

Chapter 3

Grid Quality Measures

3.1 Introduction

It is very important to develop grid generation techniques which sense grid quality features and possess means to eliminate the deficiencies of the grids. These requirements give rise to the problem of selecting and adequately formulating the necessary grid quality measures and finding out how they affect the solution error and the solution efficiency, in order to control the performance of the numerical analysis of physical problems with grids. Commonly, these quality measures encompass grid skewness, stretching, torsion, cell aspect ratio, cell volume, departure from conformality, cell deformation and various related constructions (centroids, circumcenters, circumcircles, incircles, etc.).

In this chapter, we utilize the notions and relations discussed in Sects. 2.2 and 2.3 to describe some qualitative and quantitative characteristics of structured grids. The structured grid concept allows one to define the grid characteristics through coordinate transformations as features of the coordinate curves, coordinate surfaces, coordinate volumes, etc. In general, these features are determined through the elements of the metric tensors and their derivatives. In particular, some grid properties can be described in terms of the invariants of the covariant metric tensor.

The chapter starts with an introduction to the elementary theory of curves and surfaces, necessary for the description of the quality measures of the coordinate curves and coordinate surfaces. It also includes a discussion of the metric invariants. Various grid characteristics are then formulated through quantities which measure the features of the coordinate curves, surfaces, and transformations.

3.2 Curve Geometry

Commonly, the curves lying in the n -dimensional space R^n are represented by smooth nondegenerate parametrizations

$$\mathbf{x}(\varphi) : [a, b] \rightarrow R^n, \quad \mathbf{x}(\varphi) = [x^1(\varphi), \dots, x^n(\varphi)]. \quad (3.1)$$

In our considerations, we will use the designation S^{x^1} for the curve with the parametrization $\mathbf{x}(\varphi)$. In this chapter, we discuss the important measures of the local curve quality known as curvature and torsion. These measures are derived by some manipulations of basic curve vectors using the operations of dot and cross products.

3.2.1 Basic Curve Vectors

Tangent Vector

The first derivative of the parametrization $\mathbf{x}(\varphi)$ in (3.1) is a tangential vector

$$\mathbf{x}_\varphi = (x_\varphi^1, \dots, x_\varphi^n)$$

to the curve S^{x^1} . The quantity

$$g^{x\varphi} = \mathbf{x}_\varphi \cdot \mathbf{x}_\varphi = x_\varphi^i x_\varphi^i, \quad i = 1, \dots, n,$$

is the metric tensor of the curve and its square root is the length of the tangent vector \mathbf{x}_φ . Thus, the length l of the curve S^{x^1} is computed from the integral

$$l = \int_a^b \sqrt{g^{x\varphi}} d\varphi.$$

The most important notions related to curves are connected with the arc length parameter s defined by the equation

$$s(\varphi) = \int_0^\varphi \sqrt{g^{x\varphi}} d\varphi. \quad (3.2)$$

The vector $d\mathbf{x}[\varphi(s)]/ds$, where $\varphi(s)$ is the inverse of $s(\varphi)$, is a tangent vector designated by \mathbf{t} . From (3.2), we obtain

$$\mathbf{t} = \frac{d}{ds} \mathbf{x}[\varphi(s)] = \frac{d\varphi}{ds} \mathbf{x}_\varphi = \frac{1}{\sqrt{g^{x\varphi}}} \mathbf{x}_\varphi.$$

Therefore, \mathbf{t} is the unit tangent vector and, after differentiating the relation $\mathbf{t} \cdot \mathbf{t} = 1$, we find that the derivative \mathbf{t}_s is orthogonal to \mathbf{t} . The vector \mathbf{t}_s is called the curvature vector and denoted by \mathbf{k} . Let \mathbf{n} be a unit vector that is parallel to \mathbf{t}_s ; there then exists a scalar k , such that

$$\mathbf{t}_s = \mathbf{k} = k\mathbf{n}, \quad k = (\mathbf{t}_s \cdot \mathbf{t}_s)^{1/2} = \alpha|\mathbf{k}|, \tag{3.3}$$

where $\alpha = 1$ or $\alpha = -1$.

The magnitude k is called the curvature, while the quantity $\rho = 1/k$ is called the radius of curvature of the curve.

Using the identity $\mathbf{x}_{\varphi\varphi} = \sqrt{g^{x\varphi}}\mathbf{t}$, we obtain, from (3.3),

$$\mathbf{x}_{\varphi\varphi} = \frac{1}{\sqrt{g^{x\varphi}}}(\mathbf{x}_{\varphi\varphi} \cdot \mathbf{x}_{\varphi})\mathbf{t} + g^{x\varphi}k\mathbf{n}. \tag{3.4}$$

The identity (3.4) is an analog of the Gauss relations (2.36). This identity shows that the vector $\mathbf{x}_{\varphi\varphi}$ lies in the \mathbf{t} - \mathbf{n} plane.

Curves in Three-Dimensional Space

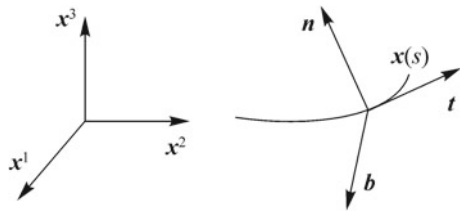
In three dimensions, we can apply the operation of the cross product to the basic tangential and normal vectors. The vector $\mathbf{b} = \mathbf{t} \times \mathbf{n}$ is a unit vector which is orthogonal to both \mathbf{t} and \mathbf{n} . It is called the binormal vector. From (3.4), we find that \mathbf{b} is orthogonal to $\mathbf{x}_{\varphi\varphi}$.

The three vectors (\mathbf{t} , \mathbf{n} , \mathbf{b}) form a right-handed triad (Fig. 3.1). Note that if the curve lies in a plane, then the vectors \mathbf{t} and \mathbf{n} lie in the plane as well and \mathbf{b} is a constant unit vector normal to the plane.

The vectors \mathbf{t} , \mathbf{n} , and \mathbf{b} are connected by the Serret–Frenet equations

$$\begin{aligned} \frac{d\mathbf{t}}{ds} &= k\mathbf{n}, \\ \frac{d\mathbf{n}}{ds} &= -k\mathbf{t} + \tau\mathbf{b}, \\ \frac{d\mathbf{b}}{ds} &= -\tau\mathbf{n}, \end{aligned} \tag{3.5}$$

Fig. 3.1 Base curve vectors



where the coefficient τ is called the torsion of the curve. The first equation of the system (3.5) is taken from (3.3). The second and third equations are readily obtained from the formula (2.6) by replacing the \mathbf{b} in (2.6) with the vectors on the left-hand side of (3.5), while the vectors \mathbf{t} , \mathbf{n} , and \mathbf{b} substitute for \mathbf{e}_1 , \mathbf{e}_2 , and \mathbf{e}_3 , respectively. The vectors \mathbf{t} , \mathbf{n} , and \mathbf{b} constitute an orthonormal basis, i.e.

$$a_{ij} = a^{ij} = \delta_j^i, \quad i, j = 1, 2, 3,$$

where, in accordance with Sect. 2.2.4, $a_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j$, and the tensor $\{a^{ij}\}$ is the inverse of the tensor $\{a_{ij}\}$. Now, using (2.6), we obtain

$$\frac{d\mathbf{n}}{ds} = \left(\frac{d\mathbf{n}}{ds} \cdot \mathbf{t} \right) \mathbf{t} + \left(\frac{d\mathbf{n}}{ds} \cdot \mathbf{n} \right) \mathbf{n} + \left(\frac{d\mathbf{n}}{ds} \cdot \mathbf{b} \right) \mathbf{b} = -k\mathbf{t} + \left(\frac{d\mathbf{n}}{ds} \cdot \mathbf{b} \right) \mathbf{b},$$

since $\mathbf{n}_s \cdot \mathbf{t} = -\mathbf{n} \cdot \mathbf{t}_s$, $\mathbf{n}_s \cdot \mathbf{n} = 0$. Thus, we obtain the second equation of (3.5) with $\tau = \mathbf{n}_s \cdot \mathbf{b}$. Analogously, we obtain the last equation of (3.5) by expanding the vector \mathbf{b}_s through \mathbf{t} , \mathbf{n} , and \mathbf{b} using the relation (2.6):

$$\frac{d\mathbf{b}}{ds} = \left(\frac{d\mathbf{b}}{ds} \cdot \mathbf{t} \right) \mathbf{t} + \left(\frac{d\mathbf{b}}{ds} \cdot \mathbf{n} \right) \mathbf{n} + \left(\frac{d\mathbf{b}}{ds} \cdot \mathbf{b} \right) \mathbf{b} = - \left(\frac{d\mathbf{n}}{ds} \cdot \mathbf{b} \right) \mathbf{n} = -\tau \mathbf{n},$$

as $\mathbf{b}_s \cdot \mathbf{t} = -\mathbf{b} \cdot \mathbf{t}_s = 0$, $\mathbf{b}_s \cdot \mathbf{b} = 0$.

3.2.2 Curvature

A very important characteristic of a curve which is related to grid generation is the curvature k . This quantity is used as a measure of coordinate line bending.

One way to compute the curvature is to multiply (3.3) by \mathbf{n} using the dot product operation. As

$$\frac{d\mathbf{t}}{ds} = \frac{1}{\sqrt{g^{x\varphi}}} \frac{d}{d\varphi} \left(\frac{1}{\sqrt{g^{x\varphi}}} \mathbf{x}_\varphi \right) = \frac{1}{g^{x\varphi}} \mathbf{x}_{\varphi\varphi} - \frac{1}{(g^{x\varphi})^2} (\mathbf{x}_\varphi \cdot \mathbf{x}_{\varphi\varphi}) \mathbf{x}_\varphi,$$

from (3.2), (3.3), the result is

$$k = \frac{1}{g^{x\varphi}} \mathbf{x}_{\varphi\varphi} \cdot \mathbf{n}. \quad (3.6)$$

The vector \mathbf{n} is independent of the curve parametrization, and therefore we find from (3.4), (3.6) that k is an invariant of parametrizations of the curve.

In two dimensions,

$$\mathbf{n} = \frac{1}{\sqrt{g^{x\varphi}}} (-x_\varphi^2, x_\varphi^1),$$

therefore, in this case, we obtain, from (3.6),

$$k^2 = \frac{(x_\varphi y_{\varphi\varphi} - y_\varphi x_{\varphi\varphi})^2}{[(x_\varphi)^2 + (y_\varphi)^2]^3} \quad (3.7)$$

with the convention $x = x^1$, $y = x^2$. In particular, when the curve in R^2 is defined by a function $u = u(x)$, we obtain from (3.7), assuming in (3.1) $\mathbf{x}(\varphi) = [\varphi, u(\varphi)]$, $\varphi = x$,

$$k^2 = (u_{xx})^2 / [1 + (u_x)^2]^3 .$$

In the case of three-dimensional space, the curvature k can also be computed from the relation obtained by multiplying (3.4) by \mathbf{x}_φ with the cross product operation:

$$\mathbf{x}_\varphi \times \mathbf{x}_{\varphi\varphi} = g^{x\varphi} k (\mathbf{x}_\varphi \times \mathbf{n}) = (g^{x\varphi})^{3/2} k \mathbf{b} .$$

Thus, we obtain

$$k^2 = \frac{|\mathbf{x}_\varphi \times \mathbf{x}_{\varphi\varphi}|^2}{(g^{x\varphi})^3} \quad (3.8)$$

and consequently, from (2.26),

$$k^2 = \frac{(x_\varphi^1 x_{\varphi\varphi}^2 - x_\varphi^2 x_{\varphi\varphi}^1)^2 + (x_\varphi^2 x_{\varphi\varphi}^3 - x_\varphi^3 x_{\varphi\varphi}^2)^2 + (x_\varphi^3 x_{\varphi\varphi}^1 - x_\varphi^1 x_{\varphi\varphi}^3)^2}{[(x_\varphi^1)^2 + (x_\varphi^2)^2 + (x_\varphi^3)^2]^3} .$$

3.2.3 Torsion

Another important quality measure of curves in three-dimensional space is the torsion τ . This quantity is suitable for measuring the rate of twisting of the lines of coordinate grids.

