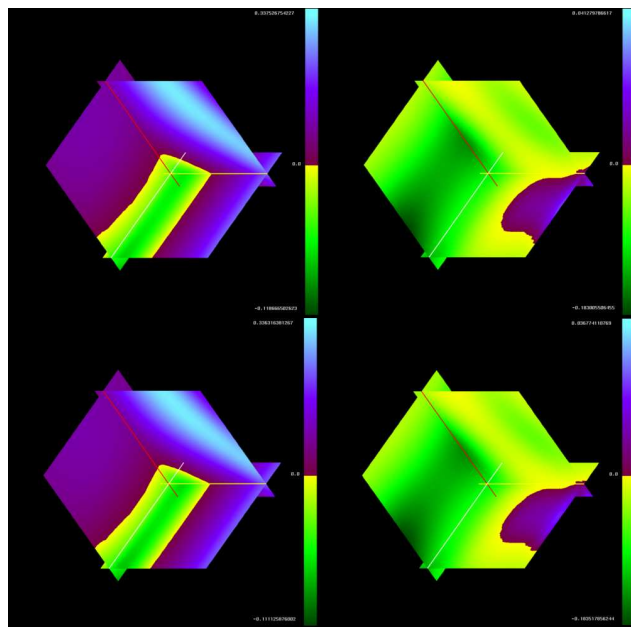


Fig. 4.11. Exact and approximated mean and Gaussian curvatures of the graph of $f(x, y, z) = .15 (x^3 + 2x^2y - xz^2 + 2y^2)$, $x, y, z \in [-1, 1]$.

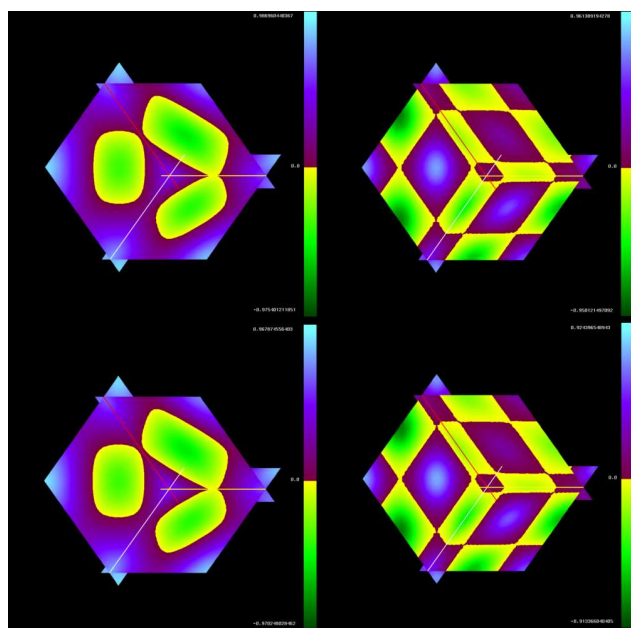


Fig. 4.12. Exact and approximated mean and Gaussian curvatures of the graph of $f(x, y, z) = .1 (\cos(\pi x) + \cos(\pi y) + \cos(\pi z))$, $x, y, z \in [-1, 1]$.