2
Constructing MDS Representations

An MDS representation is found by using an appropriate computer program. The program, of course, proceeds by computation. But one- or two-dimensional MDS representations can also be constructed by hand, using nothing but a ruler and compass. In the following, we discuss such constructions in some detail for both ratio MDS and for ordinal MDS. This leads to a better understanding of the geometry of MDS. In this context, it is also important to see that MDS is almost always done in a particular family of geometries, that is, in flat geometries.

2.1 Constructing Ratio MDS Solutions

An MDS representation is in practice always found by using an appropriate computer program (see Appendix A for a review of such programs). A computer program is, however, like a black box. It yields a result, hopefully a good one, but does not reveal how it finds this solution.

A good way to build an intuitive understanding for what an MDS program does is to proceed by hand. Consider an example. Table 2.1 shows the distances between 10 cities measured on a map of Europe. We now try to reverse the measurement process. That is, based only on the values in Table 2.1, we want to find a configuration of 10 points such that the distances between these points correspond to the distances between the 10 cities on the original map. The reconstructed map should be proportional in size to the original map, which means that the ratios of its distances

TABLE 2.1. Distances between ten cities.

	1	2	3	4	5	6	7	8	9	10
1	0	569	667	530	141	140	357	396	570	190
2	569	0	1212	1043	617	446	325	423	787	648
3	667	1212	0	201	596	768	923	882	714	714
4	530	1043	201	0	431	608	740	690	516	622
5	141	617	596	431	0	177	340	337	436	320
6	140	446	768	608	177	0	218	272	519	302
7	357	325	923	740	340	218	0	114	472	514
8	396	423	882	690	337	272	114	0	364	573
9	569	787	714	516	436	519	472	364	0	755
10	190	648	714	622	320	302	514	573	755	0

should correspond to the ratios of the values in Table 2.1. This defines the
task of *ratio MDS*. We find the *solution* of this task as follows.

A Ruler-and-Compass Approach to Ratio MDS

For convenience in laying out the map, we first identify those cities that are
farthest from each other. Table 2.1 shows that these are the cities 2 and 3,
whose distance is $d_{23} = 1212$ units. We then want to place two points on a
piece of paper such that their distance is proportional to $d_{23} = 1212$ units.
To do this, we choose a *scale factor*, s, so that the reconstructed map has a
convenient overall size. If, for example, we want the largest distance in the
map to be equal to 5 cm, then $s = 0.004125$ so that $s \cdot 1212 = 5$. All values
in Table 2.1 are then multiplied by s. The scale factor s leaves invariant
the proportions or ratios of the data in Table 2.1.

Having fixed the scale factor, we draw a line segment with a length of
$s \cdot 1212$ cm on a piece of paper. Its endpoints are called 2 and 3 (Figure
2.1).

We now elaborate our two-point configuration by picking one of the re-
maining cities for the next point. Assume that we pick city 9. Where must
point 9 lie relative to points 2 and 3? In Table 2.1 we see that the distance
between cities 2 and 9 on the original map is 787 units. Thus, point 9 must
lie anywhere on the circle with radius $s \cdot 787$ cm around point 2. At the
same time, point 9 must have a distance of $s \cdot 714$ cm to point 3. Conse-
quently, point 9 also must lie on the circle with radius $s \cdot 714$ cm around
point 3 (Figure 2.2). Hence, for point 9, there are exactly two *solutions*—
labeled as 9 and 9′, respectively, in Figure 2.1—that satisfy the conditions
$d_{29} = s \cdot 787$ cm and $d_{39} = s \cdot 714$ cm. We arbitrarily choose point 9.

We continue by adding further points to our MDS configuration. It does
not matter which city we pick next. Assume that it is city 5. Where, relative
to points 2, 3, and 9, should point 5 lie? It should lie on (a) the circle
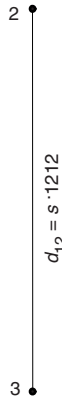around point 2 with radius $s \cdot d_{25}$, (b) on the circle around point 3 with

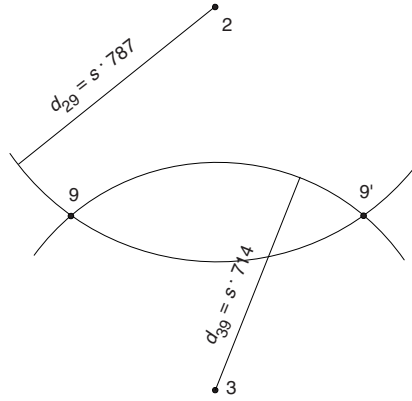FIGURE 2.1. First construction step for MDS representation of distances in Table 2.1.

