Chapter 3

Trilinear contour approximation for trivariate data

3.1. Previous work and basic definitions

Visualizing contour levels of a trivariate function is another possibility to obtain insight into a function's behavior by displaying them as surfaces. This has not yet been examined in greater detail in chapter 2, due to the fact that contours are not primarily approximated for rendering purposes, but for modeling the contours themselves as surfaces in three-dimensional space.

In principle, a point set is determined such that each point in this set is close to a certain contour, the point set is triangulated (yielding a two-dimensional triangulation in three-dimensional space), the neighbors for each triangle in the resulting triangulation are determined, and each triangle is associated with a particular part of the contour. Normal vectors are estimated for each point, needed for further modeling the data.

In [Bloomquist '90], [Petersen '84], and [Petersen et al. '87] different approaches are described to contour trivariate functions given in explicit form. Other references can be found there as well. Approximating contours from rectilinear trivariate data sets alone is explored in [Hamann '90b], [Lorensen & Cline '87], and [Nielson & Hamann '91b]. An error in the *marching-cubes method* by Lorensen has been pointed out in [Dürst '88]: Approximating a contour using Lorensen's technique results in a triangulation which might lead to "holes" (locally missing or improperly constructed triangles) for special data configurations. An optimization algorithm for a two-dimensional triangulation in three-dimensional space is given in [Choi et al. '88].

Ways for resolving the inaccuracy in Lorensen's contouring method are shown in 3.2. For further modeling this piecewise planar contour approximation, derivative information must be provided. Estimating gradients for trivariate functions is discussed in [Stead '84] and [Zucker & Hummel '81]. These estimates determining additional geometrical information (tangent planes with orientation) for the vertices in the triangulation are needed to create overall tangent-plane-continuous surfaces for each part of a contour. Again, contours of trivariate functions are interpreted here as two-dimensional boundaries of objects. Therefore, triangulations approximating such contours are used as input for a surface scheme.

Definition 3.1. Let $f : I\!R^3 \to I\!R$; a trivariate **contour** is the point set

$$C_f(\alpha) \;=\; \{\; \mathbf{x} \mid f(\mathbf{x}) = \alpha,\; \alpha \in I\!R \;\} \;\subset\; I\!R^3. \tag{3.1.}$$

Contours of trivariate functions are also referred to as **contour surfaces**, **isosurfaces**, **level surfaces** or **niveau sets**.

A contour might be partitioned into several unconnected subsets. This motivates the next definition.

Definition 3.2. Let $f : I\!R^3 \to I\!R$ be a continuous function; a **component** $C_f^j(\alpha) \subseteq C_f(\alpha)$ is the set of points such that for each pair of points $\mathbf{x}, \mathbf{y} \in C_f^j(\alpha)$ a curve $\mathbf{c} \subset C_f^j(\alpha)$ exists connecting $\mathbf{x}$ and $\mathbf{y}$.

Definition 3.3. Let $f : I\!R^3 \to I\!R$ be a partially differentiable function (a C^1 function). The **gradient** of f in $\mathbf{x} \in I\!R^3$ is the triple

$$\bigtriangledown f(\mathbf{x}) = \Big(\frac{\partial f}{\partial x}(\mathbf{x}),\ \frac{\partial f}{\partial y}(\mathbf{x}),\ \frac{\partial f}{\partial z}(\mathbf{x}) \Big) = \big(f_x(\mathbf{x}),\ f_y(\mathbf{x}),\ f_z(\mathbf{x}) \big). \tag{3.2.}$$

Theorem 3.1. *Let $f : I\!R^3 \to I\!R$ be a C^1 function and $\bigtriangledown f(\mathbf{x}) \neq (0,0,0)$ for all $\mathbf{x} \in I\!R^3$. Then, every contour $C_f(\alpha)$ is a surface (a two-dimensional manifold).*

Proof. The Taylor series for f at a point $\mathbf{x}_0 \in C_f(\alpha)$ is

$$f(\mathbf{x}) = \bigtriangledown f(\mathbf{x}_0)\ (x - x_0, y - y_0, z - z_0)^T + R(\mathbf{x}) = 0.$$

This is the equation of an implicitly defined surface of at least first degree.

q.e.d.

Remark 3.1. For computing purposes it must be assured that a contour of a trivariate function is not (locally) a three-dimensional volume. This would be the case if $f = \alpha$ on such a volume, implying a vanishing gradient.

For the further discussion the domain of the triavariate function is restricted to a subset of $I\!R^3$. In most applications this subset is a box. This restriction implies that a single component of a contour can be divided into several unconnected parts inside a subset. Therefore, the following definitions are necessary.

Definition 3.4. Let $U = (x_0, x_1) \times (y_0, y_1) \times (z_0, z_1) \subset I\!R^3$ and $\overline{U}$ be the closure of U. If

$$B = (\overline{U} \setminus U) \cap C_f(\alpha) \neq \emptyset,$$

then B is called the **boundary** of $C_f(\alpha)$ with respect to U.

Remark 3.2. $\overline{U} \setminus U$ constitutes the faces of $\overline{U}$.

Definition 3.5. Let U be defined as in 3.4. and $C_f(\alpha) = \bigcup_{j=1}^{m} C_f^j(\alpha)$ be a contour of a function $f : I\!R^3 \rightarrow I\!R$; a **part**

$$P_j^k|_{\overline{U}},\ j = 1...m,\ k = 1...m_j, \text{ of a component } C_f^j(\alpha),\ P_j^k(\overline{U}) \subseteq C_f^j(\alpha),$$

is the subset of points such that for each pair of points $\mathbf{x}, \mathbf{y} \in P_j^k|_{\overline{U}}$ a curve $\mathbf{c} \subset P_j^k|_{\overline{U}}$ exists connecting $\mathbf{x}$ and $\mathbf{y}$.

