2

Preliminaries: Size Measures and Shape Coordinates

2.1 Configuration Space

Definition 2.1 *The* **configuration** *is the set of landmarks on a particular object. The* **configuration matrix** X *is the* $k \times m$ *matrix of Cartesian coordinates of the* k *landmarks in* m *dimensions. The* **configuration space** *is the space of all possible landmark coordinates.*

In our applications we have $k \geq 3$ landmarks in $m = 2$ or $m = 3$ dimensions and the configuration space is typically $\mathbb{R}^{km}$ with possibly some special cases removed, such as coincident points.

2.2 Size

Before defining shape we should define what we mean by size, so that it can be removed from a configuration. Consider X to be a $k \times m$ matrix of the Cartesian coordinates of k landmarks in m real dimensions, i.e. the configuration matrix of the object.

Definition 2.2 *A* **size measure** $g(X)$ *is any positive real valued function of the configuration matrix such that*

$$g(aX) = ag(X) \tag{2.1}$$

for any positive scalar a*.*

Definition 2.3 *The* **centroid size** *is given by*

$$S(X) = \|CX\| = \sqrt{\sum_{i=1}^{k}\sum_{j=1}^{m}(X_{ij} - \bar{X}_j)^2}\,, \quad X \in \mathbb{R}^{km}, \tag{2.2}$$

where X_{ij} is the (i, j)th entry of X, the arithmetic mean of the jth dimension is $\bar{X}_j = \frac{1}{k}\sum_{i=1}^{k} X_{ij}$,

$$C = I_k - \frac{1}{k} 1_k 1_k^{\mathrm{T}} \tag{2.3}$$

is the centring matrix, $\|X\| = \sqrt{\mathrm{trace}(X^{\mathrm{T}}X)}$ is the Euclidean norm, I_k is the $k \times k$ identity matrix, and 1_k is the $k \times 1$ vector of ones.

Obviously $S(aX) = aS(X)$ thus satisfying Equation (2.1). The centroid size $S(X)$ is the square root of the sum of squared Euclidean distances from each landmark to the centroid, namely

$$S(X) = \sqrt{\sum_{i=1}^{k} \|(X)_i - \bar{X}\|^2},$$

where $(X)_i$ is the ith row of $X(i = 1, \ldots, k)$ and $\bar{X} = (\bar{X}_1, \ldots, \bar{X}_m)$ is the centroid. This measure of size will be used throughout the book. In fact, the centroid size is the most commonly used size measure in geometrical shape analysis (e.g. Bookstein, 1986; Kendall, 1984; Goodall, 1991; Dryden and Mardia, 1992). The centroid size could also be used in a normalized form, e.g. $S(X)/\sqrt{k}$ or $S(X)/(km)^{1/2}$, and this would be particularly appropriate when comparing configurations with different numbers of landmarks. The squared centroid size can also be interpreted as $(2k)^{-1}$ times the sum of the squared inter-landmark distances since

$$\begin{aligned}
\sum_{j=1}^{m}\sum_{i=1}^{k}\sum_{l=1}^{k}(X_{ij}-X_{lj})^2 &= \sum_{j=1}^{m}\sum_{i=1}^{k}\sum_{l=1}^{k}(X_{ij}-\bar{X}_j+\bar{X}_j-X_{lj})^2 \\
&= \sum_{j=1}^{m}\sum_{i=1}^{k}\sum_{l=1}^{k}(X_{ij}-\bar{X}_j)^2+\sum_{j=1}^{m}\sum_{i=1}^{k}\sum_{l=1}^{k}(\bar{X}_j-X_{lj})^2 \\
&\quad +2\sum_{j=1}^{m}\sum_{i=1}^{k}\sum_{l=1}^{k}(X_{ij}-\bar{X}_j)(\bar{X}_j-X_{lj}) \\
&= 2k\sum_{i=1}^{k}\sum_{j=1}^{m}(X_{ij}-\bar{X}_j)^2 \\
&= 2kS(X)^2.
\end{aligned}$$

An alternative size measure is the baseline size, i.e. the length between landmarks 1 and 2:

$$D_{12}(X) = \|(X)_2 - (X)_1\|. \tag{2.4}$$

The baseline size was used as early as 1907 by Galton for normalizing faces and its use came into prominence with Bookstein coordinates, described in Section 2.3.2.