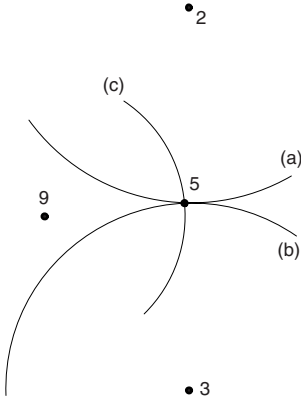FIGURE 2.2. Positioning point 9 on the map.

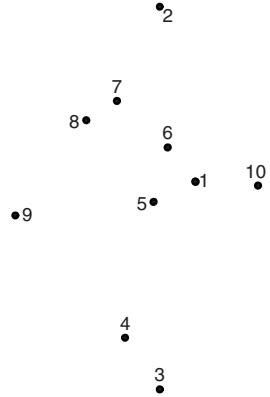FIGURE 2.3. Positioning point 5 on the map.

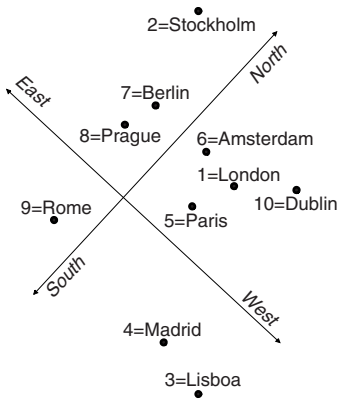FIGURE 2.4. Final MDS representation for data in Table 2.1.

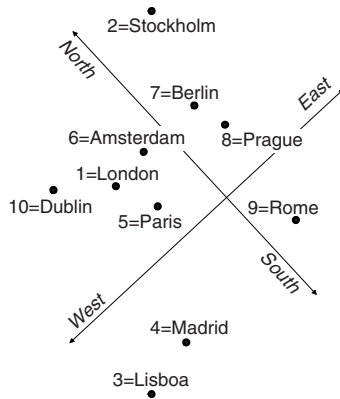FIGURE 2.5. Identification of points and geographical compass.

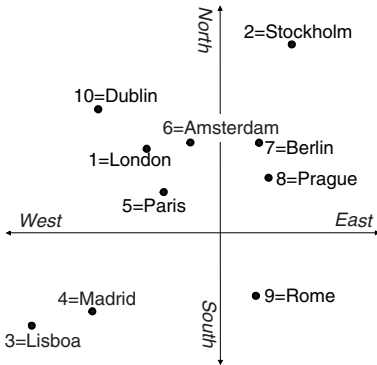FIGURE 2.6. Horizontal reflection of configuration in Fig. 2.5 so that East is to the right.

FIGURE 2.7. Rotation of configuration in Fig. 2.5 so that North is up.
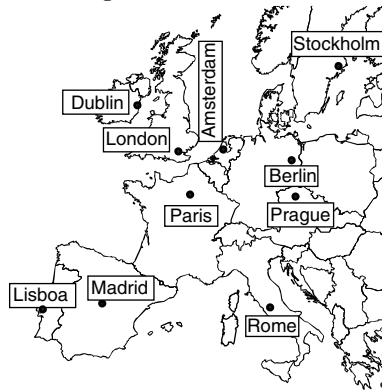

FIGURE 2.8. Configuration of Fig. 2.7 over a map of Europe.

radius $s \cdot d_{35}$, and (c) on the circle around point 9 with radius $s \cdot d_{95}$, as in Figure 2.3. Point 5 satisfies all three conditions and, in contrast to the above construction for point 9, there is only one solution point.

Once all of the cities have been considered, the configuration in Figure 2.4 is obtained. The configuration *solves* the representation problem, because the distances between its points correspond to the distances in Table 2.1, except for an overall scale factor s.

If we replace the numbers with city names, then Figure 2.5 shows that the reconstructed map has an unconventional orientation. But this can be easily adjusted. We first *reflect* the map along the horizontal direction so that West is on the left-hand side, and East is on the right-hand side (Figure

2.6). Second, we *rotate* the map somewhat in a clockwise direction so that the North–South arrow runs in the vertical direction, as usual (Figure 2.7).

Admissible Transformations of Ratio MDS Configuration

The final "cosmetic" *transformations* of the MDS configuration—rotation and reflection—are obviously without consequence for the reconstruction problem, because they leave the distances unchanged (*invariant*). Rotations and reflections are thus said to be *rigid motions*. Another form of a rigid motion is a *translation*, that is, a displacement of the entire configuration relative to a fixed point. A translation of the configuration in Figure 2.7 would, for example, move all points the same distance to the left and leave the compass where it is.

There are two ways to think of rigid motions, the *alibi* and the *alias*. The former conceives of the transformation as a motion of the points relative to a fixed frame of reference (e.g., the pages of this book) and the latter as a motion of the frame of reference relative to points that stay put in their positions in space.

