

# Escape from Boxland

## Generating a Library of High-Dimensional Geometric Shapes

Barret Schloerke, Hadley Wickham, Dianne Cook, and Heike Hofmann

**Abstract** A library of common geometric shapes can be used to calibrate your eyes for understanding data structure in high-dimensional Euclidean space. This article describes the methods for producing cubes, spheres, simplexes, and tori in multiple dimensions. It also describes new ways to define and generate high-dimensional tori. The algorithms are described, critical code chunks are given, and a large collection of generated data are provided. These are available in the R package `geozoo`, and selected movies and images, are available on the GeoZoo web site (<http://schloerke.github.io/geozoo/>).

## Introduction

This paper describes how to build a library of high-dimensional geometric shapes: cubes, spheres, simplexes, and tori. Data describing numerous 4D polytopes and polyhedra generated by other researchers are included in the library. The purpose is to enable people to calibrate their eyes for understanding data structures residing in high-dimensional Euclidean space. This work extends the work described in Cook (1997) which concentrated on samples from statistical distributions.

The `geozoo` package in R (R Development Core Team, 2003) contains the code to create the geometric shapes. Code fragments, describing the key components of the algorithms for generating the shapes, are included in this paper. The shapes in the library are best viewed using the dynamic graphical method called a tour (Asimov, 1985; Buja et al., 2005; Cook et al., 2007), such as that available in GGobi (Swayne et al., 2003) and the `tourr` R package (Wickham et al., 2011).

The structure of the paper is that basic shapes are described first followed by more complex shapes, in this order, cubes, spheres, simplexes, polyhedra, polytopes, tori.

## Cubes

Cubes are the first shape that a person should examine when starting to learn about higher dimensions. Cubes are relatively simple to understand: they have orthogonal, uniform length sides and they are convex shapes. A 1-D cube is a line segment. A 2-D cube is a square and a 3-D cube is a box.

The 4-D cube may be hard to imagine, partly because we are accustomed to describing our physical world using only three dimensions. The leap to 4-D is more understandable after watching the movie “Flatland” (Martin, 1965) or reading the novella of the same name (Abbott, 1884). In “Flatland”, the world is 2-D and characters struggle with the concept of 3-D.

Working from this name, we might think of our world as “Boxland”: we live in 3-D and see struggle with the concept of higher dimensions. Shadows created by light sources help perceive the third dimension. In Flatland, the inhabitants see only 1-D line segments. For a Flatlander who has never seen the world we live in, the third dimension is hard to understand. Similarly, for inhabitants of our world, it might seem daunting to imagine the fourth dimension. But it’s not that difficult!

Figure 1 shows the evolution of the cube from 2-D to 5-D. Each figure is a projection of a wireframe cube from two to five dimensions. To increase the dimension, double the cube and connect the corresponding vertices. The 3-D cube grows from  $2 \times 2$ -D squares, connected with four more edges. The 4-D cube is born from  $2 \times 3$ -D cubes and a 5-D cube emerges from  $2 \times 4$ -D cubes.

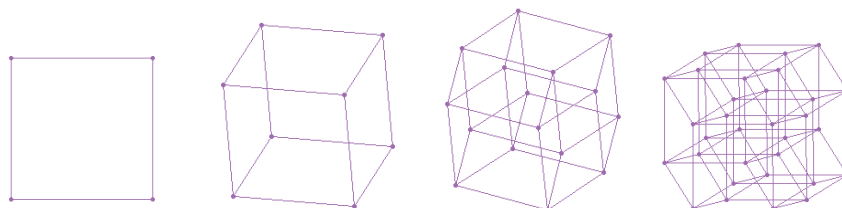


Figure 1: Wireframe cubes, (from left to right) 2-D, 3-D, 4-D, 5-D.