Other alternative size measures include the square root of the area of the convex hull for planar configurations or the cube root of the volume of the convex hull for configurations in $\mathbb{R}^3$ which intuitively describes size, but these measures have not become popular. For triangles with coordinates $(X_1, Y_1), (X_2, Y_2)$ and (X_3, Y_3) the area is simply given by

$$A = \frac{1}{2}(base\ \ length \times height).$$

or alternatively

$$A = \tfrac{1}{2}\left|(Y_3 - Y_1)(X_2 - X_1) - (X_3 - X_1)(Y_2 - Y_1)\right|.$$

Other size measures for triangles include the radius of the inscribed circle and the circumradius (e.g. Miles, 1970), the latter being equal to $S(X)/\sqrt{3}$.

In general the choice of size will affect reported conclusions. In particular, if object A has twice the centroid size of object B it doesn't necessarily follow that object A is twice the size of object B when using a different measure. When reporting size differences one needs to state which size measure was used. The exception is when both objects have the same shape, in which case the ratio of sizes will be the same regardless of the choice of size variable. If comparing sets of collinear points, then very different conclusions about size are reached, with these pathological configurations all having zero area but non-zero centroid size for non-coincident collinear points.

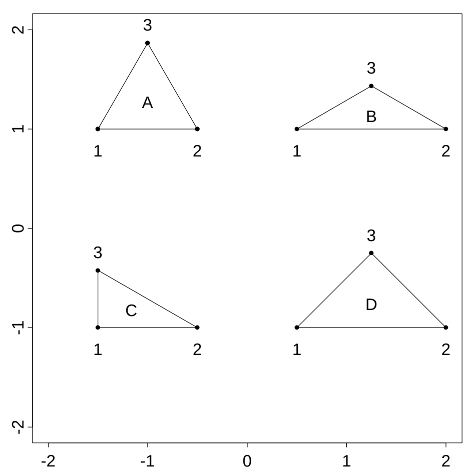

Figure 20 Four example triangles. The ranking of the triangles in terms of size differs when different choices of size measure are considered.

Example 2.1 Consider the triangles in Figure 20. The centroid sizes of the triangles are

$$A : 1,\ B : 1.118,\ C : 0.943,\ D : 1.225.$$

The baseline sizes are

$$A : 1,\ B : 1.5,\ C :1,\ D : 1.5.$$

The square root of area sizes are

$$A : 0.658,\ B : 0.570,\ C : 0.538,\ D : 0.750.$$

The relative ranking of triangles in terms of size differs depending on the choice of size measure. In particular, in terms of area A is larger than B, but in terms of centroid size B is larger than A. This example demonstrates that different choices of size measure will lead to different conclusions about size. □

2.3 Some Shape Coordinate Systems

In order to describe an object's shape it is useful to specify a coordinate system. We initially consider some of the most straightforward coordinate systems. A suitable choice of coordinate system for shape will be invariant under translation, scaling and rotation of the configuration. Further coordinate systems are discussed later in Section 4.3.

2.3.1 Angles and ratios of lengths

For $k = 3$ points in $m = 2$ dimensions two internal angles are the most obvious choice of coordinates that are invariant under the similarity transformations. For example, x_1 and x_2 could measure the shape of the triangle in Figure 21, where $x_1 + x_2 + x_3 = 180°$.