Transformations often make MDS representations easier to look at. It is important, though, to restrict such transformations to *admissible* ones, that is, to those that do not change the relations among the MDS distances that we want to represent in the MDS configuration. *Inadmissible* transformations are, on the other hand, those that destroy the relationship between MDS distances and data. For the problem above, rigid motions are certainly admissible. Also admissible are *dilations*, that is, enlargements or reductions of the entire configuration. Dilations do not affect the ratios of the distances.

Rigid motions and dilations together are termed *similarity transformations*, because they leave the shape (but not necessarily the size) of a figure unchanged. For a better overview, a summary of these transformations is given in Table 2.2. The term *invariance* denotes those properties of geometrical objects or configurations that remain unaltered by the transformation. Instead of rigid motions, one also speaks of *isometries* or, equivalently, of *isometric transformations*. This terminology characterizes more directly what is being preserved under the transformation: the metric properties of the configuration, that is, the distances between its points.

2.2   Constructing Ordinal MDS Solutions

The ruler-and-compass construction in the above attempted to represent the data such that their ratios would correspond to the ratios of the distances in the MDS space. This is called ratio MDS. In *ordinal MDS*, in contrast, one only requires that the order of the data is properly reflected

TABLE 2.2. Two important transformation groups and their invariances.

Transformation Group	Transformations	Invariance
Rigid motion (isometry)	Rotation Reflection Translation	Distances
Similarity transformation	Rotation Reflection Translation Dilation	Ratio of distances

TABLE 2.3. Ranks for data in Table 2.1; the smallest distance has rank 1.

	1	2	3	4	5	6	7	8	9	10
1	–	26	34	25	3	2	14	16	27	5
2	26	–	45	44	31	20	11	17	41	33
3	34	45	–	6	29	40	43	42	36	36
4	25	44	6	–	18	30	38	35	23	32
5	3	31	29	18	–	4	13	12	19	10
6	2	20	40	30	4	–	7	8	24	9
7	14	11	43	38	13	7	–	1	21	22
8	16	17	42	35	12	8	1	–	15	28
9	27	41	36	23	19	24	21	15	–	39
10	5	33	36	32	10	9	22	28	39	–

by the order of the representing distances. The reason for such a weaker requirement is usually that the scale level of the data is taken as merely ordinal. If only greater than and equal relations are considered informative, we could simplify Table 2.1 and replace its values by ranking numbers, because the original data are (order-)equivalent to their ranking numbers. This replacement renders Table 2.3.

Ordinal MDS is a special case of MDS, and possibly the most important one in practice. Thus, we may ask how we can proceed with our geometrical tools, ruler and compass, in constructing such an ordinal MDS solution.

A Ruler-and-Compass Approach to Ordinal MDS

The first step in ordinal MDS remains the same as above. That is, we begin by picking a pair of cities that define the first two points of the configuration. If the cities 2 and 3 are picked as before, we can use Figure 2.1 as our starting configuration. Assume now that we want to add point 9 to this configuration. What can be derived from the data to find its position relative to points 2 and 3?

Clearly, the following holds: point 9 must be closer to 3 than to 2, because the distance d_{39} must be smaller than d_{29}. This follows from Table 2.3,

because the ranking number for the distance of 3 and 9 is 36, whereas the ranking number for the distance of 2 and 9 is 41. (Note that the ranking numbers here are *dissimilarities* or *distance-like* measures; hence, a greater ranking number should lead to a greater distance.) The distances in the MDS configuration are ordered as the data are only if $d_{39} < d_{29}$. Thus, the plane in Figure 2.9 is divided into two *regions* by the perpendicular line through the middle of the line segment that connects points 2 and 3. The shaded area indicates that point 9 must lie in the region below the horizontal line if the condition $d_{39} < d_{29}$ is to be met. We call the set of points below this line the *solution set* or the *solution space* for the problem of placing point 9. Each point of this region, for example, 9, 9′, or 9″, could be chosen as point 9.

But Table 2.3 also requires that point 9 must be closer to 2 than the distance between point 2 and 3, because the rank of pair 2 and 9 is 41 and that of pair 2 and 3 is 45. Hence, $d_{29} < d_{23}$, which means that point 9 must be placed within a circle around point 2 whose radius is somewhat smaller than d_{23}. This condition is graphically illustrated in Figure 2.10 by the circle with radius $\max(d_{29})$, where $\max(d_{29})$ is "somewhat" smaller than d_{23}. Moreover, point 9 must also be placed such that $d_{39} < d_{23}$. This leads to the second circle in Figure 2.10, a circle whose radius is somewhat smaller than d_{23}.