Remark 3.3. If a part $P_j^k|_{\overline{U}}$ of a component $C_f^j(\alpha)$ coincides with a face, an edge or a corner of $\overline{U}$, a special case treatment is necessary. Only for the first of these three cases a part is considered, in the other two cases the dimension of the part (relative to $\overline{U}$) is less than 2 and therefore neglected.

Remark 3.4. It is usually difficult to determine that two parts belong to the same component of a contour, if one restricts oneself to $\overline{U}$. As a result of this, the term part is used only, the connection between parts and the component they actually belong to is no longer made when limiting a contour to $\overline{U}$.

A contour of an arbitrary trivariate function usually can not be described in an explicit form. For this reason, a finite set of points is created, each point lying on the contour. This point set is then triangulated to yield a piecewise planar approximation to the true contour.

Definition 3.6. Let $P_j^k|_{\overline{U}}$ be a part of a component such that it has a non-empty intersection with the faces of $\overline{U}$, $P_j^k|_{\overline{U}} \cap (\overline{U} \setminus U) \neq \emptyset$. Let Y be a finite set of points in $P_j^k(\overline{U})$, $Y = \{\mathbf{y} | \mathbf{y} \in P_j^k|_{\overline{U}}\}$. Y is a **closed contour point set** with respect to U, if it contains points $\mathbf{y}_r$ which can be ordered such that they describe a closed polygon on the faces of U,

$$\{ \ \overline{\mathbf{y}_r\mathbf{y}_{r+1}} \mid \overline{\mathbf{y}_r\mathbf{y}_{r+1}} \cap U = \emptyset, \mathbf{y}_r \in Y, r = 0...(p_m - 1), \text{ indices } \bmod \ p_m \ \}$$

is a closed polygon.

The segments defining such a polygon are called **boundary edges**.

Definition 3.7. Two triangles T_1 and T_2 are **neighbors**, if they have exactly two vertices in common.

The above definitions allow to introduce the term of a contour triangulation.

Definition 3.8. Let $C_f(\alpha) = \bigcup_{j=1}^{m} \ C_f^j(\alpha)$, $C_f^j(\alpha) = \bigcup_{k=1}^{m_j} P_j^k(\overline{U})$ be the contour of $f : \mathbb{R}^3 \to \mathbb{R}$ restricted onto $\overline{U}$, f being a C^1 function, such that f's gradient does not vanish on $C_f(\alpha)$, $\bigtriangledown f(\mathbf{x})\big|_{C_f(\alpha)} \neq (0,0,0)$. Let

$$X = \{ \ \mathbf{x}_i \mid \mathbf{x}_i \in C_f(\alpha), \ i = 1...n \ \} \subset \overline{U}$$

be a finite set of points in $C_f(\alpha)$. A **two-dimensional contour triangulation** $\mathcal{T}$ of the point set X is the set of index triples

$$\mathcal{T} \ = \ \{ \ T_j = (r_j, s_j, t_j) \mid r_j, s_j, t_j \in \{1, ..., n\}, \ r_j \neq s_j, \ r_j \neq t_j, \ s_j \neq t_j \ \} \quad (3.3.)$$

such that

(i) $\mathbf{x}_{r_j}$, $\mathbf{x}_{s_j}$, and $\mathbf{x}_{t_j}$ are the vertices of a triangle T_j,

(ii) each point in X is the vertex of at least one triangle,

(iii) the intersection of the interior of two triangles is empty,

(iv) an edge $\overline{\mathbf{xy}}$, $\mathbf{x}, \mathbf{y} \in X$, in the triangulation is shared by at most two triangles,

(v) each point $\mathbf{y}$ on a face of $\overline{U}$ belongs to exactly one closed contour point set Y, $\mathbf{y} \in Y \subset X$,

(vi) each triangle has exactly three neighbors, except those triangles having at least one boundary edge,

(vii) there is no edge connecting points $\mathbf{x}$ and $\mathbf{y}$, if $\mathbf{x} \in C_f^j(\alpha)$ and $\mathbf{y} \in C_f^k(\alpha)$, $j \neq k$, or, if $\mathbf{x} \in P_j^l|_{\overline{U}}$ and $\mathbf{y} \in P_j^m|_{\overline{U}}$, $l \neq m$,

(viii) T_j's outward unit normal $\mathbf{n}_j$ is defined as

$$\mathbf{n}_j = (\mathbf{x}_{s_j} - \mathbf{x}_{r_j}) \times (\mathbf{x}_{t_j} - \mathbf{x}_{r_j}) \ / \ ||(\mathbf{x}_{s_j} - \mathbf{x}_{r_j}) \times (\mathbf{x}_{t_j} - \mathbf{x}_{r_j})||,$$

where $||(x, y, z)^T|| = \sqrt{x^2 + y^2 + z^2}$.

Remark 3.5. There is no distinction made between the permutations of the index triples (r_j, s_j, t_j), (s_j, t_j, r_j), and (t_j, r_j, s_j); only the sequence of three indices in a triple determining a triangle's orientation is of importance ((viii) in Definition 3.8.). The term triangulation is used instead of two-dimensional contour triangulation whenever it is obvious from the context what is meant.

Figure 3.1. illustrates the concept of a triangulated contour divided into two parts inside a box (black dots at cell corners representing function values greater than the contour level α).