In order to figure out the value of τ for a curve in R^3 , represented by (3.1) for $n = 3$, we use the last relation in (3.5), which yields

$$\tau = -\frac{d\mathbf{b}}{ds} \cdot \mathbf{n} .$$

As $\mathbf{b} = \mathbf{t} \times \mathbf{n}$, we obtain

$$\frac{d\mathbf{b}}{ds} = \frac{d\mathbf{t}}{ds} \times \mathbf{n} + \mathbf{t} \times \frac{d\mathbf{n}}{ds} = \mathbf{t} \times \frac{d\mathbf{n}}{ds} ,$$

since $dt/ds = kn$. Thus,

$$\tau = \left(-\mathbf{t} \times \frac{d\mathbf{n}}{ds} \right) \cdot \mathbf{n} . \quad (3.9)$$

From (3.2), (3.3), we have the following obvious relations for the basic vectors \mathbf{t} and \mathbf{n} in terms of the parametrization $\mathbf{x}(\varphi)$ and its derivatives:

$$\begin{aligned} \mathbf{t} &= \frac{1}{\sqrt{g^{x\varphi}}} \mathbf{x}_{\varphi} , \\ \mathbf{n} &= \frac{1}{k} \frac{d\mathbf{t}}{ds} = \frac{1}{k} \left(\frac{1}{g^{x\varphi}} \mathbf{x}_{\varphi\varphi} - \frac{\mathbf{x}_{\varphi} \cdot \mathbf{x}_{\varphi\varphi}}{(g^{x\varphi})^2} \mathbf{x}_{\varphi} \right) , \\ \frac{d\mathbf{n}}{ds} &= \frac{1}{k} \left(\frac{1}{(g^{x\varphi})^{3/2}} \mathbf{x}_{\varphi\varphi\varphi} - 2 \frac{\mathbf{x}_{\varphi} \cdot \mathbf{x}_{\varphi\varphi}}{(g^{x\varphi})^2} \mathbf{x}_{\varphi\varphi} \right. \\ &\quad \left. - \frac{d}{d\varphi} \left(\frac{\mathbf{x}_{\varphi} \cdot \mathbf{x}_{\varphi\varphi}}{(g^{x\varphi})^2} \right) \mathbf{x}_{\varphi} - \frac{1}{k} \frac{dk}{ds} \mathbf{n} \right) . \end{aligned} \quad (3.10)$$

Thus,

$$\mathbf{t} \times \frac{d\mathbf{n}}{ds} = \frac{1}{k(g^{x\varphi})^2} \mathbf{x}_{\varphi} \times \mathbf{x}_{\varphi\varphi\varphi} - 2 \frac{\mathbf{x}_{\varphi} \cdot \mathbf{x}_{\varphi\varphi}}{k(g^{x\varphi})^{5/2}} \mathbf{x}_{\varphi} \times \mathbf{x}_{\varphi\varphi} - \frac{1}{k^2 \sqrt{g^{x\varphi}}} \frac{dk}{ds} \mathbf{x}_{\varphi} \times \mathbf{n} .$$

As $(\mathbf{a} \times \mathbf{b}) \cdot \mathbf{a} = (\mathbf{a} \times \mathbf{b}) \cdot \mathbf{b} = 0$ for arbitrary vectors \mathbf{a} and \mathbf{b} , we obtain, from (3.9, 3.10),

$$\tau = -\frac{1}{k^2 (g^{x\varphi})^3} (\mathbf{x}_{\varphi} \times \mathbf{x}_{\varphi\varphi\varphi}) \cdot \mathbf{x}_{\varphi\varphi} = \frac{1}{k^2 (g^{x\varphi})^3} (\mathbf{x}_{\varphi} \times \mathbf{x}_{\varphi\varphi}) \cdot \mathbf{x}_{\varphi\varphi\varphi} . \quad (3.11)$$

And using (2.31), we also obtain

$$\tau = \frac{1}{k^2 (g^{x\varphi})^3} \det \begin{Bmatrix} x_{\varphi}^1 & x_{\varphi}^2 & x_{\varphi}^3 \\ x_{\varphi\varphi}^1 & x_{\varphi\varphi}^2 & x_{\varphi\varphi}^3 \\ x_{\varphi\varphi\varphi}^1 & x_{\varphi\varphi\varphi}^2 & x_{\varphi\varphi\varphi}^3 \end{Bmatrix} .$$

3.3 Surface Geometry

In general, a surface in the three-dimensional space R^3 is assumed to be locally represented by some parametric two-dimensional domain S^2 and a parametrization

$$\mathbf{x}(s) : S^2 \rightarrow R^3 , \quad \mathbf{x}(s) = [x^1(s), x^2(s), x^3(s)] , \quad \mathbf{s} = (s^1, s^2) , \quad (3.12)$$

where $\mathbf{x}(s)$ is a smooth nondegenerate vector function. We use the designation S^{x^2} for the surface with the parametrization $\mathbf{x}(s)$. In analogy with domains, the transformation $\mathbf{x}(s)$ defines the curvilinear coordinate system s^1, s^2 on the surface, as well as the respective base vectors and metric tensors.

For the purpose of adaptive grid generation, the so-called monitor surfaces are very important. These surfaces are defined by the values of some vector-valued function $\mathbf{u}(s)$, referred to as the height function, over the domain S^2 . The natural form (3.12) of the parametrization of the monitor surface formed with a scalar height function $u(\mathbf{x})$ is represented by the formula

$$\mathbf{x}(s) = [s^1, s^2, u(s^1, s^2)]. \quad (3.13)$$

3.3.1 Surface Base Vectors

A surface in R^3 , represented by (3.12), has three base vectors: two tangents (one to each coordinate curve) and a normal. The two tangential vectors to the coordinates s^1 and s^2 represented by $\mathbf{x}(s)$ are, respectively,

$$\mathbf{x}_{s^i} = \frac{\partial \mathbf{x}}{\partial s^i} = \left(\frac{\partial x^1}{\partial s^i}, \frac{\partial x^2}{\partial s^i}, \frac{\partial x^3}{\partial s^i} \right), \quad i = 1, 2.$$

The unit normal vector to the surface S^{x^2} is defined through the cross product of the tangent vectors \mathbf{x}_{s^1} and \mathbf{x}_{s^2} :

$$\mathbf{n} = \frac{1}{|\mathbf{x}_{s^1} \times \mathbf{x}_{s^2}|} (\mathbf{x}_{s^1} \times \mathbf{x}_{s^2}).$$

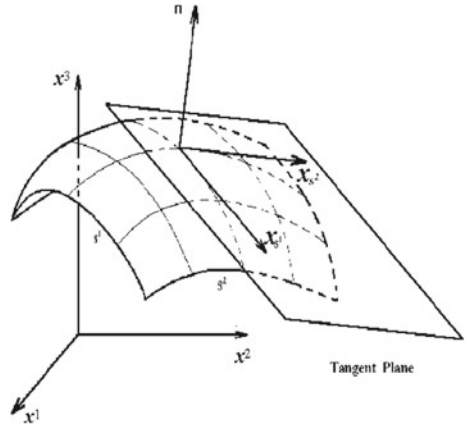
Since $(\mathbf{x}_{s^1} \times \mathbf{x}_{s^2}) \cdot \mathbf{n} > 0$, the base surface vectors \mathbf{x}_{s^1} , \mathbf{x}_{s^2} , and \mathbf{n} comprise a right-handed triad (Fig. 3.2). In accordance with (2.26) and (2.27), the unit normal \mathbf{n} can also be expressed as

$$\mathbf{n} = \frac{1}{\sqrt{g^{rs}}} \left(\frac{\partial x^{l+1}}{\partial s^1} \frac{\partial x^{l+2}}{\partial s^2} - \frac{\partial x^{l+2}}{\partial s^1} \frac{\partial x^{l+1}}{\partial s^2} \right) \mathbf{e}_l, \quad l = 1, 2, 3, \quad (3.14)$$

where $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ is the Cartesian basis of R^3 . Recall that this formula implies the identification convention for indices in three dimensions, where k is equivalent to $k \pm 3$. If the surface S^{x^2} is a monitor surface represented by a height function $u(s)$, then we obtain, from (3.14),

$$\mathbf{n} = \frac{1}{\sqrt{1 + (u_{s^1})^2 + (u_{s^2})^2}} \left(-\frac{\partial u}{\partial s^1}, -\frac{\partial u}{\partial s^2}, 1 \right).$$

Fig. 3.2 Surface base vectors



In another particular case, when the surface points are found from the equation $f(\mathbf{x}) = c$, we obtain $\nabla f \cdot \mathbf{x}_{s^i} = 0$, $i = 1, 2$, and therefore

$$\mathbf{n} = l \nabla f, \quad |l| = 1/|\nabla f|.$$

3.3.2 Metric Tensors

The surface metric tensors, like the domain metric tensors, are defined through the operation of the dot product on the vectors tangential to the coordinate lines.

Covariant Metric Tensor

We designate the covariant metric tensor of the surface S^{x^2} , represented by (3.12) in the coordinates s^1, s^2 as G^{xs} , i.e.

$$G^{xs} = \{g_{ij}^{xs}\}, \quad i, j = 1, 2,$$

where

$$g_{ij}^{xs} = \mathbf{x}_{s^i} \cdot \mathbf{x}_{s^j}, \quad i, j = 1, 2. \tag{3.15}$$

In particular, when a surface is defined by the values of some scalar function $u(\mathbf{s})$ over the domain S^2 then, from (3.13),

$$g_{ij}^{xs} = \delta_i^j + \frac{\partial u}{\partial s^i} \frac{\partial u}{\partial s^j}, \quad i, j = 1, 2.$$

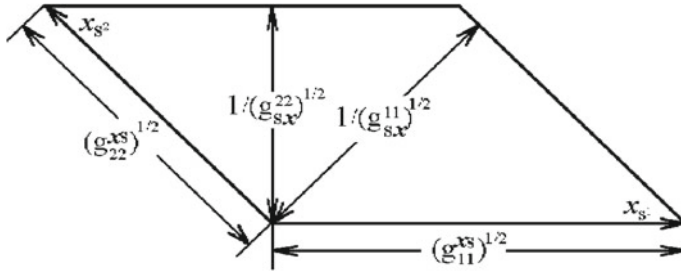


Fig. 3.3 Geometric meaning of the metric elements

The quantity $\sqrt{g_{ii}^{xs}}$ in (3.15) for a fixed i has the geometrical meaning of the length of the tangent vector \mathbf{x}_{s^i} to the coordinate curve s^i (see Fig. 3.3).

The differential quadratic form

$$g_{ij}^{xs} ds^i ds^j, \quad i, j = 1, 2,$$

relating to the line elements in space, is called the first fundamental form of the surface. It represents the value of the square of the length of an elementary displacement $d\mathbf{x}$ on the surface.