Of course, point 9 must satisfy all three conditions at the same time. Therefore, the desired solution space in Figure 2.11 results from superimposing Figures 2.9 and 2.10.

Comparing Figure 2.2 with Figure 2.11, we see that the second solution is much more *indeterminate*, offering infinitely many possible candidates for point 9, not just two. The reason for this increased indeterminacy lies in the weaker constraints that ordinal MDS puts onto the MDS configuration: only the order of the data, not their ratios, determines the distances in MDS space. In spite of that, point 9 cannot lie just anywhere. Rather, the inequalities have led to "some" reduction of freedom in placing point 9 in the given plane.

We now arbitrarily select one point from the solution set to represent object 9: let this be point 9 in Figure 2.11. We then add a fourth point representing object 5 to the present configuration consisting of points 2, 3, and 9. Table 2.3 says that the resulting configuration must satisfy (a) $d_{25} < d_{29}$, because the corresponding ranking numbers in Table 2.3 are 31 and 41, and because the distances in the MDS representation should be ordered as the data are; (b) $d_{35} < d_{39}$, because for the corresponding ranking we find 29 < 36; (c) $d_{59} < d_{35}$, because 19 < 29; (d) $d_{59} < d_{25}$, because 19 < 31; and (e) $d_{35} < d_{25}$, because 29 < 31. These conditions each induce a boundary line bisecting the plane in Figure 2.12 into a region whose points all satisfy one of the inequalities, and a complementary region whose points violate it. Point 5 must then be so placed that it satisfies all inequality conditions, (a) through (e).
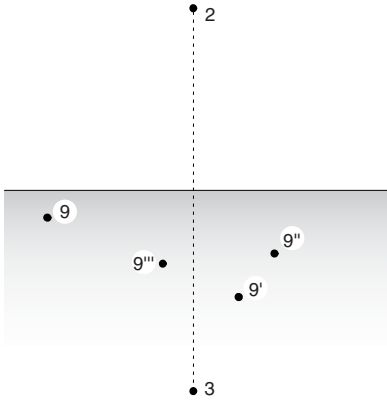
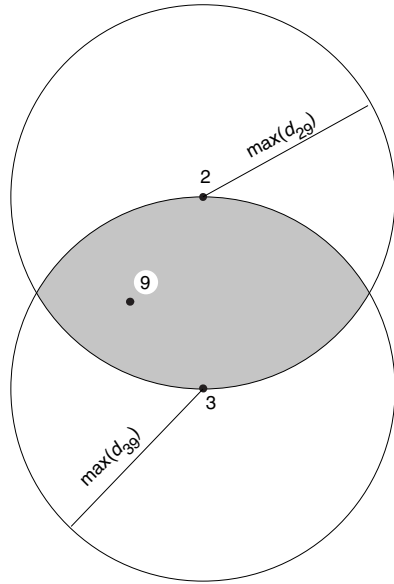FIGURE 2.9. Solution space (shaded) for all points 9 so that $d_{39} < d_{29}$.

FIGURE 2.10. Solution space (shaded) for all points 9 so that $d_{29} < d_{23}$ and $d_{39} < d_{23}$.
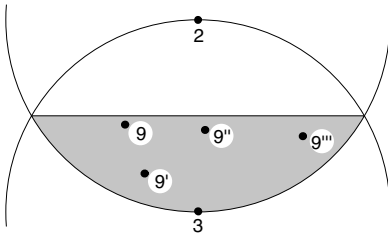

FIGURE 2.11. Solution space (shaded) for all points 9 simultaneously satisfying conditions of Figs. 2.9 and 2.10.
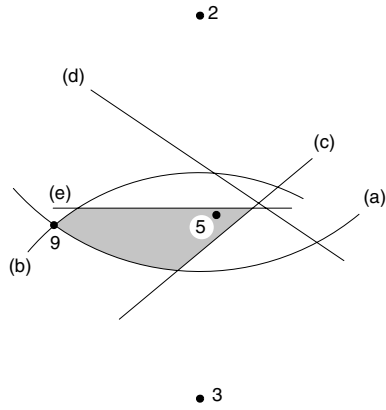

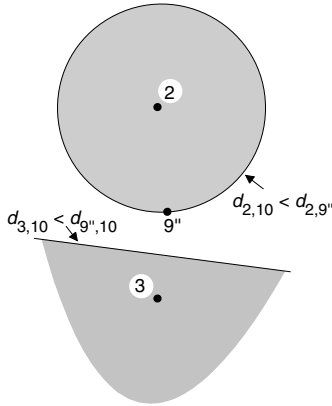FIGURE 2.12. Solution space (shaded) for point 5.

FIGURE 2.13. No point 10 can be placed into the configuration $\{2, 3, 9''\}$ so that it satisfies the shown inequalities.