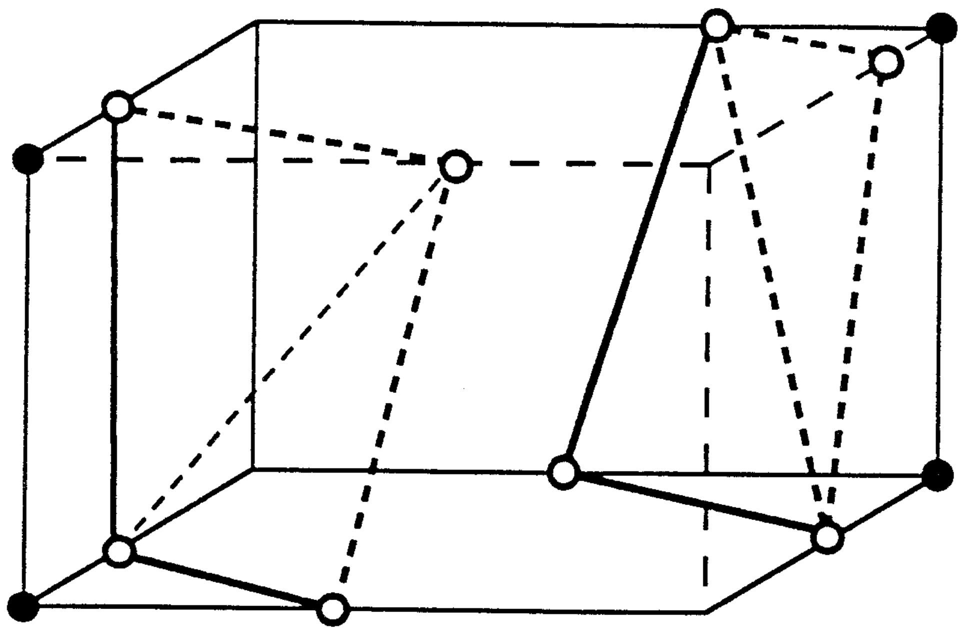

Fig. 3.1. Contour triangulation, contour divided into two parts.

To effectively test whether two triangles belong to the same part of a contour, a criterion must be given.

Definition 3.9. Two triangles $T_{l_1}, T_{l_m} \in \mathcal{T}$ **belong to the same part** $P_j^k|_{\overline{U}}$ of a component $C_f^j(\alpha)$ of a contour, if triangles $T_{l_2}, ..., T_{l_{m-1}} \in \mathcal{T}$ exist such that

$$\bigwedge_{i=1}^{m-1} \ (T_{l_i} \text{ and } T_{l_{i+1}} \text{ are neighbors }).$$

Definition 3.10. A **hole** in a contour triangulation $\mathcal{T}$ is defined by a set of m ordered edges

$$\{ \ e_i = \overline{\mathbf{x}_i \mathbf{x}_{i+1}} \mid i = 0...(m-1), \text{ indices } \bmod \ m \ \}$$

forming a closed polygon, where each edge belongs to exactly one triangle in $\mathcal{T}$. A hole is an **interior hole** if at least one edge e_i is not a boundary edge.

Remark 3.6. Holes in a contour triangulation $\mathcal{T}$ can naturally occur because the function f is restricted to $\overline{U}$. Interior holes are unnatural and undesired when approximating a trivariate contour with triangles in $\overline{U}$.

Definition 3.11. A two-dimensional contour triangulation $\mathcal{T}$ is **continuous**, if it does not contain interior holes.

3.2. Piecewise triangular contour approximation for rectilinear data

In several applications one is given a rectilinear data set as the result of physical measurements or simulations. Methods whose purpose is to approximate a contour of some underlying trivariate function (which is unknown itself) should take advantage of the structure implied by rectilinear data. An appropriate data element for a local contour approximation is a cell.

Definition 3.12. Let $X = \left\{ (\mathbf{x_i}^T, f_\mathbf{i}) \right\}$ be a rectilinear trivariate data set (Definition 2.1.). A **cell** $C_\mathbf{i}$ is the set of points

$$C_\mathbf{i} \;=\; [x_i, x_{i+1}] \times [y_j, y_{j+1}] \times [z_k, z_{k+1}], \;\; \mathbf{x_i} \in X.$$

Remark 3.7. The fact that three edges intersecting at a corner of a cell are mutually orthogonal to each other inspires the term rectilinear.

Remark 3.8. It is assumed throughout the next sections in this chapter that $f_\mathbf{i} \neq \alpha$ at all data points. If this condition is violated for a particular datum, the corresponding function value is incremented (or decremented) by $\epsilon \ll \max\{f_\mathbf{i}\} - \min\{f_\mathbf{i}\}$. This is inevitable because the number of special cases which must otherwise be taken care of is simply tremendous.

The approach described in [Lorensen & Cline '87] assumes that the underlying trivariate function f varies linearly along the edges of each cell: if $\mathbf{y}_0$ and $\mathbf{y}_1$ are the end points of an edge with corresponding function values f_0 and f_1, then

$$(\mathbf{x}^T, f)(t) = \big(\mathbf{x}^T(t), f(t)\big) = (1-t)({\mathbf{y}_0}^T, f_0) + t({\mathbf{y}_1}^T, f_1), \quad t \in [0,1].$$

If a contour intersects an edge $(f(t) = \alpha, t \in (0,1))$ the corresponding point $\mathbf{x}(t)$ is determined.

All points found on the edges of a cell are finally connected, thus forming closed polygons on the faces of a cell. These (non-planar) polygons are then triangulated. Using Lorensen's cell-by-cell method does not guarantee a continuous triangulation throughout the convex hull of the data set X (see [Dürst '88]). The reason for this is an inconsistency in constructing the polygons on a cell face shared by two neighbor cells: if four contour points are found on a face shared by two cells, they might be connected differently when the second of the two cells is considered. This is illustrated in Figure 3.2. (black dots at cell corners representing function values greater than the contour level α).