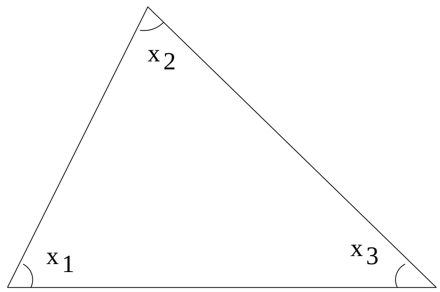

Figure 21 A labelled triangle with three internal angles marked. Two of the internal angles could be used to measure the shape of the triangle.

However, it soon becomes apparent that using angles to describe shape can be problematic. For cases such as very flat triangles (three points in a straight line) there are many different arrangements of three points. For example, see Figure 22, where the triangles all have $x_1 = 0°, x_3 = 0°, x_2 = 180°$, and yet the configurations have different shapes. For larger numbers of points ($k > 3$) one could sub-divide the configuration into triangles and so $2k - 4$ angles would be needed. For the $m = 3$ dimensional case angles could also be used, but again these suffer from problems in pathological cases.

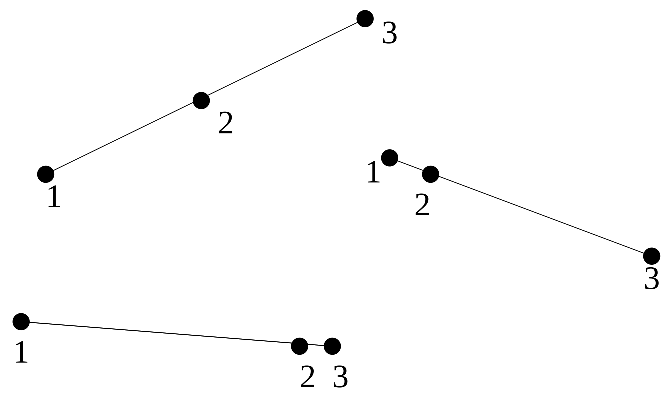

Figure 22 Examples of pathological cases where angles are an inappropriate shape measure. The landmarks are at the centre of the discs.

2.3.2 Bookstein coordinates: Planar case

Let $(x_j, y_j), j = 1, ..., k$, be $k \geq 3$ landmarks in a plane ($m = 2$ dimensions). Bookstein (1984, 1986) suggests removing the similarity transformations by translating, rotating and rescaling such that landmarks 1 and 2 are sent to a fixed position. If landmark 1 is sent to $(0, 0)$ and landmark 2 is sent to $(1, 0)$, then suitable shape variables are the coordinates of the remaining $k-2$ coordinates after these operations. To preserve symmetry, we consider the coordinate system where the baseline landmarks are sent to $(-\frac{1}{2}, 0)$ and $(\frac{1}{2}, 0)$.

Definition 2.4 Bookstein coordinates $(u_j^B, v_j^B)^{\mathrm{T}}, j = 3, \ldots, k$, *are the remaining coordinates of an object after translating, rotating and rescaling the baseline to* $(-\frac{1}{2}, 0)$ *and* $(\frac{1}{2}, 0)$ *so that*

$$
\begin{aligned}
u_j^B &= \{(x_2 - x_1)(x_j - x_1) + (y_2 - y_1)(y_j - y_1)\}/D_{12}^2 - \tfrac{1}{2}, \\
v_j^B &= \{(x_2 - x_1)(y_j - y_1) - (y_2 - y_1)(x_j - x_1)\}/D_{12}^2,
\end{aligned}
\tag{2.5}
$$

where $j = 3, ..., k$, $D_{12}^2 = (x_2 - x_1)^2 + (y_2 - y_1)^2 > 0$ *and* $-\infty < u_j^B, v_j^B < \infty$.

A geometrical illustration of these transformations is given in Figure 23. If the baseline is taken as $(0, 0)$ and $(1, 0)$, then there is no $-\frac{1}{2}$ in the equation for u_j^B. We subtract the $\frac{1}{2}$ in u_j^B to also simplify the transformation to Kendall coordinates in Section 2.3.4, although precisely where we send the baseline is an arbitrary choice. These coordinates have been used widely in shape analysis for planar data. Bookstein coordinates are the most straightforward to use for a newcomer to shape analysis. Also, many people experienced in shape analysis often use Bookstein coordinates in the first stages of an analysis. However, because of the lack of symmetry in choosing a particular baseline and the fact that correlations are induced into the coordinates, many practitioners often prefer to use the Procrustes tangent coordinates (see

Section 3.2 or 4.3.1).