An alternative way to think of a high-dimensional cube is that it can be considered to be all

permutations of binary digits (0 and 1) in  $p$ -D. A line is defined by two points: (0), (1). A square is defined by four points: (0,0), (0,1), (1,0), (1,1), which are all of the permutations of 0 and 1 in two columns, that is, the Cartesian product of two lines. A 3-D cube is the Cartesian product of two squares, and has all of the permutations of 0 and 1 in three columns.

### Points on Vertices

The two different ways to define a high-dimensional cubes leads to two different methods to create a  $p$ -D cube. Both methods yield the same result, which is shown for  $p = 1, 2, 3$  in Table 1.

1-D:

row #	1	edges
1	0	2
2	1	

2-D:

row #	1	2	edges
1	0	0	2 3
2	1	0	4
3	0	1	4
4	1	1	

3-D:

row #	1	2	3	edges
1	0	0	0	2 3 5
2	1	0	0	4 6
3	0	1	0	4 7
4	1	1	0	8
5	0	0	1	6 7
6	1	0	1	8
7	0	1	1	8
8	1	1	1	

**Table 1:** 1-D, 2-D and 3-D cube vertices and edges.

- **Method 1:** Recursively double a lower-dimensional cube.

Using the standard coordinate system, the base is 0 and 1. After establishing the base, we recursively double the base in the first column(s), and add an additional column containing a 0 in the first half of the rows and a 1 in the second half of the rows. The process is repeated  $(p - 1)$  times, to obtain a  $p$ -D cube.

```
cube_iterate <- function(p) {
  if (p == 1) {
    return(rbind(0, 1))
  }
  lower_dim_cube <- cube_iterate(p - 1)
  rbind(
    cbind(lower_dim_cube, 0),
    cbind(lower_dim_cube, 1)
  )
}
```

- **Method 2:** Generate all permutations of 0,1 in  $p$  columns.

This method takes advantage of an existing function in R, `expand.grid`. It produces all permutations by generating the Cartesian product of a set of vectors. For our purposes, the number of columns is not fixed, so we use `do.call`, to convert a function call of the form `x(a,b,c)` to `do.call(x, list(a,b,c))`, allowing specification of an arbitrary number of arguments.

```
cube_permute <- function(p) {
  as.matrix(
    do.call(
      expand.grid,
      rep(list(c(0, 1)), p)
    )
  )
}
```

### Completing the Wire Frame

The wire frame for a cube draws the edges of the cube, connecting all points that differ in one of the values, e.g. (0,0,0) and (1,0,0), or (0,0,0) and (0,1,0) for a 3-D cube. Each edge is a vector of length 1, and it is defined by specifying the row numbers of the two corresponding elements of the vertex data,

e.g. in a 3-D cube (2, 4) would connect rows (1, 0, 0) and (1, 1, 0). Table 1 gives vertex and edge lists for  $p = 1, 2$  and 3. Edges are not ordered  $(1, 2) = (2, 1)$ , and we use just one of the two, with the smaller number first. Here are three ways to generate an edge set, the last being the most computationally efficient but less intuitive.

- **Method 1:** Distance of 1.

The distance between all  $p * (p - 1) / 2$  pairs of vertices is computed, and those pairs of vertices which have distance 1 are returned. This is the simplest approach but obviously slow to compute as  $p$  increases.

```
cube_edges_length1 <- function(cube) {
  p <- ncol(cube)
  num_points <- 2 ^ p
  from_to <- matrix(NA, nrow = num_points * p / 2, ncol = 2)
  next_store_position <- 1
  for (i in 1:(num_points - 1)) {
    for (j in (i + 1):num_points) {
      d1 <- sum((cube[i, ] - cube[j, ]) ^ 2)
      if (d1 == 1) {
        from_to[next_store_position, ] <- c(i, j)
        next_store_position <- next_store_position + 1
      }
    }
  }
  from_to
}
```

- **Method 2:** The binomial approach.