Figure 2.12 shows the solution space for point 5 as a shaded area. We note that this area is smaller than the solution space for point 9 in Figure 2.11. Hence, the freedom with which we can choose a point for object 5 is less than it was for point 9 in Figure 2.11.

Proceeding in this way, we end up with an MDS representation whose distances are ordered as the ranking numbers in Table 2.3. However, finding this solution turns out not to be as straightforward as it may seem, because our construction method, in practice, would run into dead-end alleys over and over again. We show this in the next section.

Solution Spaces in Ordinal MDS

It may happen that the solution space is *empty*. In the example above, this occurs, for example, if we pick a "wrong" point for 9 in the sense that the chosen point will make it impossible to add *further* points in the desired sense. Consider an example. Assume that we had picked point $9''$ in Figure 2.11. We then would try to add a point for object 10 to the configuration $\{2, 3, 9''\}$. From Table 2.3 we note that point 10 must be closer to 2 than to $9''$, and so it must lie within the shaded circle in Figure 2.13. At the same time, point 10 must also lie below the line that is perpendicular through the midpoint of the line connecting points 3 and $9''$, because point 10 must satisfy the condition $d_{3,10} < d_{9'',10}$. But no point can simultaneously lie below this line and within the shaded circle, and so we see that the solution space for point 10 is empty. Thus, had we decided on point $9''$, we later would have had to reject this point as unacceptable for the enlarged representation problem and start all over again with a new point 9.

We also note that the solution space for each newly added point shrinks in size at a rapidly accelerating rate. Therefore, the chances for picking

wrong points for later construction steps also go up tremendously as each new point is added. Indeed, new points also have, in a way, a backwards effect: they reduce the size of the solution spaces for the old points. Every new point that cannot be properly fitted into a given configuration (as in Figure 2.13) forces one to go back and modify the given configuration until all points fit together.

The shrinkage of the solution spaces as a consequence of adding further points occurs essentially because the number of inequalities that determine the solution spaces grows much faster than the number of points in the configuration. We see this easily from our example: the solution space in Figure 2.11 is defined by three inequalities, namely, $d_{29} > d_{39}, d_{23} > d_{29}$, and $d_{23} > d_{39}$. When point 5 is added, we have four points and six distances. Because every distance can be compared to any other one, the MDS configuration must pay attention to 15 order relations.

More generally, with n points, we obtain $n \cdot n = n^2$ distances d_{ij}. Of these n^2 distances, n are irrelevant for MDS, namely, all $d_{ii} = 0, i = 1, \ldots, n$. This leaves $n^2 - n$ distances. But $d_{ij} = d_{ji}$, that is, the distance from i to j is always equal to the distance from j to i, for all points i, j. Thus, we obtain $(n^2 - n)/2 = (n)(n-1)/2$ relevant distances. This is equal to the number of pairs out of n objects, which is denoted by $\binom{n}{2}$ [read: n-take-2]. But all of these $\binom{n}{2}$ distances can be compared among each other. Consequently, we have (n-take-2)-take-2 or $\binom{\binom{n}{2}}{2}$ order relations (assuming that all values of the data matrix are different). Hence, the ranking numbers for $n = 4$ objects imply 15 inequalities; for $n = 50$, we obtain 749,700 inequalities, and for $n = 100$ there are 12,248,775 inequalities. We can understand intuitively from the sheer number of independent constraints why the ordinal MDS solution is so strongly determined, even for a fairly small n.

Isotonic Transformations

Isotonic transformations play the same role in ordinal MDS as similarity transformations in ratio MDS. Isotonic transformations comprise all transformations of a point configuration that leave the order relations of the distances unchanged (*invariant*). They include the isometric transformations discussed above as special cases.

An ordinal MDS solution is determined *up to*[1] isotonic transformations—just as the ratio MDS configurations are fixed *up to* similarity transformations—because as long as the order of the distances is not changed, any configuration is as good an ordinal MDS representation as any other. However, unless only a very small number of points is being considered, isotonic transformations allow practically no more freedom for changing the point

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[1] "Up to" means that *weaker* transformations which leave even more properties invariant are also admissible.
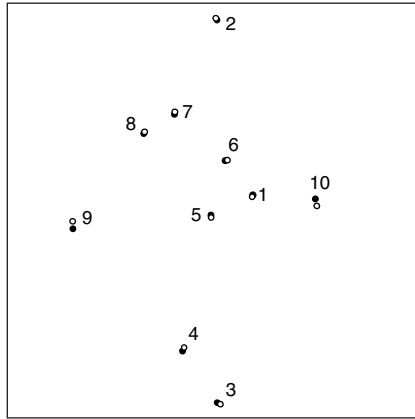
FIGURE 2.14. Comparing ratio MDS (solid points) and ordinal MDS (open circles) after fitting the latter to the former.