Galton (1907) defined precisely the same coordinates (with baseline (0,0), (1,0)) at the beginning of the century, but the statistical details of using this approach needed to be worked out.

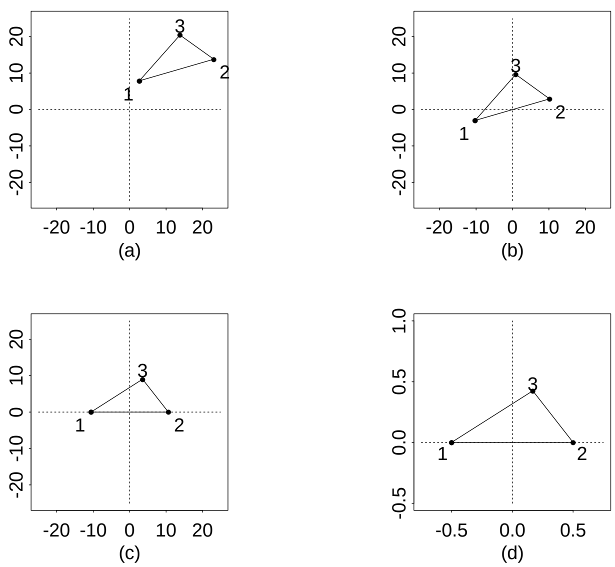

Figure 23 The geometrical interpretation of Bookstein coordinates. The original triangle in (a) is transformed by (b) translation, (c) rotation and finally (d) rescaling to give the Bookstein coordinates as the coordinates of the point labelled 3 in plot (d).

The construction of Bookstein coordinates is particularly simple if using complex arithmetic. Bookstein coordinates are obtained from the original complex coordinates $z_1^o, \ldots, z_k^o$ using

$$u_j^B + iv_j^B = \frac{z_j^o - z_1^o}{z_2^o - z_1^o} - \tfrac{1}{2} = \frac{2z_j^o - z_1^o - z_2^o}{2(z_2^o - z_1^o)}, \quad j = 3, \ldots, k. \tag{2.6}$$

Consider how the formulae in Equation (2.5) are obtained (Mardia, 1991). To find (u_j^B, v_j^B) for a fixed $j = 3, \ldots, k$, we have to find the scale $c > 0$, the rotation A, and the translation $b = (b_1, b_2)^{\mathrm{T}}$ such that

$$U = cA(X - b), \tag{2.7}$$

where $X = (x_j, y_j)^{\mathrm{T}}$ and $U = (u_j^B, v_j^B)^{\mathrm{T}}$ are the coordinates of the jth point before and after the transformation, $j = 3, \ldots, k$, and A is a 2×2 rotation matrix, namely

$$A = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}, \quad |A| = 1, \quad A^{\mathrm{T}}A = AA^{\mathrm{T}} = I_2,$$

where we rotate clockwise by θ radians. Applying the transformation to landmarks 1 and 2 gives four equations in four unknowns (c, θ, b_1, b_2)

$$cA\left(\begin{bmatrix} x_1 \\ y_1 \end{bmatrix} - b\right) = \begin{bmatrix} -\frac{1}{2} \\ 0 \end{bmatrix}, \quad cA\left(\begin{bmatrix} x_2 \\ y_2 \end{bmatrix} - b\right) = \begin{bmatrix} \frac{1}{2} \\ 0 \end{bmatrix}.$$