Let the Jacobian of G^{xs} be designated by g^{xs} . Since

$$g^{xs} = |\mathbf{x}_{s^1}|^2 |\mathbf{x}_{s^2}|^2 (1 - \cos^2 \theta) = (|\mathbf{x}_{s^1}| \cdot |\mathbf{x}_{s^2}| \sin \theta)^2 = (\mathbf{x}_{s^1} \times \mathbf{x}_{s^2})^2,$$

where θ is the angle between \mathbf{x}_{s^1} and \mathbf{x}_{s^2} , we find that the quantity g^{xs} is the area squared of the parallelogram formed by the vectors \mathbf{x}_{s^1} and \mathbf{x}_{s^2} . Therefore, the area of the surface S^{x2} is computed from the formula

$$S = \int_{S^2} \sqrt{g^{xs}} ds.$$

Contravariant Metric Tensor

Consequently, the contravariant metric tensor of the surface S^{x2} , represented by (3.12), in the coordinates s^1, s^2 is the matrix designated as G_{sx} , and consequently

$$G_{sx} = \{g_{sx}^{ij}\}, \quad i, j = 1, 2.$$

The tensors G^{xs} and G_{sx} are inverse to each other, i.e.

$$g_{ij}^{xs} g_{sx}^{jk} = \delta_k^i, \quad i, j, k = 1, 2.$$

Thus, in analogy with (2.21), we obtain

$$\begin{aligned} g_{sx}^{ij} &= (-1)^{i+j} g_{3-i}^{xs} g_{3-j}^{xs} / g^{xs}, \\ g_{ij}^{xs} &= (-1)^{i+j} g^{xs} g_{sx}^{3-i} g_{sx}^{3-j}, \quad i, j = 1, 2, \end{aligned} \quad (3.16)$$

with fixed indices i and j . The diagonal elements g_{sx}^{11} and g_{sx}^{22} of the contravariant metric tensor G_{sx} are connected with the natural geometric quantities of the parallelogram defined by the tangent vectors \mathbf{x}_{s^1} and \mathbf{x}_{s^2} (see Fig. 3.3). Namely, taking into account the relation $g^{xs} = g_{11}^{xs} / g_{sx}^{22}$, we find that $\sqrt{g_{sx}^{22}}$ is the inverse of the value of the distance between the parallel edges of the parallelogram formed by the vector \mathbf{x}_{s^1} . Analogously, $\sqrt{g_{sx}^{11}}$ is the inverse of the distance between the other pair of parallelogram edges, i.e. those formed by \mathbf{x}_{s^2} .

3.3.3 Second Fundamental Form

The coefficients of the second fundamental form

$$b_{ij} ds^i ds^j, \quad i, j = 1, 2,$$

of the surface S^{x^2} are defined by the dot products of the second derivatives of the vector function $\mathbf{x}(s)$ and the unit normal vector \mathbf{n} to the surface at the point s under consideration:

$$b_{ij} = \mathbf{x}_{s^i s^j} \cdot \mathbf{n}, \quad i, j = 1, 2. \quad (3.17)$$

Thus, from (3.14), (3.17), we obtain for b_{ij} , $i, j = 1, 2$,

$$b_{ij} = \frac{1}{\sqrt{g^{xs}}} \left[\frac{\partial^2 x^l}{\partial s^i \partial s^j} \left(\frac{\partial x^{l+1}}{\partial s^1} \frac{\partial x^{l+2}}{\partial s^2} - \frac{\partial x^{l+2}}{\partial s^1} \frac{\partial x^{l+1}}{\partial s^2} \right) \right], \quad l = 1, 2, 3, \quad (3.18)$$

with the identification convention for the superscripts that k is equivalent to $k \pm 3$. Correspondingly, for the monitor surface with the height function $u(s)$, we obtain

$$b_{ij} = \frac{1}{\sqrt{1 + (u_{s^1})^2 + (u_{s^2})^2}} u_{s^i s^j}, \quad i, j = 1, 2.$$

The tensor $\{b_{ij}\}$ reflects the local warping of the surface, namely its deviation from the tangent plane at the point under consideration. In particular, if $\{b_{ij}\} \equiv 0$ at all points of S^2 , then the surface is a plane.

3.3.4 Surface Curvatures

Principal Curvatures

Let a curve on the surface be defined by the intersection of a plane containing the normal \mathbf{n} with the surface. It is obvious that either \mathbf{n} or $-\mathbf{n}$ is also the curve normal vector. Taking into account (3.6), we obtain for the curvature of this curve

$$k = \frac{b_{ij} ds^i ds^j}{g_{ij}^x ds^i ds^j}, \quad i, j = 1, 2. \quad (3.19)$$

Here, (ds^1, ds^2) is the direction of the curve, i.e. $ds^i = c(ds^i/d\varphi)$, where $s(\varphi)$ is a curve parametrization. The two extreme quantities K_I and K_{II} of the values of k are called the principal curvatures of the surface at the point under consideration. In order to compute the principal curvatures, we consider the following relation for the value of the curvature:

$$(b_{ij} - kg_{ij}^{xs}) ds^i ds^j = 0, \quad i, j = 1, 2, \quad (3.20)$$

which follows from (3.19). In order to find the maximum and minimum values of k , the usual method of equating to zero the derivative with respect to ds^i is applied. Thus, the components of the (ds^1, ds^2) direction giving an extreme value of k are subject to the restriction

$$(b_{ij} - kg_{ij}^{xs}) ds^j = 0, \quad i, j = 1, 2,$$

which, in fact, is the eigenvalue problem for curvature. One finds the eigenvalues k by setting the determinant of this equation equal to zero, obtaining thereby the secular equation for k :

$$\det(b_{ij} - kg_{ij}^{xs}) = 0, \quad i, j = 1, 2.$$

This equation, written out in full, is a quadratic equation

$$k^2 - g_{sx}^{ij} b_{ij} k + [b_{11} b_{22} - (b_{12})^2] / g^{xs} = 0,$$

with two roots, which are the maximum and minimum values K_I and K_{II} of the curvature k :

$$K_{I,II} = \frac{1}{2} g_{sx}^{ij} b_{ij} \pm \sqrt{\frac{1}{4} (g_{sx}^{ij} b_{ij})^2 - \frac{1}{g^{xs}} [b_{11} b_{22} - (b_{12})^2]}. \quad (3.21)$$

Gaussian Curvature

The determinant of the tensor $\{K_j^i\}$ represents the Gaussian curvature of the surface (3.12)

$$K_G = \det\{K_j^i\} = \frac{1}{g^{xs}} [b_{11}b_{22} - (b_{12})^2] . \quad (3.22)$$

Taking into account (3.21), we readily see that the Gaussian curvature is the product of the two principal curvatures K_I and K_{II} , i.e.

$$K_G = K_I K_{II} .$$

In terms of the height function $u(s)$ representing the monitor surface S^{x2} , we have

$$K_G = \frac{u_{s^1s^1}u_{s^2s^2} - (u_{s^1s^2})^2}{[1 + (u_{s^1})^2 + (u_{s^2})^2]^2} .$$

A surface point is called elliptic if $K_G > 0$, i.e. both K_I and K_{II} are both negative or both positive at the point of consideration. A saddle or hyperbolic point has principal curvatures of opposite sign, and therefore has negative Gaussian curvature. A parabolic point has one principal curvature vanishing and, consequently, a vanishing Gaussian curvature. This classification of points is prompted by the form of the curve which is obtained by the intersection of the surface with a slightly offset tangent plane. For an elliptic point, the curve is an ellipse; for a saddle point, it is a hyperbola. It is a pair of lines (degenerate conic) at a parabolic point, and it vanishes at a planar point, where both principal curvatures are zero.

Mean Curvature

One half of the sum of the principal curvatures is referred to as the mean surface curvature. Taking advantage of (3.21), the mean curvature, designated by K_m , is defined through the coefficients of the second fundamental form and elements of the contravariant metric tensor by

$$K_m = \frac{1}{2}(K_I + K_{II}) = \frac{1}{2}g_{sx}^{ij}b_{ij} , \quad i, j = 1, 2 . \quad (3.23)$$

In the case of the monitor surface represented by the function $u(s^1, s^2)$, we obtain

$$K_m = \frac{u_{s^1s^1}[1 + (u_{s^2})^2] + u_{s^2s^2}[1 + (u_{s^1})^2] - 2u_{s^1s^2}u_{s^1s^2}}{2[1 + (u_{s^1})^2 + (u_{s^2})^2]^{3/2}} .$$

Now we consider the tensor

$$\{K_j^i\} \equiv \{g_{sx}^{ik}b_{kj}\} , \quad i, j, k = 1, 2 .$$

As a reminder, the repeated index k means summation over it. It is easy to see that $\{K_j^i\}$ is a mixed tensor contravariant with respect to the upper index and covariant with respect to the lower one. From (3.23), we find that the mean curvature is defined as the trace of the tensor, namely,

$$2K_m = \text{tr}\{K_j^i\}, \quad i, j = 1, 2. \quad (3.24)$$

A surface whose mean curvature is zero, i.e. $K_I = -K_{II}$, possesses the following unique property. Namely, if a surface bounded by a specified contour has a minimum area, then its mean curvature is zero. Conversely, of all the surfaces bounded by a curve whose length is sufficiently small, the minimum area is possessed by the surface whose mean curvature is zero.

It is easily shown that both the mean and the Gaussian curvatures are invariant of surface parametrizations.

3.3.5 Curvatures of Discrete Surfaces

From a computational standpoint, the discrete objects are attractive because they have been designed from the ground up with data-structures and algorithms in mind. From a mathematical standpoint, they present a great challenge: the discrete objects should have properties which are analogues of the properties of continuous objects. One important property of curves and surfaces is their curvature, which plays a significant role in many application areas. In the continuous formulations, there are remarkable theorems dealing with curvatures; a key requirement for a discrete curve or surface with discrete curvatures is that they satisfy analogous theorems.

Relying on the results presented in the paper of Sullivan (see Pinkall and Polhier 1993), we consider here some formulations of the curvatures of discrete surfaces, meaning triangulated polyhedral surfaces. Often, the most useful formulations are those which are based on integral relations for curvature, like the Gauss–Bonnet theorem or the force balance equation for mean curvature.

We assume that all cells meeting at a grid node \mathbf{P} of the discrete surface under consideration are triangles. Such a triangulation at the node \mathbf{P} can be obtained from arbitrary polyhedron triangulations by connecting the nodes adjacent to \mathbf{P} of each of the two neighboring edges emanating from \mathbf{P} .

Gauss Curvature

Gauss curvature K_G at a grid vertex \mathbf{P} must be subject to the following relation

$$\int \int_D K_G dA := \sum_{\mathbf{P} \in D} K_{\mathbf{P}}, \quad \text{with } K_{\mathbf{P}} = 2\pi - \sum_i \theta_i, \quad (3.25)$$

where the angles θ_i are the interior angles at \mathbf{P} of the triangles meeting there, and $K_{\mathbf{P}}$ is often known as the angle defect at \mathbf{P} .

From this relation, one formula for discrete Gauss curvature $K_G^d(\mathbf{P})$ at the node \mathbf{P} may be defined by

$$K_G^d(\mathbf{P}) = \frac{1}{A(\text{star}\mathbf{P})} (2\pi - \sum_i \theta_i), \quad (3.26)$$

where $\text{star}\mathbf{P}$ is a designation for the union of all triangles containing the vertex \mathbf{P} , and $A(\text{star}\mathbf{P})$ is the area of $\text{star}\mathbf{P}$.

One more intrinsic characterization of Gauss curvature K_G is obtained by comparing the circumferences C_ε of (intrinsic) ε -balls around \mathbf{P} to the value $2\pi\varepsilon$. We have

$$\frac{C_\varepsilon}{2\pi\varepsilon} = 1 - \frac{\varepsilon^2}{6} K_G(\mathbf{P}) + O(\varepsilon^3). \quad (3.27)$$

From this formula, discrete Gauss curvature $K_G^d(\mathbf{P})$ at the node \mathbf{P} may be defined by

$$K_G^d(\mathbf{P}) = \frac{6}{\varepsilon^2} \left(1 - \frac{S_\varepsilon}{2\pi\varepsilon} \right), \quad (3.28)$$

where S_ε is the length of the curve obtained by intersecting an ε -ball with $\text{star}\mathbf{P}$, and ε is a small number.

These formulations of the discrete Gauss curvature depend significantly on the choice of which pairs of cone points are connected by triangle edges (see Bobenko and Springorn 2005).

Mean Curvature

Suppose that the vertices adjacent to \mathbf{P} , in cyclic order, are $\mathbf{P}_1, \dots, \mathbf{P}_k$. Then, the discrete vector mean curvature $\mathbf{K}_m^d(\mathbf{P})$ can be expressed explicitly in terms of these neighbors by the following formula:

$$\mathbf{K}_m^d(\mathbf{P}) = \frac{1}{2} \sum_i (\cot \alpha_i + \cot \beta_i) (\mathbf{P} - \mathbf{P}_i), \quad (3.29)$$

where α_i and β_i are the angles opposite the edge $\mathbf{P}\mathbf{P}_i$ in the two incident triangles (see Pinkall and Polhier 1993 and Sullivan 2008).