This is faster to compute than the first method because it involves only a single loop over the cube vertices. For this approach to work, the vertices of the cube need to have been created using the methods described in Section 2.2.1. Each vertex, that has  $c$  elements equal to 0, will be connected to  $c$  other vertices, and we need to determine the row numbers for these other vertices. (The row number for a corresponding connected vertex is obtained by adding  $2^{(j-1)}$ ,  $j = 1, \dots, p$ , if column  $j$  contains a 0, to the row number,  $i$ ,  $i = 1, \dots, (\#vertices - 1)$  of the originating vertex.) For example, for a 3-D cube, the first vertex (0, 0, 0) will be connected to vertices  $2^0 + 1 = 2$ ,  $2^1 + 1 = 3$  and  $2^2 + 1 = 5$ .

```
cube_edges_binomial <- function(cube) {
  p <- ncol(cube)
  num_points <- 2 ^ p
  from_to <- matrix(NA, nrow = num_points * p / 2, ncol = 2)
  next_store_position <- 1
  for (i in 1:(num_points - 1)) {
    for (j in 1:p) {
      if (cube[i, j] == 0) {
        from_to[next_store_position, ] <- c(i, 2 ^ (j - 1) + i)
        next_store_position <- next_store_position + 1
      }
    }
  }
  from_to
}
```

- **Method 3:** Binary relationships.

The final method is the most computationally efficient, but the least intuitive. Here we will use the fact that the vertices of the cube can be represented as binary numbers, e.g.  $(0, 1, 1) = 011_2 = 3_{10}$ . This allows us to both vectorize the code, and use the very fast C bitwise operations provided by the **bitops** package.

The key insight is to note that edges connect vertices which have a single bit flipped. For example, 011 connects to 111, 001 and 010 (vertex 3 connects to 7, 1, and 2). We can flip a single bit with the exclusive or function,  $011 \oplus 100 = 111$ ,  $011 \oplus 010 = 001$ ,  $011 \oplus 001 = 010$ . This leads to a fast and efficient method for generating the edges.

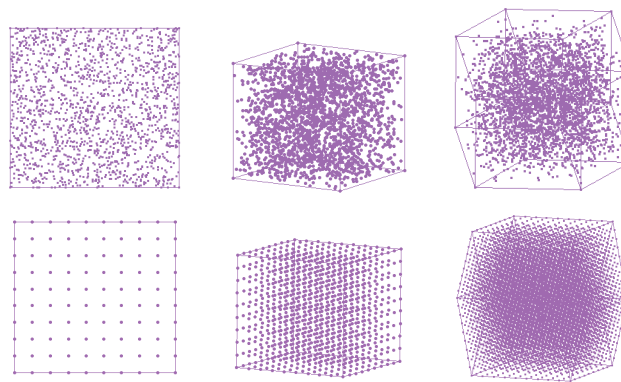
```

library(bitops)
cube_edges_binary <- function(p) {
  vertices <- 0:(2 ^ p - 1)
  from_verts <- vertices[
    rep(1:(2 ^ p), each = p)
  ]
  from_to <- data.frame(
    from = from_verts,
    to = bitXor(from_verts, 2 ^ (0:(p - 1)))
  )
  from_to <- subset(from_to, from < to) + 1
  from_to
}

```

## Solid Cube

A solid cube has points in the interior (Figure 2). It is easy to generate, using either random sampling or a fixed grid.



**Figure 2:** Solid cubes in 2-D, 3-D, and 4-D (top) independent random samples from  $p$  uniform distributions (bottom) fixed grid. As dimension increases, the vertices look sparse, more so with the random samples.

- **Method 1:** Random uniform.