Now, we can solve these equations and see that the translation is

$$b = (\tfrac{1}{2}(x_1 + x_2), \tfrac{1}{2}(y_1 + y_2))^{\mathrm{T}},$$

the rotation (in the appropriate quadrant) is

$$\theta = \arctan\{(y_2 - y_1)/(x_2 - x_1)\}$$

and the rescaling is $c = \{(x_2 - x_1)^2 + (y_2 - y_1)^2\}^{-1/2}$. So,

$$A = c\begin{pmatrix} x_2 - x_1 & y_2 - y_1 \\ -(y_2 - y_1) & x_2 - x_1 \end{pmatrix}. \qquad (2.8)$$

Substituting $X = (x_j, y_j)^{\mathrm{T}} (j = 3, ..., k)$ and c, A, b into Equation (2.7) we obtain the shape variables of Equation (2.5). This solution can also be seen from Figure 23 using geometry.

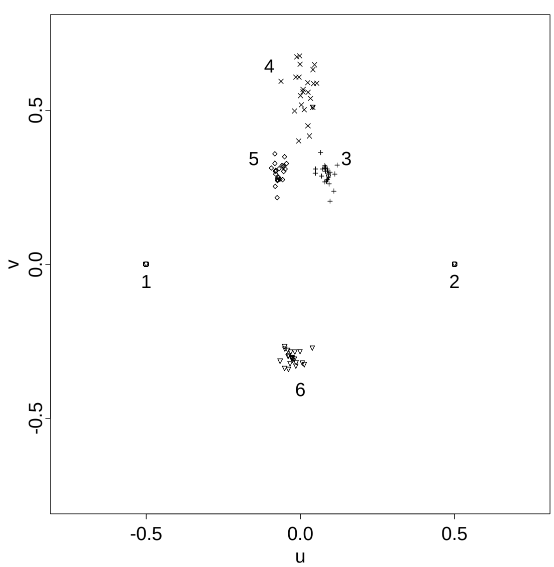

Figure 24 Scatter plots of the T2 vertebrae registered on the baseline 1, 2, giving a scatter plot of the Bookstein coordinates.

Example 2.2 In Figure 24 we see scatter plots of the

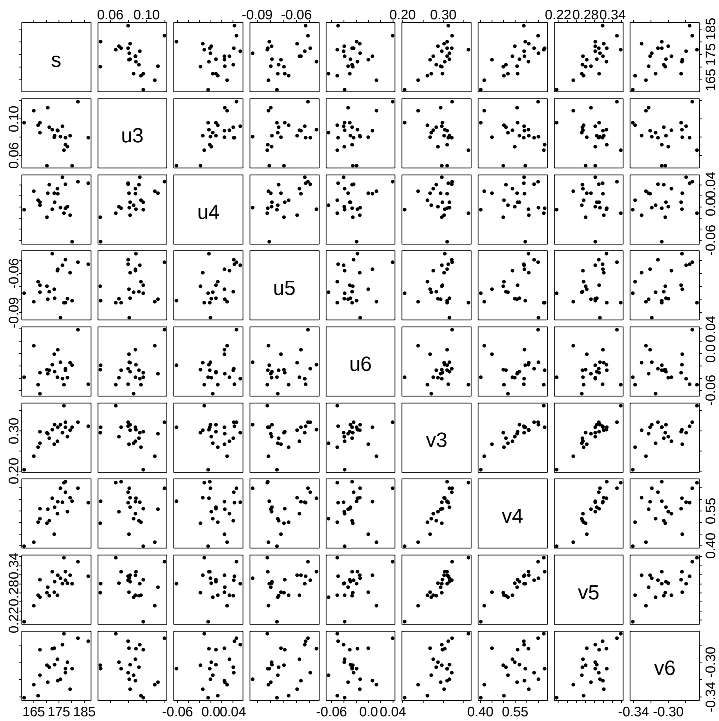

Figure 25 Pairwise scatter plots of centroid size S and Bookstein coordinates $u_3^B, \ldots, u_6^B, v_3^B, \ldots, v_6^B$ for the T2 vertebrae Small group.