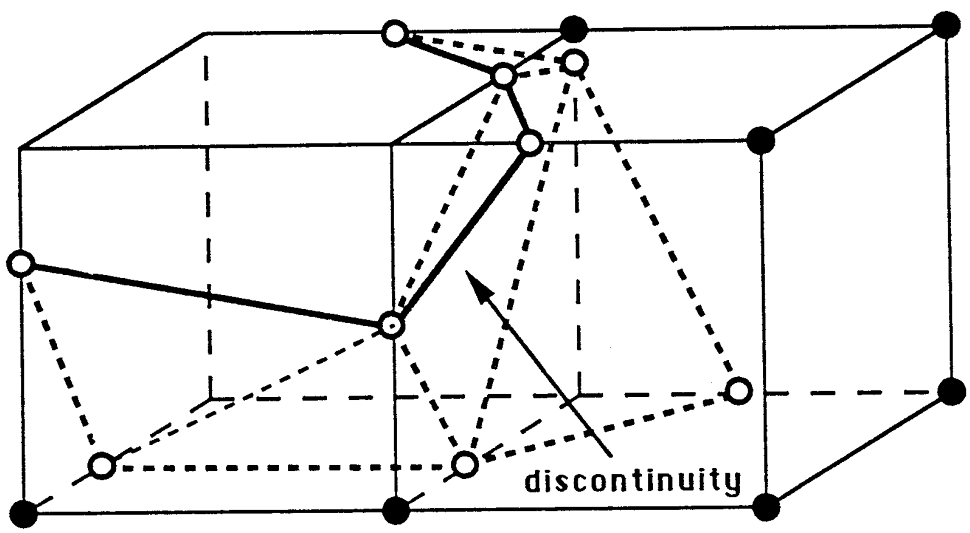

Fig. 3.2. Discontinuous piecewise planar contour approximation.

One solution to this problem is to subdivide a cell $C_{\mathbf{i}}$ into a set of tetrahedra whose union is $C_{\mathbf{i}}$ and whose intersections are tetrahedral faces. One way to split a cell $C_{\mathbf{i}}$ is to partition it into six tetrahedra:

$$
\begin{aligned}
T_{\mathbf{i}}^1 &= \{\ \mathbf{x} \mid \mathbf{x}(\mathbf{u}) = u_1\mathbf{x}_{i,j,k} + u_2\mathbf{x}_{i+1,j,k} + u_3\mathbf{x}_{i,j+1,k} + u_4\mathbf{x}_{i,j,k+1}\ \}, \\
T_{\mathbf{i}}^2 &= \{\ \mathbf{x} \mid \mathbf{x}(\mathbf{u}) = u_1\mathbf{x}_{i+1,j,k} + u_2\mathbf{x}_{i,j+1,k} + u_3\mathbf{x}_{i,j,k+1} + u_4\mathbf{x}_{i,j+1,k+1}\ \}, \\
T_{\mathbf{i}}^3 &= \{\ \mathbf{x} \mid \mathbf{x}(\mathbf{u}) = u_1\mathbf{x}_{i+1,j,k} + u_2\mathbf{x}_{i+1,j,k+1} + u_3\mathbf{x}_{i,j,k+1} + u_4\mathbf{x}_{i,j+1,k+1}\ \}, \\
T_{\mathbf{i}}^4 &= \{\ \mathbf{x} \mid \mathbf{x}(\mathbf{u}) = u_1\mathbf{x}_{i+1,j,k} + u_2\mathbf{x}_{i+1,j+1,k} + u_3\mathbf{x}_{i,j+1,k} + u_4\mathbf{x}_{i,j+1,k+1}\ \}, \\
T_{\mathbf{i}}^5 &= \{\ \mathbf{x} \mid \mathbf{x}(\mathbf{u}) = u_1\mathbf{x}_{i+1,j,k} + u_2\mathbf{x}_{i+1,j+1,k} + u_3\mathbf{x}_{i+1,j,k+1} + u_4\mathbf{x}_{i,j+1,k+1}\ \}, \\
T_{\mathbf{i}}^6 &= \{\ \mathbf{x} \mid \mathbf{x}(\mathbf{u}) = u_1\mathbf{x}_{i+1,j+1,k} + u_2\mathbf{x}_{i+1,j,k+1} + u_3\mathbf{x}_{i,j+1,k+1} + u_4\mathbf{x}_{i+1,j+1,k+1}\ \},
\end{aligned}
$$

where $\sum_{l=1}^{4} u_l = 1$, $u_l \geq 0$ (barycentric coordinates). Assuming that f is a linear polynomial over each tetrahedron, $f(\mathbf{u}) = \sum_{l=1}^{4} u_l f_l$, $\mathbf{u}$ representing the barycentric coordinates of a point $\mathbf{x}$ in a tetrahedron with function values f_l at its four vertices, the contour of f is planar whenever it passes through the interior of a tetrahedron (see [Bloomquist '90] or [Foley & Lane '90]).

Both Lorensen's and the tetrahedral split-technique yield precise contours if the underlying function f originally is a linear polynomial defined over $I\!R^3$, $f(\mathbf{x}) = \sum_{|\mathbf{l}|\leq 1} c_{\mathbf{i}}\mathbf{x}^{\mathbf{l}}$, $|\mathbf{l}| = i + j + k$, $c_l \in I\!R$, $\mathbf{x}^{\mathbf{l}} = x^i y^j z^k$. However, if one prefers to avoid the tetrahedral split-approach and derive a piecewise planar contour approximation from the cells themselves, Lorensen's method must be modified in order to achieve a continuous triangulation.

The data for a cell are interpolated over the whole cell using an appropriate and simple interpolation method.