The R function `runif` function generates samples from a uniform distribution between 0 and 1. Generating  $p$  random uniform values creates a  $p$ -dimensional vector corresponding to a point inside a  $p$ -dimensional cube. The number of points needed to make the cube appear solid increases as  $p$  increases, exponentially. For example, a 3-D cube with  $k$  points on each side has  $k^3$  total points, and a 4-D cube with the same  $k$  points per side  $k^4$  total points. Thus the number of points must be increased substantially for each increase in dimension, for the shape to look similarly solid. In our function, we use a base of 850 points, and the total number of points is capped at 50000 points for speed of viewing.

```

cube_solid_random <- function(p, n = 850 * 2 ^ p) {
  matrix(runif(n * p), ncol = p)
}

```

- **Method 2:** Equidistant.

A solid cube can also be generated with equidistant points. As with the second vertex generation method the `expand.grid` function is used. The input  $n$  allows the number of grid points to be varied.

```

cube_solid_grid <- function(p, n) {
  grid <- list(seq(0, 1, length = n))
  do.call(expand.grid, rep(grid, p))
}

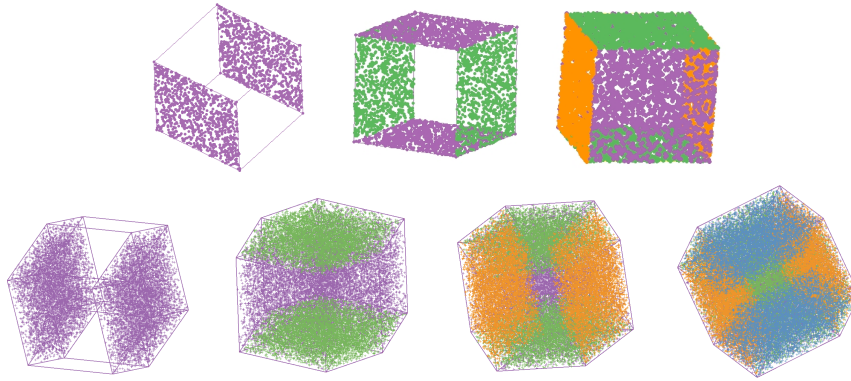
```

There are advantages and disadvantages. The first method, random points, produces a solid cube that looks more solid, but as  $p$  increases, points near the vertices become more scarce. With equidistant points the filled cubes better fills the vertex regions, but the structure produces regular patterns which can be distracting to a viewer.

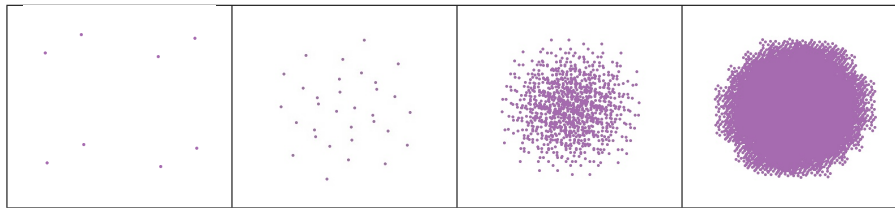
## Hollow Cube

The “face” of a cube is a surface that is one dimension lower than that of the cube. For example, a face of a 3-D cube is a 2-D square and a face of a 4-D cube is a 3-D cube. To generate points on the faces of a cube, random points are created in all dimensions except one. The last dimension is given the value of 0 or 1, to create the opposing faces.

For a 3-D cube, the  $X_1$  and  $X_2$  components of the cube are given random values and the  $X_3$  components would be set to 0 in the first half and 1 in the second half. The process would then be repeated for the remaining columns, as shown in Figure 3. This will create six 2-D squares which form the faces of a 3-D cube. The bottom row shows the faces of a 4-D cube being built. The left side plot shows the first pair of faces, a solid 3-D cube in  $X_1, X_2, X_3$ , with fixed values on the fourth dimension  $X_4$ . The subsequent plots show the remaining faces.



**Figure 3:** Faces of a 3-D cube (top row) and a 4-D cube (bottom row), obtained by fixing one column of values to be 0 or 1, and allowing the other columns to vary freely between 0 and 1.