Alternatively, we have

$$\mathbf{K}_m(\mathbf{P}) = \Delta_B[\mathbf{x}](\mathbf{P}),$$

where \mathbf{x} is the position vector, and Δ_B is the Beltrami operator. Computing the Beltrami operator numerically at each grid point of a discrete surface gives the value of $\mathbf{K}_m^d(\mathbf{P})$.

3.4 Metric-Tensor Invariants

The coordinate transformation $\mathbf{x}(\boldsymbol{\xi}) : \mathcal{E}^n \rightarrow X^n$ of a physical n -dimensional domain X^n applied to generate grids through mapping approaches can be locally interpreted as some deformation of a uniform cell in the computational domain \mathcal{E}^n into the corresponding cell in the domain X^n . The local deformation of any cell is approximated by a linear transformation represented by the Jacobi matrix $\{\partial x^i / \partial \xi^j\}$. This deformation is not changed if any orthogonal transformation is applied to the cell in X^n . The deformation is also preserved if the orientation of the computational domain \mathcal{E}^n is changed. Therefore, it is logical to formulate the features of the coordinate grid cells in terms of the invariants of the orthogonal transformations of the covariant metric tensor $\{g_{ij}\}$, in the coordinates ξ_1, \dots, ξ_n , i.e.

$$g_{ij} = \mathbf{x}_{\xi^i} \cdot \mathbf{x}_{\xi^j}, \quad i, j = 1, \dots, n. \quad (3.30)$$

3.4.1 Algebraic Expressions for the Invariants

According to the theory of matrices, a symmetric nondegenerate $(n \times n)$ matrix $\{a_{ij}\}$ has n independent invariants I_i , $i = 1, \dots, n$, of its orthogonal transformations. The i th invariant I_i is defined by summing all of the principal minors of order i of the matrix. Recall that the principal minors of a square matrix are the determinants of the square submatrices of the matrix. Thus, for example,

$$\begin{aligned} I_1 &= \sum_{i=1}^n a_{ii} = \text{tr}\{a_{ij}\}, \\ I_{n-1} &= \sum_{i=1}^n \text{cofactor } a_{ii} = \det\{a_{ij}\} \sum_{i=1}^n a^{ii} = \det\{a_{ij}\} \text{tr}\{a^{ij}\}, \\ I_n &= \det\{a_{ij}\}, \end{aligned} \quad (3.31)$$

where the matrix $\{a^{ij}\}$ is the inverse of $\{a_{ij}\}$.

When we use, for $\{a_{ij}\}$, the covariant metric tensor $\{g_{ij}\}$, $g_{ij} = \mathbf{x}_{\xi^i} \cdot \mathbf{x}_{\xi^j}$, of a domain X^n , then, taking advantage of (3.31), the invariants I_1 and I_2 in two dimensions are expressed as

$$\begin{aligned} I_1 &= g_{11} + g_{22}, \\ I_2 &= g_{11} g_{22} - (g_{12})^2 = g = J^2, \end{aligned} \quad (3.32)$$

where $J = \det\{\partial x^i / \partial \xi^j\}$. The invariants of the three-dimensional metric tensor $\{g_{ij}\}$ are expressed as follows:

$$\begin{aligned}
I_1 &= g_{11} + g_{22} + g_{33} , \\
I_2 &= g(g^{11} + g^{22} + g^{33}) \\
I_3 &= \det\{g_{ij}\} = g , \quad i, j = 1, 2, 3 ,
\end{aligned} \tag{3.33}$$

where $g^{ij} = \nabla\xi^i \cdot \nabla\xi^j$. Analogously, the invariants of the surface metric tensor G^{xs} , represented in the coordinates s^1, s^2 by (3.12), are written out as

$$\begin{aligned}
I_1 &= g_{11}^{xs} + g_{22}^{xs} \\
I_2 &= g^{xs} .
\end{aligned} \tag{3.34}$$

The notion of an invariant can be helpful to identify conformal coordinate transformations. For example, in two dimensions, we know that a conformal mapping $\mathbf{x}(\xi)$ satisfies the Cauchy–Riemann equations

$$\frac{\partial x^1}{\partial \xi^1} = \frac{\partial x^2}{\partial \xi^2} , \quad \frac{\partial x^1}{\partial \xi^2} = -\frac{\partial x^2}{\partial \xi^1} .$$

Therefore, a zero value of the quantity

$$Q = \left(\frac{\partial x^1}{\partial \xi^1} - \frac{\partial x^2}{\partial \xi^2} \right)^2 + \left(\frac{\partial x^1}{\partial \xi^2} + \frac{\partial x^2}{\partial \xi^1} \right)^2$$

is an indication of the conformality of $\mathbf{x}(\xi)$. We obtain

$$Q = g_{11} + g_{22} - 2J = I_1 - 2\sqrt{I_2} ,$$

using (3.32). Thus, the two-dimensional coordinate transformation $\mathbf{x}(\xi)$ is conformal if only if the invariants I_1 and I_2 satisfy the restriction $I_1/\sqrt{I_2} = 2$. In Sect. 3.7.7, it will be shown that an analogous relation is valid for an arbitrary dimension $n \geq 2$.

We also can see that the mean and Gaussian curvatures described by (3.24) and (3.22), respectively, are defined through the invariants of the tensor $\{K_j^i\}$, namely,

$$K_m = \frac{1}{2}I_1 , \quad K_G = I_2 .$$

3.4.2 Geometric Interpretation

The invariants of the covariant metric tensor $\{g_{ij}\}$ can also be described in terms of some geometric characteristics of the n -dimensional parallelepiped (parallelogram in two dimensions) determined by the tangent vectors \mathbf{x}_{ξ^i} , thus giving a relationship between the cell characteristics of coordinate grids and the invariants. For example, we see from (3.32), (3.34) in two dimensions that the invariant I_1 equals the sum

squares of the parallelogram edge lengths, while I_2 is equal to the parallelogram area squared. In three-dimensional space, we find, from (3.33), that I_1 equals the sum of the squares of the lengths of the base vectors \mathbf{x}_{ξ^i} , $i = 1, 2, 3$, which are the edges of the parallelepiped. The invariant I_2 is the sum of the squares of the areas of the faces of the parallelepiped, while the invariant I_3 is its volume squared.

These geometric interpretations can be extended to arbitrary dimensions by the following consideration. Every principal minor of order m is the determinant of an m -dimensional square matrix A^m obtained from the covariant tensor $\{g_{ij}\}$ by crossing out $n - m$ rows and columns that intersect pairwise on the diagonal. Therefore, the elements of A^m are the dot products of m particular vectors of the base tangential vectors \mathbf{x}_{ξ^i} , $i = 1, \dots, n$. Thus, geometrically, the determinant of A^m equals the square of the m -dimensional volume of the m -dimensional parallelepiped constructed by the vectors of the basic set \mathbf{x}_{ξ^i} , $i = 1, \dots, n$, whose dot products form the matrix A^m . Therefore, I_i , $i = 1, \dots, n$, is geometrically the sum of the squares of the i -dimensional volumes of the i -dimensional sides of the n -dimensional parallelepiped spanned by the base vectors \mathbf{x}_{ξ^i} , $i = 1, \dots, n$.

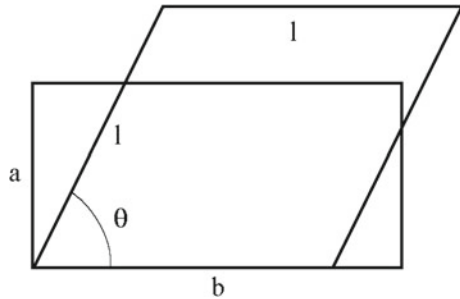
We note that the invariants do not describe all of the geometric features of the grid cells. In the two-dimensional case, the invariants I_1 and I_2 given by (3.32) can be the same for parallelepipeds that are not similar. For example, if we take a transformation $\mathbf{x}(\boldsymbol{\xi})$ whose tangential vectors \mathbf{x}_{ξ^1} and \mathbf{x}_{ξ^2} define a rectangle with sides of different lengths a and b , then we obtain

$$I_1 = a^2 + b^2, \quad I_2 = (ab)^2.$$

However, as demonstrated in Fig. 3.4, the same invariants are produced by a transformation $\mathbf{x}(\boldsymbol{\xi})$, whose tangent vectors yield a rhombus with a side length l equal to $\sqrt{(a^2 + b^2)}/2$ and an angle θ defined by

$$\theta = \arcsin \frac{2ab}{a^2 + b^2},$$

Fig. 3.4 Quadrilaterals with the same invariants



since

$$\begin{aligned} I_1 &= 2l^2 = a^2 + b^2, \\ I_2 &= l^2 \sin^2 \theta = (ab)^2. \end{aligned}$$

Thus, knowledge of the values of the invariants I_1 and I_2 alone is not sufficient to distinguish the rectangle from the rhombus. However, the value of the quantity $I_1/\sqrt{I_2}$ imposes restriction on the maximal angle between the parallelogram edges and on the maximum cell aspect ratio. These bounds will be evaluated in Sect. 3.7.7. In particular, if $I_1 = 2\sqrt{I_2}$, then we can definitely state that the parallelogram is a square.

3.5 Characteristics of Grid Lines

This section describes some characteristics of curvilinear coordinate lines in domains specified by the parametrization $\mathbf{x}(\boldsymbol{\xi}) : \mathcal{E}^n \rightarrow X^n$. These characteristics can be used for the evaluation of the grid properties and for the formulation of grid generation techniques through the calculus of variations.

All considerations in this section are concerned with a selected coordinate line ξ^i for a specified i , and therefore summation is not carried out over the repeated index i here.

3.5.1 Sum of Squares of Cell Edge Lengths

The length l_i of any cell edge along the coordinate curve ξ^i is expressed through the element g_{ii} of the covariant metric tensor $\{g_{ij}\}$:

$$l_i \approx \sqrt{g_{ii}}h.$$

The sum of the squares of the cell edge lengths equals $Q_l h^2$, where

$$Q_l = \sum_{j=1}^n g_{jj} = \text{tr} \{g_{ij}\}. \quad (3.35)$$

The quantity Q_l is one of the important characteristics of the grid cell. This characteristic is the first invariant I_1 of the tensor matrix $\{g_{ij}\}$.

3.5.2 Eccentricity

The ratio between two adjacent grid steps along any coordinate curve ξ^i is a quantity which characterizes the change of the length of the cell edge in the ξ^i direction. This quantity is designated as ϵ^i , and at the point ξ , it is expressed as follows:

$$\epsilon^i \approx \frac{|\mathbf{x}_{\xi^i}(\xi + h\mathbf{e}^i)|}{|\mathbf{x}_{\xi^i}(\xi)|} .$$

We also find that

$$\epsilon^i \approx \frac{\sqrt{g_{ii}(\xi + h\mathbf{e}^i)} - \sqrt{g_{ii}(\xi)}}{\sqrt{g_{ii}(\xi)}} + 1 \approx h \frac{1}{\sqrt{g_{ii}}} \frac{\partial}{\partial \xi^i} \sqrt{g_{ii}} + 1 ,$$

for a fixed i , since $|\mathbf{x}_{\xi^i}| = \sqrt{g_{ii}}$. The quantity

$$Q_\epsilon^i = \left(\frac{1}{\sqrt{g_{ii}}} \frac{\partial}{\partial \xi^i} \sqrt{g_{ii}} \right)^2 = \left(\frac{\partial}{\partial \xi^i} \ln \sqrt{g_{ii}} \right)^2 , \quad i \text{ fixed} \quad (3.36)$$

obtained from the expression for ϵ^i is a measure of the relative eccentricity. When $Q_\epsilon = 0$, then the length of the cell edge does not change in the ξ^i direction. With the Christoffel symbol notation (2.40), we also obtain

$$Q_\epsilon^i = \left(\frac{1}{g_{ii}} \frac{\partial \mathbf{x}}{\partial \xi^i} \cdot \frac{\partial^2 \mathbf{x}}{\partial \xi^i \partial \xi^i} \right)^2 = \left(\frac{1}{g_{ii}} [ii, i] \right)^2 , \quad i \text{ fixed} . \quad (3.37)$$

3.5.3 Curvature

The relative eccentricity Q_ϵ^i describes the change of the length of the cell edge along the coordinate curve ξ^i , however, it fails to describe the change in its direction. The quantity which characterizes this grid quality is derived through a curvature vector.