Definition 3.13. Let $C_{\mathbf{i}}$ be a cell; the associated **trilinear cell interpolant** is the trivariate polynomial

$$
\begin{aligned}
(\mathbf{x}^T, f)(u,v,w) &= \left(\mathbf{x}^T(u,v,w), f(u,v,w)\right) \\
&= \sum_{t=0}^{1}\sum_{s=0}^{1}\sum_{r=0}^{1} (\mathbf{x_r}^T, f_{\mathbf{r}})^{[\mathbf{i}]} \; B_r^1(u) B_s^1(v) B_t^1(w),
\end{aligned}
\tag{3.4.}
$$

where $(\mathbf{x_r}^T, f_{\mathbf{r}})^{[\mathbf{i}]} = (\mathbf{x}_{i+r,j+s,k+t}{}^T, f_{i+r,j+s,k+t})$ are so-called Bézier points, $B_l^1(t) = (1-t)^{1-l} t^l$, $t \in [0,1]$, $l = 0, 1$, are the Bernstein polynomials of degree one and $u, v, w \in [0,1]$.

Theorem 3.2. *The component $f(u,v,w)$ of the trilinear cell interpolant is a linear polynomial along each cell edge and a bilinear polynomial over each cell face.*

Proof. It is

$$f(u,v,w) = \textstyle\sum_{r=0}^{1} f_{\mathbf{r}}^{[\mathbf{i}]} \; B_r^1(u)$$

for $v, w \in \{0,1\}$, $u \in [0,1]$, $s, t \in \{0,1\}$ (analogous for the other edges, given by $u, w \in \{0,1\}$, $v \in [0,1]$, $r, t \in \{0,1\}$ and $u, v \in \{0,1\}$, $w \in [0,1]$, $r, s \in \{0,1\}$), and it is

$$f(u,v,w) = \textstyle\sum_{s=0}^{1} \sum_{r=0}^{1} f_{\mathbf{r}}^{[\mathbf{i}]} B_r^1(u) B_s^1(v)$$

for $w \in \{0,1\}$, $u, v \in [0,1]$, $t \in \{0,1\}$ (analogous for the other faces, $v \in \{0,1\}$, $u, w \in [0,1]$, $s \in \{0,1\}$, and $u \in \{0,1\}$, $v, w \in [0,1]$, $r \in \{0,1\}$).

q.e.d.

If a face shared by two cells contains two contour points on two edges of that face, only one possibility exists to connect them by a line segment. If there are four contour points (one on each edge of a face), an ambiguity arises for connecting pairs of points on that face to construct two line segments. It is this case that leads to discontinuities in the contour triangulation obtained from Lorensen's technique. The trilinear cell interpolant solves this problem. Denoting the four corner data on a cell face by $(\mathbf{x}_{i,j}{}^T, f_{i,j})$, $i, j \in \{0, 1\}$, one is concerned with the ambiguous case if

$$f_{0,0}, f_{1,1} > (<)\ \alpha \quad \text{and} \quad f_{1,0}, f_{0,1} < (>)\ \alpha. \tag{3.5.}$$

The contour points on the edges are again obtained from linear interpolation along the edges, consistent connections between them are assured by considering the contour

$$f(u,v) \;=\; \sum_{j=0}^{1}\sum_{i=0}^{1} f_{i,j}\ B_i^1(u)B_j^1(v) \;=\; \alpha, \tag{3.6.}$$

$u, v \in [0,1]$, over the whole face. Equation (3.6.) is equivalent to the equation

$$f(u,v) \;=\; \sum_{j=0}^{1}\sum_{i=0}^{1} \triangle^{i,j} f_{0,0}\ u^i v^j \;=\; \alpha, \tag{3.7.}$$

where

$$\triangle^{1,0} f_{0,0} = f_{1,0} - f_{0,0}, \quad \triangle^{0,1} f_{0,0} = f_{0,1} - f_{0,0} \quad \text{and}$$
$$\triangle^{1,1} f_{0,0} = \triangle^{1,0}(f_{0,1} - f_{0,0}) = (f_{1,1} - f_{1,0}) - (f_{0,1} - f_{0,0})$$

are the forward differences for two indices.

Theorem 3.3. *The contour defined by equation* (3.7.) *is a hyperbola with asymptotes given by*

$$u = u_0 = -\frac{\triangle^{0,1} f_{0,0}}{\triangle^{1,1} f_{0,0}} \quad \textit{and} \quad v = v_0 = -\frac{\triangle^{1,0} f_{0,0}}{\triangle^{1,1} f_{0,0}}, \quad u_0, v_0 \in [0,1]. \tag{3.8.}$$

Proof. Let $\triangle^{i,j}$ be the abbreviation for $\triangle^{i,j} f_{0,0}$ and equation (3.5.) be satisfied (ambiguous case). The asymptotic behavior for $f(u, v) = \alpha$ is proven quite easily:

$$\lim_{v\to\infty} u(v) = \lim_{v\to\infty} \frac{\alpha - \triangle^{0,0} - \triangle^{0,1} v}{\triangle^{1,0} + \triangle^{1,1} v} = -\frac{\triangle^{0,1}}{\triangle^{1,1}},$$

$$\lim_{u\to\infty} v(u) = \lim_{u\to\infty} \frac{\alpha - \triangle^{0,0} - \triangle^{1,0} u}{\triangle^{0,1} + \triangle^{1,1} u} = -\frac{\triangle^{1,0}}{\triangle^{1,1}}.$$

By performing an appropriate coordinate transformation it can be shown that $f(u, v) = \alpha$ is a hyperbola. A new coordinate system $\overline{S}$ is defined by its origin (u_0, v_0) and $\frac{\sqrt{2}}{2}(1, -1)$ and $\frac{\sqrt{2}}{2}(1, 1)$ as its two orthogonal unit vectors determining a right-handed system. A point (u, v) is linearly mapped by the composition of a translation by $-(u_0, v_0)$ followed by a rotation by $-\frac{\pi}{4}$ onto the point $(\overline{u}, \overline{v})$,

$$\overline{u} = \tfrac{\sqrt{2}}{2} \; \big(\; (u - u_0) + (v - v_0) \; \big),$$

$$\overline{v} = \tfrac{\sqrt{2}}{2} \; \big(\; -(u - u_0) + (v - v_0) \; \big).$$