Bookstein coordinates for the T2 Small vertebrae of Section 1.2.1. Producing such a plot is often the first stage in any simple shape analysis. We take landmarks 1 and 2 as the baseline. Note that the marginal scatter plots at landmarks 4 and possibly 3 and 5 are elliptical in nature. For practical data analysis it is sensible to choose the baseline as landmarks that are not too close together, as in this example. As often happens with using Bookstein coordinates, the variability in the points away from the origin appears larger than the points nearer to the origin.

In Figure 25 we see pairwise scatter plots of Bookstein coordinates. There are strong positive correlations in the v_3^B, v_4^B and v_5^B coordinates. There are also positive correlations between v_3^B and v_6^B, between v_5^B and v_6^B, and between u_3^B and u_4^B. However, it is also an artifact of the coordinate system that correlations are induced into the shape variables, even when the landmarks themselves are uncorrelated (see Section 6.6.4), and so correlations can be difficult to interpret.

We can also examine the joint relationship between size and shape, which will be considered in more detail in Chapter 8. Scatter plots of the centroid size S versus each of the shape coordinates are also given in Figure 25. We see that there are quite strong positive correlations between S and each of v_3^B, v_4^B and v_5^B. $\square$

Throughout the text we shall often refer to the real $(2k-4)$-vector of Bookstein coordinates $u^B = (u_3^B, \ldots, u_k^B, v_3^B, \ldots, v_k^B)^{\mathrm{T}}$, stacking the coordinates in this particular order.

One approach to shape analysis is to use standard multivariate analysis on Bookstein coordinates, ignoring the non-Euclidean nature of the space. Provided variations in the data are small, then the method is adequate for mean estimation and hypothesis testing. For example, we could obtain an estimate of the mean shape of the configuration by taking the arithmetic average of the Bookstein coordinates (the **Bookstein mean shape**). For example, the Bookstein mean shape for the T2 Small mouse vertebrae of Example 2.2 is given by

$$\bar{u}^B = (0.085, 0.012, 0.069, -0.025, 0.292, 0.559, 0.298, -0.304)^{\mathrm{T}}.$$

The variability of the shape variables is less straightforward to interpret. Transforming the objects (or registering) to a given edge induces correlations into the shape variables in general and this can lead to spurious correlations.

So the method should not be used to interpret the structure of shape variability unless there is a good reason to believe that two landmarks are essentially fixed (see Section 7.3).

2.3.3 Triangle case

For the case of a triangle of landmarks we have two shape coordinates.

Example 2.3 In Figure 20 we see the triangles with internal angles at points 1, 2, 3 given by

A: $60^\circ, 60^\circ, 60^\circ$ (equilateral),

B: $30^\circ, 30^\circ, 120^\circ$ (isosceles) ,

C: $90^\circ, 30^\circ, 60^\circ$ (right-angled),

D: $45^\circ, 45^\circ, 90^\circ$ (right-angled and isosceles).

Bookstein coordinates for these three triangles with baseline points 1, 2 are

A: $U_3^B = 0, V_3^B = \frac{\sqrt{3}}{2}$,

B: $U_3^B = 0, V_3^B = \frac{1}{2\sqrt{3}}$,

C: $U_3^B = -\frac{1}{2}, V_3^B = \frac{1}{\sqrt{3}}$,

D: $U_3^B = 0, V_3^B = \frac{1}{2}$. □

A plot of the shape space of triangles for Bookstein coordinates is given in Figure 26. Each triangle shape is drawn with its centroid in the position of the Bookstein coordinates (U^B, V^B) corresponding to its shape in the shape space. For example, the equilateral triangles are at $(0, \sqrt{3}/2)$ and $(0, -\sqrt{3}/2)$ (marked E and F). The right-angled triangles are located on the lines $U^B = -0.5, U^B = 0.5$ and on the circle $(U^B)^2 + (V^B)^2 = 0.5$; the isosceles triangles are located on the line $U^B = 0$ and on the circles $(U^B + 0.5)^2 + (V^B)^2 = 1$ and $(U^B - 0.5)^2 + (V^B)^2 = 1$; and the flat triangles (3 points in a straight line) are located on $V^B = 0$.