In accordance with (3.3), the curvature vector \mathbf{k}_i of the coordinate line ξ^i for a fixed i is defined by the relation $\mathbf{k}_i = \mathbf{x}_{ss}$, where s is the arc length parametrization of the coordinate line ξ^i , i.e. the variable s is defined by the transformation $s(\xi^i)$ satisfying the equation

$$\frac{ds}{d\xi^i} = \sqrt{g_{ii}} , \quad i \text{ fixed} .$$

Therefore,

$$\frac{\partial}{\partial s} = \frac{1}{\sqrt{g_{ii}}} \frac{\partial}{\partial \xi^i} , \quad i \text{ fixed}$$

and consequently

$$\mathbf{k}_i = \frac{1}{g_{ii}} \mathbf{x}_{\xi^i \xi^i} - \frac{\mathbf{x}_{\xi^i}}{(g_{ii})^2} \mathbf{x}_{\xi^i} \cdot \mathbf{x}_{\xi^i \xi^i}, \quad i \text{ fixed.} \quad (3.38)$$

Local Straightness of the Coordinate Line

Equation (3.38) shows that if the curvature vector \mathbf{k}_i equals zero ($\mathbf{k}_i = \mathbf{0}$), then the vector $\mathbf{x}_{\xi^i \xi^i}$ is parallel to the vector \mathbf{x}_{ξ^i} , i.e. the tangential vector does not change its direction. Therefore, the coordinate line ξ^i is locally straight at a point of zero curvature. From (3.38), we obtain, in this case,

$$\mathbf{x}_{\xi^i \xi^i} = \frac{(\mathbf{x}_{\xi^i \xi^i} \cdot \mathbf{x}_{\xi^i})}{g_{ii}} \mathbf{x}_{\xi^i}, \quad i \text{ fixed.}$$

Using the Gauss relations (2.36), we also obtain

$$\mathbf{x}_{\xi^i \xi^l} = \Gamma_{ii}^l \mathbf{x}_{\xi^l}, \quad l = 1, \dots, n, \quad i \text{ fixed.}$$

Comparing these two expansions of $\mathbf{x}_{\xi^i \xi^l}$, we see that the vector $\mathbf{x}_{\xi^i \xi^l}$ is parallel to \mathbf{x}_{ξ^l} if

$$\Gamma_{ii}^l = 0 \quad \text{for all } l \neq i, \quad i \text{ fixed.} \quad (3.39)$$

The relation (3.39) is a criterion of local straightness of the coordinate curve ξ^i . A measure of the deviation of the curve ξ^i from a straight line may, therefore, be determined as

$$Q_{st}^i = d_{lm} \Gamma_{ii}^l \Gamma_{ii}^m, \quad l, m \neq i, \quad i \text{ fixed,} \quad (3.40)$$

where d_{lm} is a positive $(n-1) \times (n-1)$ tensor.

Expansion of the Curvature Vector in the Normal Vectors

We know that the curvature vector \mathbf{k}_i is orthogonal to the unit tangential vector \mathbf{x}_s . On the other hand, the normal base vectors $\nabla \xi^j$, $j \neq i$, are also orthogonal to the tangential vector \mathbf{x}_{ξ^i} and therefore to \mathbf{x}_s . Thus, the curvature vector \mathbf{k}_i of the coordinate curve ξ^i can be expanded in the $n-1$ normal vectors $\nabla \xi^j$, $j \neq i$. In order to find such an expansion, we first recall that in accordance with (2.41),

$$\mathbf{x}_{\xi^i \xi^i} = [ii, m] \nabla \xi^m, \quad m = 1, \dots, n, \quad i \text{ fixed}$$

with summation over m , where

$$[ii, m] = \mathbf{x}_{\xi^i \xi^i} \cdot \mathbf{x}_{\xi^m} = \frac{\partial g_{im}}{\partial \xi^i} - \frac{1}{2} \frac{\partial g_{ii}}{\partial \xi^m}, \quad i \text{ fixed,}$$

from (2.45). Furthermore, from (2.23),

$$\mathbf{x}^{\xi^i} = g_{im} \nabla \xi^m, \quad m = 1, \dots, n.$$

Therefore, the relation (3.38) is equivalent to

$$\begin{aligned} \mathbf{k}_i &= \frac{1}{g_{ii}} \left([ii, m] \nabla \xi^m - \frac{1}{g_{ii}} [ii, i] \right) g_{im} \nabla \xi^m \\ &= \frac{1}{(g_{ii})^2} (g_{ii} [ii, l] - g_{il} [ii, i]) \nabla \xi^l, \\ & \quad m = 1, \dots, n, \quad l = 1, \dots, n, \quad l \neq i, \quad i \text{ fixed}. \end{aligned} \quad (3.41)$$

This equation represents the curvature vector \mathbf{k}_i through the $n-1$ normal base vectors $\nabla \xi^l$, $l \neq i$.

In particular, in two dimensions, the relation (3.41) for $i = 1$ becomes

$$\mathbf{k}_1 = \frac{1}{(g_{11})^2} (g_{11} [11, 2] - g_{12} [11, 1]) \nabla \xi^2. \quad (3.42)$$

And, from (2.21),

$$\mathbf{k}_1 = \frac{g}{(g_{11})^2} (g^{22} [11, 2] + g^{21} [11, 1]) \nabla \xi^2.$$

Therefore, using (2.43), we obtain

$$\mathbf{k}_1 = \frac{g}{(g_{11})^2} \Gamma_{11}^2 \nabla \xi^2. \quad (3.43)$$

Analogously, the curvature vector \mathbf{k}_2 along the coordinate ξ^2 is expressed as follows:

$$\mathbf{k}_2 = \frac{g}{(g_{22})^2} \Gamma_{22}^1 \nabla \xi^1. \quad (3.44)$$

In the same way, the curvature vector of the coordinate curves in the case of three-dimensional space R^3 is computed. For example, in accordance with (3.41), the vector \mathbf{k}_1 can be expanded in the normal vectors $\nabla \xi^2$ and $\nabla \xi^3$ as

$$\begin{aligned} \mathbf{k}_1 &= \frac{1}{(g_{11})^2} \{ (g_{11} [11, 2] - g_{12} [11, 1]) \nabla \xi^2 \\ & \quad + (g_{11} [11, 3] - g_{13} [11, 1]) \nabla \xi^3 \}. \end{aligned} \quad (3.45)$$

Measure of Coordinate Line Curvature

The length of the vector k_i is the modulus of the curvature and denoted by $|k_i|$. Thus, for the curvature k_1 of the coordinate line ξ^1 in the two-dimensional domain X^2 , we obtain, from (3.43),

$$|k_1| = \frac{g\sqrt{g^{22}}}{(g_{11})^2} |\Gamma_{11}^2| = \frac{g\sqrt{g^{22}}}{(g_{11})^2} \left| \frac{\partial^2 x^1}{\partial \xi^1 \partial \xi^1} \frac{\partial \xi^2}{\partial x^1} + \frac{\partial^2 x^2}{\partial \xi^1 \partial \xi^1} \frac{\partial \xi^2}{\partial x^2} \right|. \quad (3.46)$$

Taking into account the two-dimensional relation (2.4)

$$\frac{\partial \xi^i}{\partial x^j} = (-1)^{i+j} \frac{1}{J} \frac{\partial x^{3-j}}{\partial \xi^{3-i}}, \quad i, j = 1, 2, \quad J = \sqrt{g},$$

with i, j fixed, we find that

$$\Gamma_{11}^2 = \frac{1}{J} \left(\frac{\partial x^1}{\partial \xi^1} \frac{\partial^2 x^2}{\partial \xi^1 \partial \xi^1} - \frac{\partial x^2}{\partial \xi^1} \frac{\partial^2 x^1}{\partial \xi^1 \partial \xi^1} \right).$$

Therefore, for the curvature of the coordinate ξ^1 , we also obtain, from (2.21) and (3.46),

$$|k_1| = \frac{1}{(g_{11})^{3/2}} \left| \frac{\partial x^1}{\partial \xi^1} \frac{\partial^2 x^2}{\partial \xi^1 \partial \xi^1} - \frac{\partial x^2}{\partial \xi^1} \frac{\partial^2 x^1}{\partial \xi^1 \partial \xi^1} \right|. \quad (3.47)$$

Analogously, using the relation (3.44), we get for the curvature of the coordinate curve ξ^2

$$|k_2| = \frac{1}{(g_{22})^{3/2}} \left| \frac{\partial x^2}{\partial \xi^2} \frac{\partial^2 x^1}{\partial \xi^2 \partial \xi^2} - \frac{\partial x^1}{\partial \xi^2} \frac{\partial^2 x^2}{\partial \xi^2 \partial \xi^2} \right|. \quad (3.48)$$

In the case of three-dimensional space, the curvature measure of the coordinate line ξ^i is computed from the relation (3.8):

$$|k_i| = \frac{1}{\sqrt{(g_{ii})^3}} |\mathbf{x}_{\xi^i} \times \mathbf{x}_{\xi^i \xi^i}|, \quad i = 1, 2, 3, \quad i \text{ fixed}. \quad (3.49)$$

The curvature representation can provide various measures of the curvature of the coordinate line ξ^i . The simplest measure may be described in the common manner as the square of the curvature

$$Q_k^i = (k_i)^2. \quad (3.50)$$

In analogy with (3.40), the quantity Q_k^i is also a measure of the departure of the coordinate line ξ^i from a straight line.

3.5.4 Measure of Coordinate Line Torsion

The square of the torsion is another measure of a coordinate line ξ^i lying in three-dimensional space. This measure is computed in accordance with (3.11) from the relation

$$\begin{aligned} Q_\tau^i &= \frac{1}{(k_i)^4 (g_{ii})^6} [(\mathbf{x}_{\xi^i} \times \mathbf{x}_{\xi^i \xi^i}) \cdot \mathbf{x}_{\xi^i \xi^i \xi^i}]^2 \\ &= \frac{1}{(k_i)^4 (g_{ii})^6} \det^2 \begin{pmatrix} \mathbf{x}_{\xi^i} \\ \mathbf{x}_{\xi^i \xi^i} \\ \mathbf{x}_{\xi^i \xi^i \xi^i} \end{pmatrix}, \quad i \text{ fixed}. \end{aligned} \quad (3.51)$$

The condition $Q_\tau^i \equiv 0$ means that the coordinate line ξ^i lies in a plane. Thus, the quantity Q_τ^i is a measure of the departure of the coordinate line ξ^i from a plane line.

3.6 Characteristics of Faces of Three-Dimensional Cells

A coordinate grid in a three-dimensional domain X^3 is composed of three-dimensional curvilinear hexahedral cells which are images of elementary cubes obtained through a coordinate transformation

$$\mathbf{x}(\boldsymbol{\xi}) : \mathcal{E}^3 \rightarrow X^3.$$

The boundary of each cell is segmented into six curvilinear quadrilaterals, through which some characteristics of the cell can be defined. This section describes some important quality measures of the faces of three-dimensional coordinate cells.