locations than isometric transformations. This is a consequence of the rapid shrinkage of the solution sets for the points.[2]

2.3   Comparing Ordinal and Ratio MDS Solutions

The solutions of both the ratio MDS and the ordinal MDS are shown together in Figure 2.14. The solid black points are the ratio MDS solution, and the open circles are the ordinal MDS configuration. We notice that the two configurations are very similar. This similarity has been brought out by admissibly transforming the ordinal MDS configuration so that it matches the ratio MDS configuration as much as possible. That is, leaving the former configuration fixed, we shifted, rotated, reflected, and dilated the ordinal MDS configuration so that its points $1, \ldots, 10$ would lie as close as possible to their respective target points $1, \ldots, 10$ in the ratio MDS configuration. (How this fitting is done is shown in Chapter 20.)

The fact that we obtain such highly similar structures demonstrates that treating the data as ordinal information only may be sufficient for reconstructing the original map. This seems to suggest that one gets something for free, but it really is a consequence of the fact that the order relations in a data matrix like Table 2.3 are on *pairs of pairs* of objects, not just on *pairs* of objects. In the second case, we would have weak information, indeed, and in the first, obviously not.

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[2]The solution sets in ordinal MDS are also called *isotonic regions*, because the distances of each point in this set to a set of particular points outside of this set are ordered in the same way.

Ratio and ordinal MDS solutions are almost always very similar in practice. However, there are some instances when an ordinal MDS will yield a degenerate solution (see Chapter 13). Also, the positions of the points in an ordinal MDS are practically just as unique as they are in ratio MDS, unless one has only very few points. With few points, the solution spaces remain relatively large, allowing for much freedom to position the points (see, e.g., Figure 2.11).

But why do ordinal MDS at all? The answer typically relates to scale level considerations on the data. Consider the following experiment: a subject is given a 9-point rating scale; its categories range from 1 = very poor to 9 = very good; the subject judges three pictures (A, B, and C) on this scale and arrives at the judgments $A = 5, B = 7$, and $C = 1$. Undoubtedly, it is correct to say that the subject has assigned the pictures A and B more similar ratings than A and C, because $|A-B| = 2$ and $|A-C| = 4$. But it is not so clear whether the subject really felt that pictures A and B were more alike in their quality than pictures A and C. The categories of the rating scale, as used by the subject, need not correspond in meaning to the arithmetical properties of the numbers $1, 2, \ldots, 9$. For example, it is conceivable that the subject really only makes a poor-average-good distinction, or that she understands the category "very good" as "truly extraordinary", which might mean that 8 is much farther from 9 than 5 is from 6. In this case, the assigned scores 5, 7, and 1 would have a much weaker interpretability, and we could really only assert that the subject regarded B as best, A as next best, and C as worst.

2.4   On Flat and Curved Geometries

Taking a closer look at the European map in Figure 2.8, one notes that Stockholm has about the same Y-coordinate as points in Scotland. Geographically, however, Stockholm lies farther to the north than Scotland. Hence, the map is incorrect in the sense suggested by the compass in Figure 2.8, because points with the same Y-coordinates generally do not have the same geographical latitude. The distances in Table 2.1 are, on the other hand, correctly represented in Figure 2.8. But these distances were measured on a map printed on the pages of an atlas, and not measured over the *curved* surface of the globe.

Any geographical map that is *flat* is wrong in one way or another. Consider the globe in Figure 2.15, and assume that we want to produce a flat map of a relatively small region of its surface such as, for example, one of the shown spherical rectangles. This can only be done by *projecting* this region onto a flat plane, and any such projection will distort some feature of the original geometry. The usual method, for example, projects the globe's surface (except for the areas close to the poles) by rays emanating
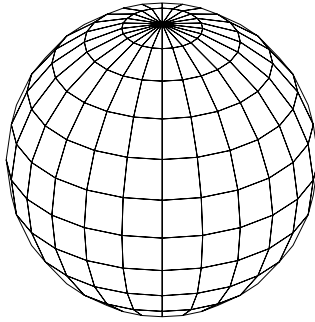
FIGURE 2.15. Globe with meridians (North–South lines) and parallels (East–West lines).

from the globe's center onto the surface of a cylinder that encompasses the globe and touches it on the Equator. The converging meridians—the lines running from the North Pole to the South Pole in Figure 2.15—thus are mapped onto parallel lines on the flat map. This projection properly represents the points' North–South coordinates on the Y-axis of the flat map. It also preserves the points' meridians as lines with the same X-coordinates. However, although the map is quite accurate for small areas, the size of the polar regions is greatly exaggerated so that, for example, Alaska looks much larger than it is. There are many other projections, which are used for different purposes. The map in Figure 2.8 is a projection that preserves area, but it is misleading when one naively reads its X–Y-coordinates as geographical longitude and latitude, respectively.