The plane can be partitioned into two half-planes – all triangles below $V^B = 0$ can be reflected to lie above $V^B = 0$. In addition, each half-plane can be partitioned into six regions where the triangles have their labels permuted. If a triangle has baseline 1, 2 and apex 3 and side lengths d_{12}, d_{13} and d_{23}, then the six regions are

$$d_{23} \geq d_{13} \geq d_{12},$$

$$d_{23} \geq d_{12} \geq d_{13},$$

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$$d_{12} \geq d_{13} \geq d_{23},$$

$$d_{13} \geq d_{12} \geq d_{23},$$

$$d_{13} \geq d_{23} \geq d_{12}.$$

Thus, if invariance under relabelling and reflection of the landmarks was required, then we would be restricted to one of the 12 regions, for example the region AOE, bounded by the arc of isosceles triangles AE, the line of isosceles triangles OE and the line of flat triangles AO in Figure 26.

It is quite apparent from Figure 26 that only a non-Euclidean distance in (U^B, V^B) is appropriate for the shape space. For example, two triangles near the origin that are a Euclidean distance of 1 apart are very different in shape, but two triangles away from the origin that are a Euclidean distance of 1 apart are quite similar in shape.

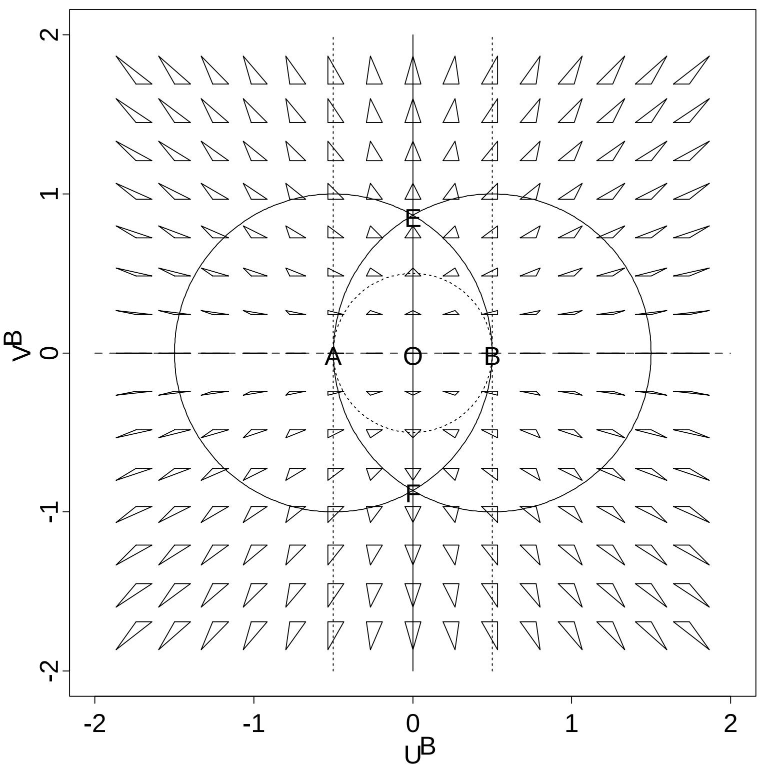

Figure 26 The shape space of triangles, using the Bookstein coordinates (U^B, V^B). Each triangle is plotted with its centre at the shape coordinates (U^B, V^B). The equilateral triangles are located at the points marked E and F. The isosceles triangles are located on the unbroken lines and circles (——-) and the right-angled triangles are located on the broken lines and circles (- - - -). The flat (collinear) triangles are located on the $V^B = 0$ line (the U^B axis). All triangles could be relabelled and reflected to lie in the region AOE, bounded by the arc of isosceles triangles AE, the line of isosceles triangles OE and the line of flat triangles AO.