**Figure 4:** Vertices of cubes, (left to right) 3-D, 5-D, 10-D, and 15-D. Cubes look more rounded in projections as the dimension increases.

## High-D Cubes Look Spherical!

As the dimension increases, the shape the cube takes in a 2-D projection looks more rounded than square. The reason is explained in [Diaconis and Freedman \(1984\)](#) and is related to the Central Limit Theorem. When we use a tour to visualize high-dimensional data we examine low-dimensional projections. Consider the axes for a  $p$ -dimensional space labeled as  $X_1, \dots, X_p$ . A 1-D projection is generated by taking a linear combination of these axes, such as  $a_1 X_1 + \dots + a_p X_p$ . The squared values of  $a_j, j = 1, \dots, p$  are constrained to sum to 1. As  $p$  increases, the combining the values operates like averaging the values in many dimensions, resulting in views that look Gaussian. Another way to think about it is that we are looking at rotated cubes rather than a cube through its square face and this gets increasingly rounded as the dimension of increases.

## Spheres

A sphere can be described as all points within a fixed radius of zero,  $\{X : X_1^2 + \dots + X_p^2 \leq 1\}$ . A hollow sphere is the set of points with radius equal to 1,  $\{X : X_1^2 + \dots + X_p^2 = 1\}$ . Generating the hollow sphere is simpler than the solid sphere.

## Hollow Sphere

To generate points uniformly distributed on the surface of a sphere we use a trick: First, generate a random vector from a multivariate standard normal distribution and then normalize its length. The top row of Figure 5 shows the results.

```
norm_vec <- function(x) {
  x / sqrt(sum(x ^ 2))
}

sphere_hollow <- function(p, n = p * 500) {
  x <- matrix(rnorm(n * p), ncol = p)
  t(apply(x, 1, norm_vec))
}
```

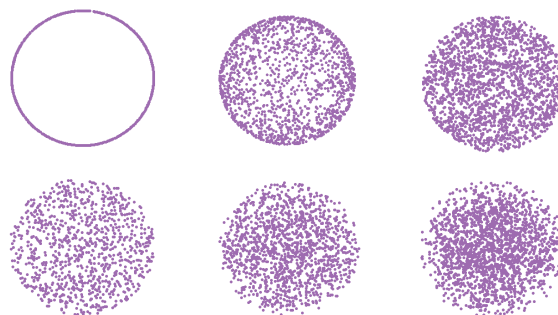


Figure 5: Hollow (top row) and solid spheres (bottom row) for 2-D, 3-D, 4-D.

## Don't Reject the Solid Sphere!

Solid spheres can be generated in much the same way as solid cubes; use random points to fill the object. While the solid cube fills the box, the sphere's points are inside a radius of 1 from the center. A simple approach would be to use a rejection method: generate points in the solid cube and discard those with radius more than 1. This is problematic as  $p$  increases. Most points will eventually be rejected. For example, to generate the points of a 3-D sphere, around 50% of the points are kept, but for a 10-D sphere only 0.25% of the points are kept. The space in the corners of the box, outside the sphere increases dramatically with  $p$ .

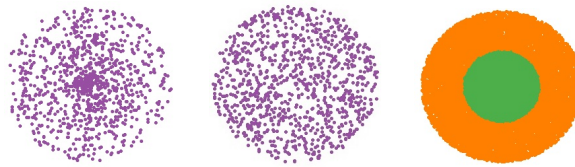
The approach we used is a minor modification to the method used to generate a hollow sphere. Figure 5 illustrates the process. The vector length is randomly sampled from a uniform distribution on  $(0, 1)$  (left plot). The result is raised to the power  $1/p$  to adjust for the volume increase with  $p$ , resulting in points spread evenly throughout the inside of the sphere (middle plot). Taking the sphere to the  $1/p$  power may seem ad hoc, but the operation ensures that the density is uniform within the sphere. To see this, compare circles of radius 1 and 2 (right plot). The area of the smaller circle equals  $\pi = 1^2\pi$ . The area of the whole circle equals  $4\pi = 2^2\pi$ . This is four times as large, but only twice the radius. Thus without accounting for radial distance more points will be generated closer to the center than is warranted by the area. Raising the vector length to the power  $1/p$ ,  $1/2$  in our example, corrects for the volume.

```
sphere_solid_random <- function(p, n = p * 500) {
  sphere_hollow(p, n) * runif(n) ^ (1 / p)
}
```