The inverse map is given by

$$u = \tfrac{\sqrt{2}}{2} \; (\; \overline{u} - \overline{v} \;) \; + \; u_0,$$

$$v = \tfrac{\sqrt{2}}{2} \; (\; \overline{u} + \overline{v} \;) \; + \; v_0.$$

Expressing the function f in terms of $\overline{u}$ and $\overline{v}$ and inserting it into equation (3.7.) yields the equation of a hyperbola in standard position:

$$\overline{u}^2 - \overline{v}^2 \quad = \quad \tfrac{2}{(\triangle^{1,1})^2} \; \big(\; \triangle^{1,1}(\alpha - \triangle^{0,0}) + \triangle^{1,0}\triangle^{0,1} \; \big) \quad = \quad (-) \; a^2,$$

which is equivalent to

$$\frac{\overline{u}^2}{a^2} - \frac{\overline{v}^2}{a^2} \quad = \quad 1 \quad \left(\frac{\overline{v}^2}{a^2} - \frac{\overline{u}^2}{a^2} \quad = \quad 1 \right), \qquad a \neq 0. \tag{3.9}$$

q.e.d.

It is now obvious how to derive a criterion for a proper connection of pairs of contour points on a cell face in the ambiguous case. The asymptotes $u = u_0$ and $v = v_0$ define four quadrants in the $uv-$domain square $[0,1]^2$, namely

$$[0, u_0] \times [0, v_0], \quad [u_0, 1] \times [0, v_0],$$
$$[0, u_0] \times [v_0, 1], \quad \text{and} \quad [u_0, 1] \times [v_0, 1].$$

Two contour points are connected to form a line segment if they lie in the same quadrant. The problem for the special case that the contour $f(u, v) = \alpha$ coincides with the two straight lines $u = u_0$ and $v = v_0$ (which is the case when equation (3.9.) collapses to $\overline{u}^2 = \overline{v}^2$) still remains. The ambiguity can be solved in two different ways. Either, one decides to connect pairs of contour points on opposite edges on the face (which is in accordance with the fact that the contour actually consists of two straight lines intersecting somewhere in the face's interior), or, one chooses an adhoc solution: connect pairs of contour points such that the quadrants in which the constructed line segments are lying in satisfy the condition to contain a corner (i, j), $i, j \in \{0, 1\}$, for which $f(i, j) > \alpha$. Connecting pairs of points on opposite edges might lead to problems in the triangulation process of the constructed contour polygons later on, thus making the adhoc solution preferable.

In Figure 3.3., the ambiguous case is shown. The trilinear cell interpolant is restricted to a single cell face whose edges all yield a point on the contour $f(u, v) = \alpha$ (corner ordinates drawn as black dots representing function values greater than the contour level α). Contour points are drawn as circles, their connection is based on the asymptotes $u = u_0$ and $v = v_0$ of $f(u, v) = \alpha$.

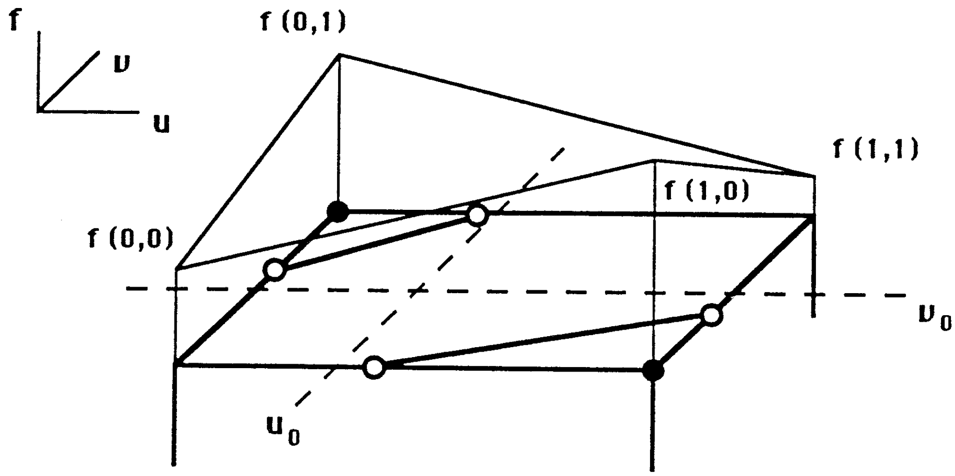

Fig. 3.3. Trilinear cell interpolant restricted to a cell face, solution for the ambiguous case.

Connecting all contour points found along the edges of a cell obviously yields a set of usually non-planar, closed polygons consisting of three (minimal number) to twelve (maximal number) of vertices. A polygon of length twelve can only be created if there are four contour points on each cell face, and all line segments belong to the same polygon. These polygons are interpreted as polygonal boundaries of a piecewise planar (triangular) approximation of a contour of a trivariate function with respect to a particular cell. Therefore, points of each polygon must be connected in order to constitute a contour triangulation inside a cell. Consistency constraints with respect to cells sharing faces require that the following condition is always satisfied:

Condition 3.1. *The only edges on cell faces in the contour triangulation are the line segments constituting the closed polygons constructed over the cells' faces. No other edges connecting contour points on cell faces are allowed.*

This rule guarantees that triangles completely lying on a cell face are never constructed. Only in the case that a cell face contains four contour points belonging to the same polygon one must assure that the above condition is not violated.

Theorem 3.4. (i) *If a closed contour polygon P consisting of the line segments* $\overline{\mathbf{y}_i\mathbf{y}_{i+1}}$, $i = 0...(n-1)$, *indices mod n, has at most one line segment on each cell face, every triangulation of P satisfies condition* 3.1.