3.6.1 Cell Face Skewness

The skewness of a cell face is described through the angle between the two tangent vectors defining the cell face. Let the cell face lie in the surface $\xi^l = \text{const}$; the tangent vectors of the surface are then the vectors \mathbf{x}_{ξ^i} and \mathbf{x}_{ξ^j} , $i = l + 1$, $j = l + 2$, with the identification convention for the index m that m is equivalent to $m \pm 3$. One of the cell face skewness characteristics can be determined as the square of the cosine of the angle between the vectors. Thus, for a fixed l ,

$$Q_{\text{sk},1}^l = \cos^2 \theta = \frac{(g_{ij})^2}{g_{ii} g_{jj}}, \quad i = l + 1, \quad j = l + 2. \quad (3.52)$$

Another expression for the cell face skewness is specified by the cotangent squared of the angle θ :

$$Q'_{\text{sk},2} = \cot^2 \theta = \frac{(g_{ij})^2}{g_{ii}g_{jj} - (g_{ij})^2}, \quad i = l + 1, \quad j = l + 2. \quad (3.53)$$

Taking into account the relations (2.29) and (2.33), this can also be written in the form

$$Q'_{\text{sk},2} = \frac{(g_{ij})^2}{(\mathbf{x}_{\xi^i} \times \mathbf{x}_{\xi^j})^2} = \frac{(g_{ij})^2}{gg^{ll}}, \quad i = l + 1, \quad j = l + 2.$$

Since $(g_{ij})^2 = g_{ii}g_{jj}(1 - \sin^2 \theta)$, we also obtain

$$Q'_{\text{sk},2} = \frac{g_{ii}g_{jj}}{(\mathbf{x}_{\xi^i} \times \mathbf{x}_{\xi^j})^2} - 1 = \frac{g_{ii}g_{jj}}{gg^{ll}}, \quad i = l + 1, \quad j = l + 2.$$

The quantities for the grid face skewness introduced above equal zero when the edges of the cell face are orthogonal. Therefore, these quantities characterize the departure of the cell face from a rectangle. One more characteristic of the cell face nonorthogonality is defined as square of the dot product of the vectors \mathbf{x}_{ξ^i} and \mathbf{x}_{ξ^j} :

$$Q'_{\text{o},1} = (g_{ij})^2, \quad i = l + 1, \quad j = l + 2. \quad (3.54)$$

3.6.2 Face Aspect-Ratio

A measure of the aspect-ratio of the cell face formed by the tangent vectors \mathbf{x}_{ξ^i} and \mathbf{x}_{ξ^j} is defined through the diagonal elements g_{ii} and g_{jj} of the covariant metric tensor $\{g_{km}\}$, $k, m = 1, 2, 3$. One form of this measure is given by the expression

$$Q'_{\text{as}} = \frac{g_{ii}}{g_{jj}} + \frac{g_{jj}}{g_{ii}} = \frac{(g_{ii} + g_{jj})^2}{g_{ii}g_{jj}} - 2, \quad (3.55)$$

where $i = l + 1$, $j = l + 2$, and $m + 3$ is equivalent to $\pm m$. We have the inequality $Q'_{\text{as}} \geq 2$, which is an equality if and only if $g_{ii} = g_{jj}$, i.e. the parallelogram formed by the vectors \mathbf{x}_{ξ^i} and \mathbf{x}_{ξ^j} is a rhombus. Thus, (3.55) is a measure of the departure of the cell from a rhombus.

3.6.3 Cell Face Area Squared

The square of the area of the face of the basic parallelepiped formed by the two tangential vectors \mathbf{x}_{ξ^i} and \mathbf{x}_{ξ^j} is expressed as follows:

$$Q_{\text{ar}}^l = |\mathbf{x}_{\xi^i}|^2 |\mathbf{x}_{\xi^j}|^2 \sin^2 \theta = g_{ii} g_{jj} - (g_{ij})^2, \quad i = l + 1, \quad j = l + 2, \quad (3.56)$$

where θ is the angle of intersection of the vectors and i and j are chosen to satisfy the condition $l \neq i$ and $l \neq j$. Taking advantage of (2.29) and (2.33), we see that

$$Q_{\text{ar}}^l = |\mathbf{x}_{\xi^i} \times \mathbf{x}_{\xi^j}|^2 = g |\nabla \xi^l|^2 = g g^{ll}, \quad l \text{ fixed}. \quad (3.57)$$

As the square of the area of the coordinate cell face which corresponds to the parallelogram defined by the vectors \mathbf{x}_{ξ^i} and \mathbf{x}_{ξ^j} equals $h^2 Q_{\text{ar}} + O(h^3)$, the quantity Q_{ar}^l can be applied to characterize the area of the cell face.

3.6.4 Cell Face Warping

Measures of the cell face warping are obtained through the curvatures of the coordinate surface on which the face lies. Let this be the coordinate surface $\xi^3 = \xi_0^3$. Then, a natural parametrization $\mathbf{x}(\boldsymbol{\xi}) : \mathcal{E}^2 \rightarrow R^3$, $\boldsymbol{\xi} = (\xi^1, \xi^2)$ of the surface is represented by $\mathbf{x}(\xi^1, \xi^2, \xi_0^3)$.

Mean Curvature of the Coordinate Surface

Twice the mean curvature of the coordinate surface is defined through the formula (3.23) or (3.24) as

$$2K_{3,m} = g_{\xi^i \xi^j}^{ij} b_{ij}, \quad i, j = 1, 2, \quad (3.58)$$

where $b_{ij} = \mathbf{x}_{\xi^i \xi^j} \cdot \mathbf{n}$. It is obvious that the contravariant metric tensor $\{g_{\xi^i \xi^j}^{ij}\}$ of the surface $\xi^3 = \xi_0^3$ in the coordinates ξ^1, ξ^2 is the inverse of the 2×2 matrix $\{g_{ij}^{x\xi}\}$ whose elements are the elements of the volume metric tensor $\{g_{ij}\}$ with the indices $i, j = 1, 2$, i.e.

$$g_{ij}^{x\xi} = g_{ij} = \mathbf{x}_{\xi^i} \cdot \mathbf{x}_{\xi^j}, \quad i, j = 1, 2.$$

Therefore, using (3.16) and (2.33), we have

$$g_{\xi^i \xi^j}^{ij} = (-1)^{i+j} g_{3-i \ 3-j} / (\mathbf{x}_{\xi^1} \times \mathbf{x}_{\xi^2})^2 = \frac{(-1)^{i+j} g^{33}}{g} g_{3-i \ 3-j}, \quad i, j = 1, 2,$$

without summation over i or j . Also, it is clear that

$$\mathbf{n} = \frac{1}{\sqrt{g^{33}}} \nabla \xi^3,$$

and consequently the coefficients of the second fundamental form of the coordinate surface $\xi^3 = \xi_0^3$ are expressed as follows:

$$b_{ij} = \frac{1}{\sqrt{g^{33}}} \mathbf{x}_{\xi^i \xi^j} \cdot \nabla \xi^3 = \frac{1}{\sqrt{g^{33}}} \Gamma_{ij}^3.$$

Thus, (3.58) results in

$$2K_{3,m} = \frac{(-1)^{i+j} \sqrt{g^{33}}}{g} g_{3-i \ 3-j} \Gamma_{ij}^3, \quad i, j = 1, 2.$$

Analogously, we obtain a general formula for the coefficients of the second fundamental form of the coordinate surface $\xi^l = \xi_0^l$, $l = 1, 2, 3$:

$$b_{ij} = \frac{1}{\sqrt{g^{ll}}} \Gamma_{l+i \ l+j}^l, \quad i, j = 1, 2, \quad (3.59)$$

with l fixed and where m is equivalent to $m \pm 3$. Thus, twice the mean curvature of the coordinate surface $\xi^l = \xi_0^l$, $l = 1, 2$, is expressed by

$$2K_{l,m} = \frac{(-1)^{i+j} \sqrt{g^{ll}}}{g} g_{l-i \ l-j} \Gamma_{l+i \ l+j}^l, \quad i, j = 1, 2, \quad (3.60)$$

with l fixed.

Gaussian Curvature of the Coordinate Surface

Taking advantage of (3.22) and (3.59), the Gaussian curvature of the coordinate surface $\xi^l = \xi_0^l$ can be expressed as follows:

$$K_{l,G} = \frac{\sqrt{g^{ll}}}{g} [\Gamma_{l+1 \ l+1}^l \Gamma_{l+2 \ l+2}^l - (\Gamma_{l+1 \ l+2}^l)^2], \quad (3.61)$$

with the index l fixed.

Measures of Face Warping

The quantities which measure the warping of the face of a three-dimensional cell are obtained through the coefficients of the second fundamental form or through the mean and Gaussian curvatures of a coordinate surface containing the face. Let this be the surface $\xi^l = \xi_0^l$. Then, taking advantage of (3.60) and (3.61), the measures may be expressed as follows:

$$\begin{aligned}
Q_{w,1}^l &= (K_{l,m})^2 = \frac{g^{ll}}{g^2} [(-1)^{i+j} g_{l-i} g_{l-j} \Gamma_{l+i}^l \Gamma_{l+j}^l]^2, \\
Q_{w,2}^l &= (K_{l,g})^2 = \frac{g^{ll}}{g^2} [\Gamma_{l+1}^l \Gamma_{l+2}^l - (\Gamma_{l+1}^l \Gamma_{l+2}^l)^2], \quad (3.62)
\end{aligned}$$

with l fixed.

Equation (3.59) for the second fundamental form of the surface $\xi^l = \xi_0^l$ also gives an expression for the third measure of the cell face warpage:

$$Q_{w,3}^l = \sum_{i,j=1}^2 (b_{ij})^2 = \frac{1}{g^{ll}} \sum_{i,j=1}^2 (\Gamma_{l+i}^l \Gamma_{l+j}^l)^2, \quad l \text{ fixed}. \quad (3.63)$$

3.7 Characteristics of Grid Cells

Cell features are described by the cell volume (area in two dimensions) and by the characteristics of the cell edges and faces.

3.7.1 Cell Aspect-Ratio

A measure of the aspect-ratio of a three-dimensional cell is formulated through the measures of the aspect-ratio of its faces described by (3.55). The simplest formulation is provided by summing these measures, which results in

$$Q_{as} = \sum_{l=1}^3 Q_{as}^l. \quad (3.64)$$

3.7.2 Square of Cell Volume

The characteristic related to the square of the cell volume is

$$Q_V = g = \det\{g_{ij}\} = I_n. \quad (3.65)$$

In three dimensions, we also obtain, from (2.32),

$$Q_V = [\mathbf{x}_{\xi^1} \cdot (\mathbf{x}_{\xi^2} \times \mathbf{x}_{\xi^3})]^2.$$

3.7.3 Cell Area Squared

We denote by Q_{ar} the sum of the quantities Q_{ar}^{ij} , $i \neq j$, from (3.57). These quantities are the area characteristics of the faces of a three-dimensional cell; thus, in accordance with (3.33), the magnitude Q_{ar} coincides with the invariant I_2 :

$$Q_{\text{ar}} = \sum_{i=1}^3 g g^{ii} = I_2 . \quad (3.66)$$

3.7.4 Cell Skewness

One way to describe the cell skewness characteristics of three-dimensional grids utilizes the angles between the tangential vectors in the forms of the corresponding expressions (3.52) and (3.53) introduced for the formulation of the face skewness. For example, summation of these quantities gives the following expressions for the cell skewness measures:

$$\begin{aligned} Q_{\text{sk},1} &= \frac{(g_{12})^2}{g_{11}g_{22}} + \frac{(g_{23})^2}{g_{22}g_{33}} + \frac{(g_{13})^2}{g_{11}g_{33}} \\ Q_{\text{sk},2} &= \frac{(g_{12})^2}{g_{11}g_{22} - (g_{12})^2} + \frac{(g_{13})^2}{g_{11}g_{33} - (g_{13})^2} + \frac{(g_{23})^2}{g_{22}g_{33} - (g_{23})^2} \\ &= \frac{1}{g} \left(\frac{(g_{12})^2}{g^{33}} + \frac{(g_{13})^2}{g^{22}} + \frac{(g_{23})^2}{g^{11}} \right) . \end{aligned} \quad (3.67)$$

Here, $Q_{\text{sk},1}$ is the sum of the squares of the cosines of the angles between the edges of the cell, while $Q_{\text{sk},2}$ is the sum of the squares of the cotangents of the angles.