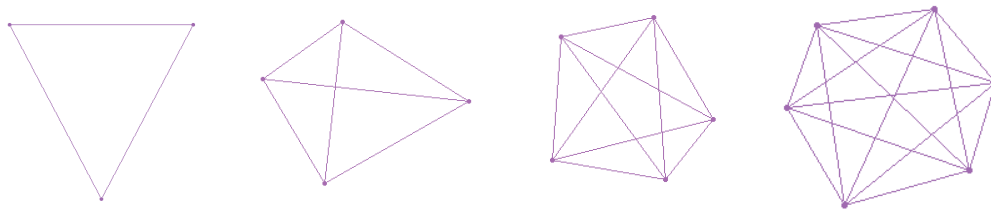
## Simplexes

Simplexes are one of the simplest objects to create and view. A  $p$ -D simplex is a shape that lives in one dimension less than  $p$ . It has vertices corresponding to the coordinate axes. The simplex vertices are then projected, using a Helmert matrix, into the  $(p - 1)$ -dimensional space in which it exists.

For example, a 3-D simplex has vertices at  $(1,0,0)$ ,  $(0,1,0)$ ,  $(0,0,1)$ , which are reduced by the Helmert transformation to points a 2-D equilateral triangle,  $(0.7071, 0.4082)$ ,  $(-0.7071, 0.4082)$ ,  $(0.0000, -0.8165)$ .



**Figure 6:** Solid sphere in 2-D: (left) generated randomly results in an over-concentration of points in the center, (middle) adjusted for volume generates a uniform distribution inside the sphere, and (right) comparison of areas of circles of radius 1 and 2.



**Figure 7:** Wireframe simplexes: 2-D, 3-D, 4-D, 5-D.

```
helmert <- function(d) {
  helmert_mat <- matrix(NA, nrow = d, ncol = d)
  helmert_mat[1, ] <- rep(1 / sqrt(d), d)
  for (i in 1:(d - 1)) {
    helmert_mat[i + 1, ] <- c(
      rep(1 / sqrt(i * (i + 1))), i),
      -i / sqrt(i * (i + 1)),
      rep(0, d - i - 1)
    )
  }
  helmert_mat
}

simplex <- function(p) {
  x <- diag(p)
  # center simplex
  x <- x - matrix(1 / p, p, p)
  hm <- helmert(p)
  final <- (x %*% t(hm))[, -1]
  final
}
```

The wire frame for a simplex connects every point to every other point, and can be computed in just two lines of code, following method 2 of the cube vertices. It makes a list of all combinations of each row number and then removes the lines that connect a point to itself.

```
simplex_wires <- function(simplex) {
  wires <- do.call(
    expand.grid,
    list(
      c(1:nrow(simplex)),
      c(1:nrow(simplex))
    )
  )
  wires[!wires[,1] == wires[,2],]
}
```

## Polyhedra

A polyhedron is a three dimensional object that contains straight edges and has flat faces. Our polyhedra data comes from George W. Hart's website ([Hart, 2000](#)). Hart's website contains an extensive



collection of polyhedra, ranging from Platonic Solids to Stellations of the Rhombic Triacontahedron. In our data sets, we used the information from Platonic Solids, Kepler-Poinsot Polyhedra, Archimedean Polyhedra and its duals, Prisms. The data was reformatted from VRML into XML. The vertices and wire frames from separate files were compiled into tables. Some reformatting of edges was also necessary.