(ii) *If a closed contour polygon has two line segments on the same face of a cell, condition* 3.1. *is violated by at least one triangulation of P.*

Proof. (i) All edges besides the line segments constituting P additionally needed for any of P's triangulations necessarily pass through the cells' interior.

(ii) If $\overline{\mathbf{y}_k\mathbf{y}_{k+1}}$ and $\overline{\mathbf{y}_l\mathbf{y}_{l+1}}$ are two line segments on the same face constituting P, there is at least one triangulation of P with the edge $\overline{\mathbf{y}_k\mathbf{y}_l}$

q.e.d.

Cells containing polygons whose triangulation might lead to a violation of condition 3.1. are illustrated in Figure 3.4. Polygons of length six, eight, nine, and twelve are shown. Black dots represent function values greater than α, circles are the polygons' vertices.

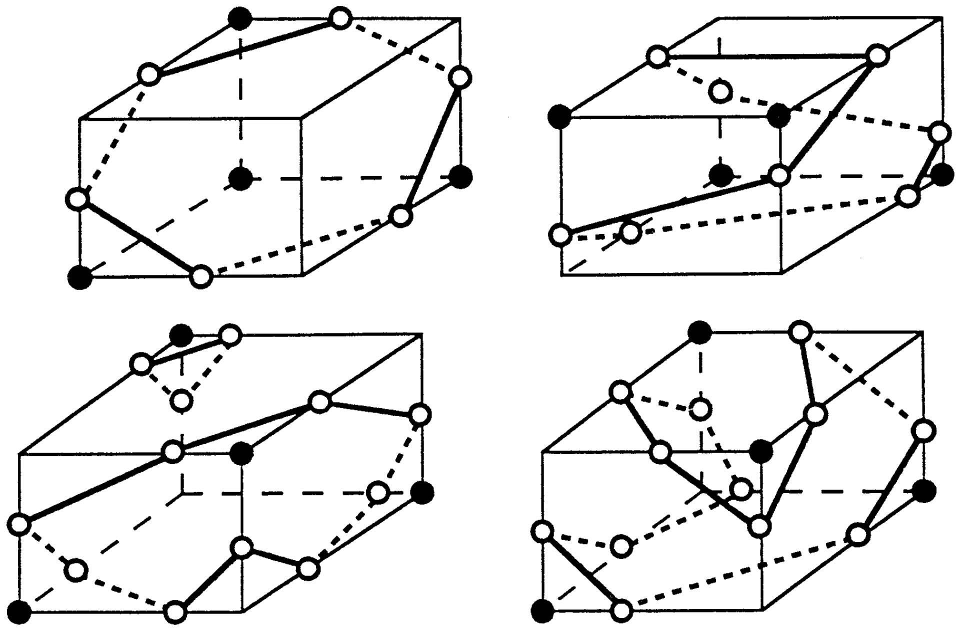

Fig. 3.4. Cells containing contour polygons
of length six, eight, nine, and twelve.

Theorem 3.5. *Let P be a closed contour polygon with line segments $\overline{\mathbf{y}_i\mathbf{y}_{i+1}}$, $i = 0...(n-1)$, with four contour points on at least one cell face F. Let $\mathbf{y}_n$ be a point not in the same plane as F. Then the point set $\{\mathbf{y}_0, ..., \mathbf{y}_n\}$ can be triangulated using only P's line segments without any other edges on F than two of P's line segments.*

Proof. The triangulation $\mathcal{T} = \left\{ \ (i, i+1, n) \mid i = 0...(n-1), \text{ indices } \bmod \ n \ \right\}$ is a triangulation not violating condition 3.1.

q.e.d.

An appropriate choice for $\mathbf{y}_n$ must be made in the case that a contour polygon has four points on the same cell face. The obvious way to choose $\mathbf{y}_n$ is to calculate a point on the contour $f(\mathbf{u}) = \alpha$.

Theorem 3.6. *Let P be a contour polygon in a cell $C_{\mathbf{i}}$ with four points on the cell face F_L (without loss of generality) given by*

$$F_L \;=\; [y_j, y_{j+1}] \times [z_k, z_{k+1}], \quad x = x_i.$$

Let P consist of the line segments $\overline{\mathbf{y}_i\mathbf{y}_{i+1}}$, $i = 0...(n-1)$, indices mod n, and $[0,1]^3$ be the associated domain in uvw-space and

$$\{\ (u = 0, v = v_0, w) \mid v_0 \in (0,1),\ w \in I\!R\ \} \qquad \textit{and}$$

$$\{\ (u = 0, v, w = w_0) \mid w_0 \in (0,1),\ v \in I\!R\ \}$$

be the two asymptotes for the hyperbola $f(\mathbf{u}) = \alpha$ (equation (3.8.) on F_L's corresponding face in uvw-space. Then, the point

$$\mathbf{y}_n\big(\mathbf{u}(t_0)\big) \;=\; \mathbf{y}_n\big((0, v_0, w_0) + t_0(1,0,0)\big), \tag{3.10.}$$

where

$$t_0 = \frac{\alpha - \sum_{k=0}^{1}\sum_{j=0}^{1}\ \triangle^{0,j,k} f_{0,0,0}\ v_0^j w_0^k}{\sum_{k=0}^{1}\sum_{j=0}^{1}\ \triangle^{1,j,k} f_{0,0,0}\ v_0^j w_0^k,} \tag{3.11.}$$

is a point on the contour $f(\mathbf{u}) = \alpha$.