Other quantities for expressing the three-dimensional cell skewness can be defined through the angles between the normals to the coordinate surfaces. Any normal to the coordinate surface $\xi^i = \xi_0^i$ is parallel to the normal vector $\nabla \xi^i$. Therefore, the cell skewness can be derived through the angles between the base normal vectors $\nabla \xi^i$. The quantity

$$\frac{(\nabla \xi^i \cdot \nabla \xi^j)^2}{g^{ii} g^{jj}} = \frac{(g^{ij})^2}{g^{ii} g^{jj}} , \quad i, j \text{ fixed}$$

is the cosine squared of the angle between the respective faces of the coordinate cell. This characteristic is a dimensionless magnitude. The sum of such quantities is the third characteristic of the three-dimensional cell skewness:

$$Q_{\text{sk},3} = \frac{(g^{12})^2}{g^{11} g^{22}} + \frac{(g^{13})^2}{g^{11} g^{33}} + \frac{(g^{23})^2}{g^{22} g^{33}} . \quad (3.68)$$

Another dimensionless quantity which characterizes the mutual skewness of two faces of the cell is the cotangent squared of the angle between the normal vectors $\nabla\xi^i$ and $\nabla\xi^j$:

$$\frac{(\nabla\xi^i \cdot \nabla\xi^j)^2}{|\nabla\xi^i \times \nabla\xi^j|^2} = \frac{g(g^{ij})^2}{g_{kk}} = \frac{(g^{ij})^2}{g^{ii}g^{jj} - (g^{ij})^2},$$

where (i, j, k) are cyclic and fixed. The summation of this over k defines the fourth grid skewness characteristic

$$\begin{aligned} Q_{sk,4} &= \frac{(g^{12})^2}{g^{11}g^{22} - (g^{12})^2} + \frac{(g^{13})^2}{g^{11}g^{33} - (g^{13})^2} + \frac{(g^{23})^2}{g^{22}g^{33} - (g^{23})^2} \\ &= g \left(\frac{(g^{12})^2}{g_{33}} + \frac{(g^{13})^2}{g_{22}} + \frac{(g^{23})^2}{g_{11}} \right). \end{aligned} \quad (3.69)$$

Note that the three-dimensional cell skewness quantities $Q_{sk,1}$ and $Q_{sk,3}$ can be readily extended to arbitrary dimensions $n \geq 2$.

3.7.5 Characteristics of Nonorthogonality

The quantities $Q_{sk,i}$, $i = 1, 2, 3, 4$, from (3.67)–(3.69) reach their minimum values equal to zero only when the three-dimensional transformation $\mathbf{x}(\boldsymbol{\xi})$ is orthogonal at the respective point, and vice-versa. Therefore, these quantities, which provide the possibility to detect orthogonal grids, may be considered as some measures of grid nonorthogonality.

Other quantities characterizing the departure of a three-dimensional grid from an orthogonal one are as follows:

$$\begin{aligned} Q_{o,1} &= \frac{g_{11}g_{22}g_{33}}{g}, \\ Q_{o,2} &= g (g^{11}g^{22}g^{33}). \end{aligned} \quad (3.70)$$

Obviously, these quantities $Q_{o,1}$ and $Q_{o,2}$ are dimensionless and reach their minimum equal to 1 if and only if the coordinate transformation $\mathbf{x}(\boldsymbol{\xi})$ is orthogonal.

The sum of the squares of the nondiagonal elements of the covariant metric tensor $\{g_{ij}\}$ yields another characteristic of cell nonorthogonality,

$$Q_{o,3} = (g_{12})^2 + (g_{13})^2 + (g_{23})^2. \quad (3.71)$$

An analogous formulation is given through the elements of the contravariant metric tensor,

$$Q_{o,4} = (g^{12})^2 + (g^{13})^2 + (g^{23})^2. \quad (3.72)$$

Note that, in contrast to $Q_{0,1}$ and $Q_{0,2}$, the quantities $Q_{0,3}$ and $Q_{0,4}$ are dimensionally heterogeneous.

3.7.6 Grid Density

The invariants of the tensor $\{g_{ij}\}$ can be useful for specifying some characteristics of grid quality. For example, one important characteristic describing the concentration of grid nodes can be derived from the ratio I_{n-1}/I_n .

In order to show this, we first note that in accordance with the geometrical interpretation of the invariants given in Sect. 3.4.2, we can write

$$\frac{I_{n-1}}{I_n} = \sum_{m=1}^n (V_m^{n-1})^2 / (V^n)^2, \quad (3.73)$$

where V_m^{n-1} is the space of the boundary segment $\xi^m = \text{const}$ of the basic parallelepiped defined by the tangential vectors \mathbf{x}_{ξ^i} , $i = 1, \dots, n$.

It is evident that

$$V^n = d_m V_m^{n-1}, \quad m = 1, \dots, n,$$

where d_m is the distance between the vertex of the tangential vector \mathbf{x}_{ξ^m} and the $(n-1)$ -dimensional plane P^{n-1} spanned by the vectors \mathbf{x}_{ξ^i} , $i \neq m$. Hence, from (3.73),

$$\frac{I_{n-1}}{I_n} = \sum_{m=1}^n (1/d_m)^2. \quad (3.74)$$

Now let us consider two grid surfaces $\xi^m = c$ and $\xi^m = c+h$ obtained by mapping a uniform rectangular grid with a step size h in the computational domain \mathcal{E}^n onto X^n . Let us denote by l_m the distance between a node on the coordinate surface $\xi^m = c$ and the nearest node on the surface $\xi^m = c+h$ (Fig. 3.5). We have

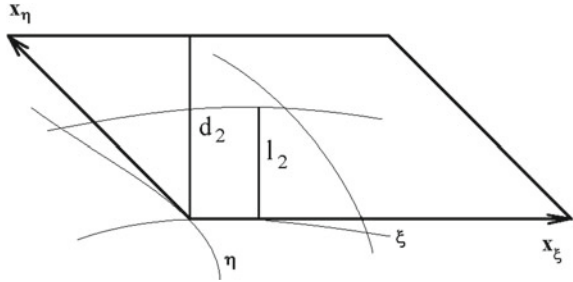
$$l_m = d_m h + O(h)^2$$

and therefore, from (3.74),

$$\frac{I_{n-1}}{I_n} = \sum_{m=1}^n (h/l_m)^2 + O(h).$$

The quantity $(h/l_m)^2$ increases if the grid nodes cluster in the direction normal to the surface $\xi^m = c$. Therefore, this quantity can be considered as some measure of the grid concentration in the normal direction and, consequently, the magnitude $1/d_m$

Fig. 3.5 Illustration of invariants



means the density of the grid concentration in the $\nabla \xi^m$ direction. In particular, we readily see that $1/d_m = \sqrt{g^{mm}}$, with m fixed. Thus, the expression (3.74) defines a measure of the grid density in all directions. We denote this quantity by Q_{cn} , where the subscript “cn” represents “concentration”. Note that, in accordance with (3.31), this measure can be expressed as follows:

$$Q_{cn} = \frac{I_{n-1}}{I_n} = g^{11} + \dots + g^{nn} . \tag{3.75}$$

3.7.7 Characteristics of Deviation from Conformality

Conformal coordinate transformations are distinguished by the fact that the Jacobi matrix J is orthonormal, and consequently the metric tensor $\{g_{ij}\}$ is a multiple of the unit matrix:

$$\{g_{ij}\} = g(\boldsymbol{\xi})I = g(\boldsymbol{\xi})\{\delta_j^i\} , \quad i, j = 1, \dots, n .$$

The cells of the coordinate grid derived from the conformal mapping $\mathbf{x}(\boldsymbol{\xi})$ are close to n -dimensional cubes (squares in two dimensions). Grids with such cells are attractive from the computational point of view. Therefore, it is desirable to define simple grid quantities which can allow one to detect grids whose cells are close to n -dimensional cubes. It is clear that the condition of conformality can be described by the system

$$\begin{aligned} g_{ij} &= 0 , & i &\neq j , \\ g_{11} &= g_{22} = \dots = g_{nn} . \end{aligned}$$

These relations give rise to a natural quantity

$$Q = \sum_{i \neq j} (g_{ij})^2 + \sum_{i=2}^n (g_{ii} - g_{11})^2 ,$$

which is zero if and only if the coordinate transformation $\mathbf{x}(\boldsymbol{\xi})$ is conformal. So, this quantity can help one to detect when the grid is conformal. However, the above formula is too cumbersome, as well as being dimensionally heterogeneous. More compact expressions for the analysis of the conformality or nonconformality of grid cells and for the formulation of algorithms to construct nearly conformal grids are obtained through the use of the metric-tensor invariants.

Two-Dimensional Space

The departure from conformality of the two-dimensional transformation $\mathbf{x}(\boldsymbol{\xi}) : \mathcal{E}^2 \rightarrow X^2$ is expressed by the quantity

$$Q_{\text{cf},1} = \frac{I_1}{\sqrt{I_2}} = \frac{|\mathbf{x}_{\xi^1}|^2 + |\mathbf{x}_{\xi^2}|^2}{|\mathbf{x}_{\xi^1}| |\mathbf{r}_{\xi^2}| |\sin \theta|} = \frac{g_{11} + g_{22}}{\sqrt{g_{11}g_{22}} |\sin \theta|}, \quad (3.76)$$

where θ is the angle between the tangent vectors \mathbf{x}_{ξ^1} and \mathbf{x}_{ξ^2} . Since

$$Q_{\text{cf},1} \geq \frac{g_{11} + g_{22}}{\sqrt{g_{11}g_{22}}},$$

it is clear that the value of $I_1/\sqrt{I_2}$ exceeds 2. The minimum value 2 is achieved only if $g_{11} = g_{22}$ and $\theta = \pi/2$, i.e. when the parallelogram with sides defined by the vectors \mathbf{x}_{ξ^1} and \mathbf{x}_{ξ^2} is a square. Thus, the characteristic $Q_{\text{cf},1}$ allows one to state with certainty when the coordinate transformation $\mathbf{x}(\boldsymbol{\xi})$ is conformal at a point $\boldsymbol{\xi}$, namely when $Q_{\text{cf},1}(\boldsymbol{\xi}) = 2$. Therefore, in the two-dimensional case, the quantity

$$Q_{\text{cf},1} - 2 = I_1/\sqrt{I_2} - 2$$

reflects some measure of the deviation of the cell from a square. We see that the quantity $Q_{\text{cf},1}$ given by (3.76) is dimensionally homogeneous.

Through the quantity $Q_{\text{cf},1}$, we can also estimate the bounds of the aspect ratio of the two-dimensional cell and the angle between the edges of this cell.

Evaluation of the Cell Angles

First, we obtain an estimate of the angle between the cell edges. From (3.76), we have

$$\sin^2 \theta = \frac{(F^2 + 1)^2}{F^2} / Q_{\text{cf},1}^2, \quad (3.77)$$

where $F^2 = g_{11}/g_{22}$. As $(F^2 + 1)^2/F^2 \geq 4$, we have from (3.77) that

$$\sin^2 \theta \geq 4/Q_{\text{cf},1}^2 \quad (3.78)$$

and, accordingly, we obtain the following estimate for the angle θ :

$$\pi - \arcsin(2/Q_{cf,1}) \geq \theta \geq \arcsin(2/Q_{cf,1}) . \quad (3.79)$$

From (3.77), we find that the minimum value $4/Q_{cf,1}^2$ of $\sin^2 \theta$ for a fixed value of $Q_{cf,1}$ is achieved when $F = 1$, i.e. when the parallelogram is the rhombus.

Although it is desirable to generate orthogonal grids, a departure from orthogonality is practically inevitable when grid adaptation is performed. Commonly, this departure is required to be restricted to 45° . Beyond this range, the contribution of the grid skewness to the truncation error may become unacceptable. The inequality (3.79) shows that this barrier of 45° is not broken if $Q_{cf,1} \leq 2\sqrt{2}$.