Anyone who approaches a point configuration first looks at it in the Euclidean sense. Euclidean geometry is *flat* geometry, with the flat plane as its most prominent example. Euclidean geometry is the *natural* geometry, because its properties are what they appear to be: circles look like circles, perpendicular lines look perpendicular, and the distance between two points can be measured by a straight ruler, for example. Euclidean geometry is a formalization of man's experience in a spatially limited environment. Other geometries besides the Euclidean one were discovered only by a tremendous effort of abstraction that took some 2000 years.[3] The surface of the globe

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[3]Euclid, in his *Elements*, had systematically explained and proved well-known theorems of geometry such as the theorem of Pythagoras. The proofs rely on propositions that are not proved (*axioms*). One of these axioms is the parallel postulate. It says that through a point outside a straight line there passes precisely one straight line parallel to the first one. This seems to be a very special axiom. Many attempts were made to show that it is superfluous, because it can be deduced from the other axioms. "The mystery of why Euclid's parallel postulate could not be proved remained unsolved for over two thousand years, until the discovery of non-Euclidean geometry and its Euclidean models revealed the impossibility of any such proof. This discovery shattered the traditional conception of geometry as the true description of physical space ... a new conception

in Figure 2.15 is an example for a *curved* geometry. Distance is measured on the globe not with a straight ruler but with a thread stretched over its surface. This yields the shortest path between any two points and thus defines their distance. Extending the path of the thread into both directions defines a straight line, just as in Euclidean geometry. (From the outside, this path appears curved, but for the earthbound, it is "straight".) On the globe, any two straight lines will meet and, hence, there are no parallels in this kind of plane. Moreover, they will intersect in two points. For example, any two meridians meet both at the North and the South pole. Following any straight line brings you back to the point you started from, and so the globe's surface is a finite but unbounded plane. Another one of its "odd" properties is that the sum of the angles in a triangle on this plane is not a fixed quantity, but depends on the size of the triangle, whereas in Euclidean geometry these angles always add up to 180°.

Thus, the globe's surface is a geometry with many properties that differ from Euclidean geometry. Indeed, most people would probably argue that this surface is not a plane at all, because it does not correspond to our intuitive notion of a plane as a flat surface. Mathematically, however, the surface of the sphere is a consistent geometry, that is, a system with two sets of objects (called points and lines) that are linked by geometrical relations such as: for every point P and for every point Q not equal to P there exists a unique line L that passes through P and Q.

Some curved geometries are even stranger than the sphere surface geometry (e.g., the locally curved four-dimensional space used in modern physics) but none ever became important in MDS. MDS almost always is carried out in Euclidean geometry. If MDS is used as a technique for data analysis, then it is supposed to make the data accessible to the eye, and this is, of course, only possible if the geometric properties of the representation space are what they seem to be. Conversely, if MDS is non-Euclidean, then it is never used as a tool for data explorations. Rather, in this case, the properties of the representing geometry are interpreted as a substantive theory. Curved geometries play a minor role in this context. Drösler (1981), for example, used the properties of a particular two-dimensional constant-curvature geometry to model monocular depth perception. Most non-Euclidean modeling efforts remained, however, restricted to flat geometries such as the city-block plane discussed in Chapter 1, Section 1.4. In this book, we only utilize flat geometries and, indeed, mostly Euclidean geometry, unless stated otherwise.

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emerged in which the existence of many equally consistent geometries was acknowledged, each being a purely formal logical discipline that may or may not be useful for modeling physical reality" (Greenberg, 1980, p. xi).

2.5 General Properties of Distance Representations

A geometry—whether flat or curved—that allows one to measure the distances between its points is called a metric geometry. There are usually many ways to define distances. In the flat plane, the natural way to think of a distance is the Euclidean distance that measures the length of the ruler-drawn line between two points. Another example is the city-block distance as shown in Figure 1.7. These two variants of a distance, as well as all other distances in any geometry, have a number of properties in common. These properties are important for MDS because they imply that proximities can be mapped into distances only if they too satisfy certain properties.

Consider a plane filled with points. For any two points i and j, it holds that

$$d_{ii} = d_{jj} = 0 \le d_{ij}; \tag{2.1}$$

that is, the distance between any two points i and j is greater than 0 or equal to 0 (if $i = j$). This property is called *nonnegativity* of the distance function. Furthermore, for any two points i and j, it is true that

$$d_{ij} = d_{ji}; \tag{2.2}$$

that is, the distance between i and j is the same as the distance between j and i (*symmetry*). Finally, for all points i, j, k, it holds that

$$d_{ij} \le d_{ik} + d_{kj}. \tag{2.3}$$

This *triangle inequality* says that going directly from i to j will never be farther than going from i to j via an intermediate point k. If k happens to be on the way, then (2.3) is an equality.