Proof. Calculating the intersection of the line

$$\mathbf{u}(t) \;=\; (0, v_0, w_0) + t(1,0,0)$$

$t \in I\!R$, in $uvw-$space and the contour $f(\mathbf{u}) = \alpha$ of the trilinear cell interpolant

$$f(\mathbf{u}) \;=\; \sum_{k=0}^{1}\sum_{j=0}^{1}\sum_{i=0}^{1}\ \triangle^{i,j,k} f_{0,0,0}\ u^i v^j w^k \;=\; \alpha$$

and abbreviating the forward differences for three indices as $\triangle^{i,j,k} \;=\; \triangle^{i,j,k} f_{0,0,0}$ yields

$$t_0 = \frac{\alpha - (\triangle^{0,0,0} + \triangle^{0,1,0} v_0 + \triangle^{0,0,1} w_0 + \triangle^{0,1,1} v_0 w_0)}{\triangle^{1,0,0} + \triangle^{1,1,0} v_0 + \triangle^{1,0,1} w_0 + \triangle^{1,1,1} v_0 w_0}$$

$$= \frac{\alpha - \sum_{k=0}^{1} \sum_{j=0}^{1} \ \triangle^{0,j,k} f_{0,0,0} \ v_0^j w_0^k}{\sum_{k=0}^{1} \sum_{j=0}^{1} \ \triangle^{1,j,k} f_{0,0,0} \ v_0^j w_0^k}$$

determining a point in $xyz-$space serving as the additional point $\mathbf{y}_n$.

q.e.d.

Remark 3.9. The denominator in equation (3.11.) must not vanish. If it does vanish, the centroid of all contour points $\mathbf{y}_i$, $i = 0...(n-1)$,

$$\mathbf{y}_n = \frac{1}{n} \sum_{i=0}^{n-1} \mathbf{y}_i,$$

is chosen. This choice guarantees that $\mathbf{y}_n$ always is a point in the cell's interior.

Remark 3.10. The additional contour point $\mathbf{y}_n$ does not necessarily lie in a cell's interior (using the method from Theorem 3.6.). This might eventually lead to a contour triangulation violating (iii) in Definition 3.8. (the intersection of the interior of two triangles must be empty).

Figure 3.5. shows the exact and the piecewise linearly approximated contour $f(\mathbf{x}) = 1.5$ using the trilinear approach described above including the construction of an additional contour point $\mathbf{y}_n$ in a single domain cell's interior for the trilinear function

$$f\ (\mathbf{x}) \ = \ 2\ (1-x)(1-y)(1-z) + 1.6\ x(1-y)(1-z) + 1.4\ (1-x)y(1-z)$$

$$+1.4\ (1-x)(1-y)z + .4\ x(1-y)z + 2\ (1-x)yz + 2\ xyz,$$

where the cell is given by $[0,1] \times [0,1] \times [0,1]$.

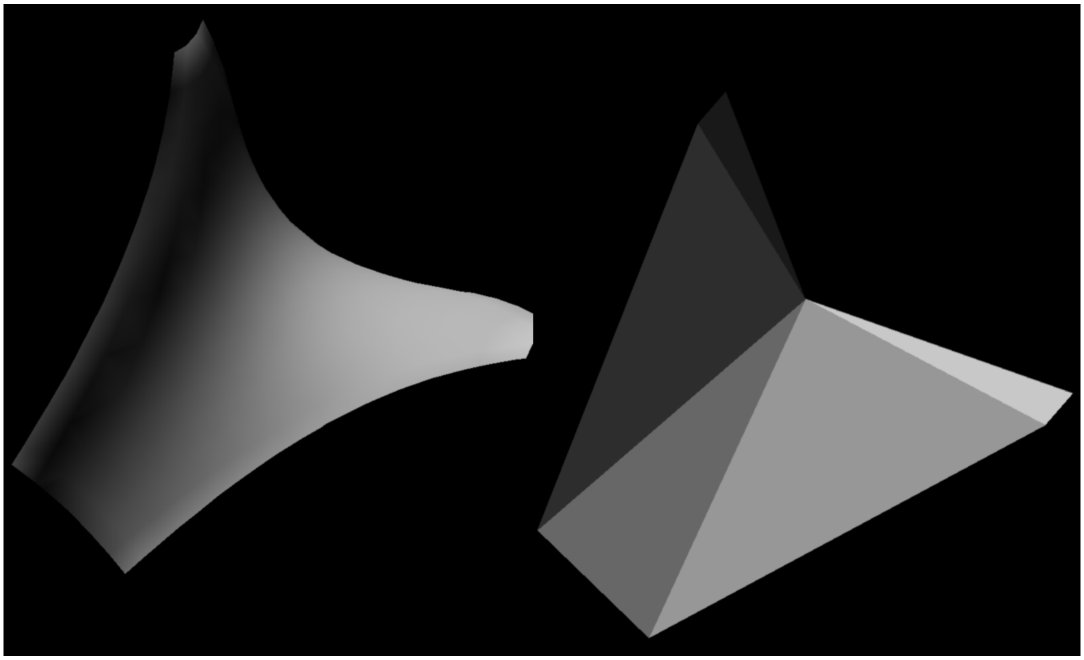

Fig. 3.5. Exact and piecewise linearly approximated contour in a cell,
$$f(x,y,z) \;=\; 2(1-x)(1-y)(1-z) + 1.6x(1-y)(1-z) + 1.4(1-x)y(1-z)$$
$$+1.4(1-x)(1-y)z + .4x(1-y)z + 2(1-x)yz + 2xyz \;=\; 1.5,\;\; x,y,z \in [0,1].$$

Remark 3.11. The piecewise planar contour approximation is trilinearly precise with respect to a single cell in the sense that all the contour points used for the approximation are points of a contour of the trilinear cell interpolant. By construction it is a continuous two-dimensional contour triangulation in the sense of the Definitions (3.8.) and (3.11.).

Remark 3.12. The problem of consistently connecting contour points on cells' faces does not arise when using convex polyhedra having triangular faces only. Therefore, it might be worth considering a decomposition of a subset of $I\!R^3$ into a set of octahedra as well. In this case, contour polygons would have maximally one line segment on a face of an octahedron (using a linear interpolation approach).