Evaluation of the Cell Aspect Ratio

Now we estimate the quantity $F = \sqrt{g_{11}/g_{22}}$. The quantity F , called the cell aspect-ratio, is the ratio of the lengths of the edges of the cell. By computing F from (3.77), we obtain

$$F = \frac{\alpha}{2} - 1 \pm \sqrt{\frac{\alpha^2}{4} - \alpha} , \quad \alpha = Q_{cf,1}^2 \sin^2 \theta . \quad (3.80)$$

Equation (3.80) gives two values of the cell aspect-ratio,

$$F_1 = \frac{\alpha}{2} - 1 + \sqrt{\frac{\alpha^2}{4} - \alpha} \quad \text{and} \quad F_2 = \frac{\alpha}{2} - 1 - \sqrt{\frac{\alpha^2}{4} - \alpha} ,$$

satisfying the relation $F_1 F_2 = 1$. We find that

$$F_1 = \max(\sqrt{g_{11}/g_{22}}, \sqrt{g_{22}/g_{11}})$$

and

$$F_2 = \min(\sqrt{g_{11}/g_{22}}, \sqrt{g_{22}/g_{11}}) .$$

Thus,

$$\frac{\alpha}{2} - 1 - \sqrt{\frac{\alpha^2}{4} - \alpha} \leq F_i \leq \frac{\alpha}{2} - 1 + \sqrt{\frac{\alpha^2}{4} - \alpha} , \quad i = 1, 2 , \quad (3.81)$$

and consequently

$$2 \leq F_i + 1/F_i \leq \alpha - 2 , \quad i = 1, 2 . \quad (3.82)$$

As $Q_{cf,1}^2 \geq \alpha \geq 4$, from (3.78), we also obtain, from (3.81) and (3.82), the following upper and lower estimates of the aspect ratios F_i , $i = 1, 2$, which depend only on the quantity $Q_{cf,1}$:

$$\frac{Q_{cf,1}^2}{2} - 1 - Q_{cf,1} \sqrt{\frac{Q_{cf,1}^2}{4} - 1} \leq F_i \leq \frac{Q_{cf,1}^2}{2} - 1 + Q_{cf,1} \sqrt{\frac{Q_{cf,1}^2}{4} - 1}, \quad (3.83)$$

and

$$2 \leq F_i + 1/F_i \leq Q_{cf,1}^2 - 2, \quad i = 1, 2. \quad (3.84)$$

The maximum value of F_i for a given value of $Q_{cf,1}$ is realized when $\sin^2 \theta = 1$, i.e. the parallelogram is a rectangle.

Three-Dimensional Space

In three-dimensional space, the deviation from conformality can be described by the dimensionless magnitude

$$Q_{cf,1} = (g)^{1/3} (g^{11} + g^{22} + g^{33}), \quad (3.85)$$

which, in accordance with (3.33), is expressed by means of the invariants I_2 and I_3 as follows:

$$Q_{cf,1} = I_2 / (I_3)^{2/3}. \quad (3.86)$$

The value of (3.86) reaches its minimum only if

$$g^{11} = g^{22} = g^{33} \quad \text{and} \quad g^{-1} = g^{11} g^{22} g^{33}, \quad (3.87)$$

i.e. when the parallelogram defined by the basic normal vectors $\nabla \xi^i$ is a cube. To prove this fact, we note that

$$\frac{1}{g} \leq g^{11} g^{22} g^{33}.$$

Therefore, from (3.85),

$$Q_{cf,1} \geq \frac{g^{11} + g^{22} + g^{33}}{\sqrt[3]{g^{11} g^{22} g^{33}}}$$

and, taking into account the general inequality for arbitrary positive numbers a_1, \dots, a_n

$$\frac{1}{n} \sum_{i=1}^n a_i \geq \sqrt[n]{\prod_{i=1}^n a_i},$$

we find that $Q_{cf,1} \geq 3$. Obviously, $Q_{cf,1} = 3$ when the relations (3.87) are satisfied. From (2.35),

$$\frac{1}{g} = |\nabla \xi^1 \cdot \nabla \xi^2 \times \nabla \xi^3|^2$$

and therefore (3.87) is satisfied only when the normal vectors $\nabla \xi^i$, $i = 1, 2, 3$, are orthogonal to each other and have the same length. But then this is valid for the base tangential vectors \mathbf{x}_{ξ^i} , $i = 1, 2, 3$, as well. Thus, (3.87) is satisfied only when the transformation $\mathbf{x}(\xi)$ is conformal.

In the same manner as in the two-dimensional case, one can derive bounds on the angles of the parallelepiped and on the ratio of the lengths of its edges that depend on the quantity $Q_{cf,1}$.

Generalization to Arbitrary Dimensions

Analogously, in the n -dimensional case, a local measure of the deviation of the transformation $\mathbf{x}(\xi)$ from a conformal one is expressed by the quantity $Q_{cf,1} - n$, where

$$Q_{cf,1} = I_{n-1}/(I_n)^{1-1/n} = g^{1/n}(g^{11} + \dots + g^{nn}) . \tag{3.88}$$

The quantity $Q_{cf,1}$ equals n if and only if the mapping $\mathbf{x}(\xi)$ is conformal.

Another local characteristic of the deviation from conformality is described by the quantity $Q_{cf,2} - n$, where

$$Q_{cf,2} = I_1/(I_n)^{1/n} . \tag{3.89}$$

As for $Q_{cf,1}$, we can show that $Q_{cf,2} \geq n$ and that $Q_{cf,2} = n$ if the transformation $\mathbf{x}(\xi)$ is conformal at the point under consideration. Note also that $Q_{cf,1} = Q_{cf,2}$ in two dimensions.

3.7.8 Grid Eccentricity

One grid eccentricity characteristic is defined by summing the squares of the coordinate-line eccentricities (3.36). Thus, the quantity

$$Q_{\epsilon,1} = \sum_{i=1}^n \left(\frac{\partial}{\partial \xi^i} \ln \sqrt{g_{ii}} \right)^2 \tag{3.90}$$

is a measure of the change of the lengths of all of the grid cell edges.

A similar characteristic of eccentricity can be formulated through the terms g^{ii} , namely

$$Q_{\epsilon,2} = \sum_{i=1}^n \left(\frac{\partial}{\partial x^i} \ln \sqrt{g^{ii}} \right)^2 . \tag{3.91}$$

3.7.9 Measures of Grid Warping and Grid Torsion

In the same way as for grid eccentricity, we may formulate measures of three-dimensional grid warping by summing the surface-coordinate characteristics (3.62) and (3.63). As a result, we obtain

$$\begin{aligned}
 Q_{w,1} &= \frac{1}{g^2} \sum_{l=1}^3 g^{ll} \left((-1)^{i+j} g_{l-i \ l-j} \Gamma_{l+i \ l+j}^l \right)^2, \\
 Q_{w,2} &= \frac{1}{g^2} \sum_{l=1}^3 g^{ll} \left[\Gamma_{l+1 \ l+1}^l \Gamma_{l+2 \ l+2}^l - (\Gamma_{l+1 \ l+1}^l)^2 \right], \\
 Q_{w,3} &= \sum_{l=1}^3 \sum_{i,j=1}^2 \frac{1}{g^{ll}} (\Gamma_{l+i \ l+j}^l)^2.
 \end{aligned} \tag{3.92}$$

The measure of grid torsion is formulated by summing the torsion measures (3.51) of the coordinate lines ξ^i , $i = 1, 2, 3$:

$$Q_\tau = \sum_{i=1}^3 Q_\tau^i. \tag{3.93}$$

3.7.10 Quality Measures of Simplexes

The quantities which are applied to measure the quality of triangles and tetrahedrons are the following:

- (1) the maximum edge length H ,
- (2) the minimum edge length h ,
- (3) the circum-radius R ,
- (4) the inradius r .

There are four deformation measures that allow one to characterize the quality of triangular and tetrahedral cells:

$$Q_{d,1} = \frac{H}{r}, \quad Q_{d,2} = \frac{R}{H}, \quad Q_{d,3} = \frac{H}{h}, \quad Q_{d,4} = \frac{R}{r}.$$

The uniformity condition for a cell is satisfied when $Q_{d,1} = O(1)$ or $Q_{d,4} = O(1)$.

Examples of poorly shaped cells are shown in Fig. 3.6. Cases a and c correspond to needle-shaped cells. Figure 3.6d shows a wedge-shaped cell, while Fig. 3.6b, e show sliver-shaped cells.

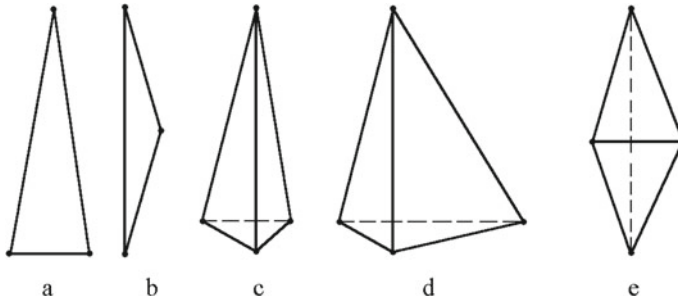


Fig. 3.6 Examples of poorly shaped triangles (a, b) and tetrahedrons (c, d, e)

The cell is excessively deformed if $Q_{d,1} \gg 1$. In this case, the cell has either a very acute or a very obtuse angle. The former case corresponds to $Q_{d,2} = O(1)$, $Q_{d,3} \gg 1$ (Fig. 3.6a, c, d), while the latter corresponds to $Q_{d,4} \gg 1$, $Q_{d,3} = O(1)$ (Fig. 3.6b, e). The condition $Q_{d,2} = O(1)$ precludes obtuse angles.

3.8 Comments

Various aspects of mesh quality were surveyed by Knupp (2001, 2007). The introduction of metric-tensor invariants to describe some of the qualitative properties of grids was originally proposed by Jacquotte (1987). The grid measures in terms of the invariants and their relations described in this chapter were obtained by the author.

Prokopov (1989) introduced the dimensionless characteristics of two-dimensional cells.

Triangular elements were extensively analyzed by Field (2000).

Some questions concerned with the assessment of the contribution of the grid quality properties to the accuracy of solutions obtained using the grid were discussed by Kerlic and Klopfer (1982), Mastin (1982), Lee and Tsuei (1992), and Huang and Prosperetti (1994).

Discrete length, area, and orthogonality grid measures using averages and deviations were formulated by Steinberg and Roache (1992).

Babuška and Aziz (1976) have shown that the minimum-angle condition in a planar triangulation is too restrictive and can be replaced by a condition that limits the maximum allowable angle. Also, the influence of grid quality measures on solution accuracy was discussed by Knupp (2007) and Shewchuck (2002).

Measures to quantify the shape of triangles and tetrahedrons were introduced by Field (1986), Baker (1989), Cougny et al. (1990), and Dannenlongue and Tanguy (1991).

A brief overview of tetrahedron quality measures with a comparison of the fidelity of these measures to a set of distortion sensitivity tests, as well as a comparison of the computational expense of such measures, was given by Parthasarathy et al. (1993).

An overview of several element quality metrics was given by Field (2000). Chen et al. (2003) extended the angle-based quality metric originally defined by Lee and Lo (1994) for use in the optimization of meshes consisting of triangles and quadrilaterals. They also extended the formulation of cell unfolding by adding a barrier part to their quality functional (2003).

A special tetrahedron shape measure was given by Liu and Joe (1994a). It is based on eigenvalues of the metric tensor for the transformation between a tetrahedron and a regular reference tetrahedron. The geometric explanation of this measure is that it characterizes the shape of the inscribed ellipsoid. Another shape regularity quality of a triangle was given Bank and Xu (1996) and Bank and Smith (1997). They showed that the quality has circular level sets, when considered a function of the location of one vertex of a triangle with the other two vertices fixed. Three tetrahedron measures – the minimum solid angle, the radius ratio, and the mean ratio – and their relations were discussed by Liu and Joe (1994b).

An algorithm for construction of solution-adapted triangular meshes within an optimization framework was considered by Buscaglia and Dari (1997). Here, the optimized quality measure is a product of “shape” quality and a function of mesh size.

A local cell quality measure as a function of Jacobian matrix and combined element-shape and size-control metrics for different cell types was analyzed by Garanzha (2000) and Branets and Carey (2005).

Dompierre et al. (2005) analyzed and generalized several simplex shape measures documented in the literature and used them for mesh adaptation and mesh optimization. Conclusions were drawn on the choice of simplex shape measures to control mesh optimization.

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