These properties, which are obviously true for distances in the familiar Euclidean geometry, are taken as the definitional characteristics (*axioms*) of the notion of distance. One can check whether any given function that assigns a numerical value to pairs of points (or to any pair of objects) possesses these three properties.

Consider, for example, the *trivial distance* defined by $d_{ij} = 1$ (if $i \ne j$) and $d_{ij} = 0$ (if $i = j$). To prove that this function is a distance, we have to show that it satisfies the three distance axioms. Starting with nonnegativity, we find that we have $d_{ii} = 0$ for all i by the second part of the definition, and that $d_{ij} > 0$ for all $i \ne j$ by the first part of the definition. Symmetry also holds because the function is equal to 1 for all $i \ne j$. Finally, for the triangle inequality, we obtain $1 < 1 + 1$ if i, j, and k are all different; $1 = 1 + 0$ if $k = j$ and so on. Hence, the left-hand side of the inequality can never be greater than the right-hand side.

Naturally, the trivial distance is not a particularly interesting function. Even so, it can still serve as a nontrivial psychological model. If it is used

as a primitive model for liking, it may turn out empirically wrong for a given set of persons if there are persons who like somebody else more than themselves.

We may also have proximities where $p_{ij} = p_{ji}$ does not hold for all i and j. The proximities, in other words, are not symmetric. Such proximities are rather typical for the social relation "liking" between persons. If such nonsymmetry is observed and if it cannot be interpreted as due to error, then the given data cannot be represented directly in *any* metric geometry. Symmetry, thus, is always a precondition for MDS.

The other properties of distances may or may not be necessary conditions for MDS. If one has observed "self"-proximities for at least two p_{ii}s and if they are not all equal or if any p_{ii} is greater than any p_{ij} (for $i \neq j$) proximity then, strictly speaking, one cannot represent these proximities by any distance. If the proximities violate the triangle inequality, it may or may not be relevant for MDS. In ordinal MDS, it is no problem because adding a sufficiently large constant to all p_{ij}s eliminates all violations (see Section 18.2). In ratio MDS, however, the proximities are assumed to have a fixed origin and no such arbitrary additive constants are admissible. Hence, violations of the triangle inequality are serious problems. If they are considered large enough, they exclude any distance representation for the data.

2.6 Exercises

Exercise 2.1 If you square the correlations in Exercises 1.1, 1.2, or 1.4, and then do ordinal MDS, you obtain exactly the same solutions as for the original values.

(a) Explain why.

(b) Specify three other transformations that change the data values substantially but lead to the same ordinal MDS solutions as the raw data.

(c) Specify a case where such a transformation of the data values changes the ordinal MDS solution.

Exercise 2.2 Specify the admissible transformations for the city-block ordinal MDS solution in Figure 1.7.

Exercise 2.3 Consider the table of distances between five objects below.

Object	1	2	3	4	5
1	0	1.41	3.16	4.00	8.06
2	1.41	0	2.00	3.16	8.54
3	3.16	2.00	0	1.41	8.06
4	4.00	3.16	1.41	0	7.00
5	8.06	8.54	8.06	7.00	0

(a) Use the ruler-and-compass method described in Section 2.1 to construct a ratio MDS solution. Choose the scale factor s equal to 1, so that the distance between points 1 and 4 should be equal to 4 cm in your solution.

(b) Connect points 1 to 2 by a line, points 2 and 3, etc. What pattern emerges?

(c) Verify your solution by using an MDS program. Explain possible differences between the two solutions obtained by hand and by using the computer program.

Exercise 2.4 A psychologist investigates the dissimilarity of the colors red, orange, green, and blue. In a small experiment, she asks a subject to rank the six pairs of colors on their dissimilarity (1 = most similar, 6 = most dissimilar). The resulting table of ranks is given below.

Item	R	O	G	B
Red	–			
Orange	1	–		
Green	3	2	–	
Blue	5	6	4	–

The psychologist wants to do an ordinal MDS in two dimensions on these data but does not have an MDS program for doing so. So far, she has found the coordinates for Red (0, 3), Orange (0, 0), and Green (4, 0).

(a) Use the ruler-and-compass method described in Section 2.2 to find a location for point Blue that satisfies the rank-order of the data. Specify the region where Blue may be located.

(b) Interpret your solution substantively.

(c) Suppose that none of the coordinates were known. Try to find an ordinal MDS solution for all four points. Does this solution differ from the one obtained in (a)? If so, explain why.