## Surfaces and Curves

Paul Bourke's website (Bourke, 1996) has equations for generating several famous objects, including the Mobius Strip, Steiner's Roman Surface and the Klein Bottle (Figure 8). It is interesting to see how each object twists onto itself. R functions based on these equations were written to produce each object. Each object was rendered by points on the surface. For each shape, a set of random angles were generated to seed the equations, producing points on the surface. For some of the objects, to view the object in its familiar form the plot limits for each variable need to use the global minimum and maximum values.

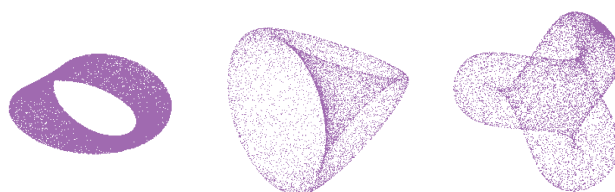


Figure 8: Mobius strip, Steiner's roman surface, and Boy's surface.

## Polytopes

A polytope is a generalized term of a geometric shape in any dimension. A polygon is a 2-D polytope. A polyhedron is a 3-D polytope. A polychoron is a 4-D polytope. Beyond that we typically use polytope to refer to any  $p$ -gon. Our polychoron data comes from Paul Bourke's website (Bourke, 2003), where there is also information on some of the objects that have been covered (hypercube, simplex) in the preceding sections of this paper, and new objects, 24-cell, 120-cell, 600-cell (Figure 9). The explanations of these polytopes is very clear. The data has been formatted into XML files allowing descriptions of the vertices and edges for each shape.

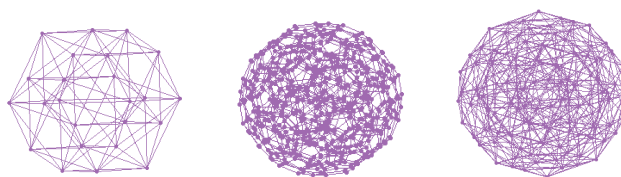


Figure 9: 24-Cell, 120-Cell, and 600-Cell.

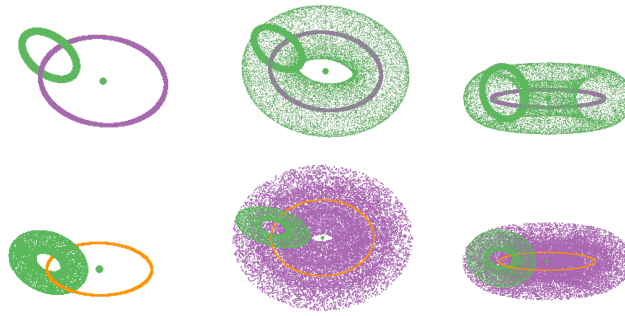
## Tori

A "doughnut" torus is known as a ring torus. Paul Bourke's website (Bourke, 1990) on "The Torus and Super Torus" provides the inspiration. The website explains how the 3-D torus is made.

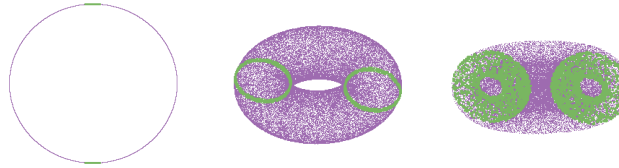
It also contains information that we used to develop the process of building high-dimensional tori. Figure 10 shows this process: a smaller circle that follows a larger circle, creating a doughnut. The points for the torus are formed by polar coordinates.

To produce a 4-D torus, a 3-D torus is rotated around a circle into the fourth dimension (Figure 10 bottom row). This torus still has a hole in the center. A way to think about the process is a recursive circle system. For a 3-D torus, the smaller radius circle follows the larger radius circle. For a 4-D torus, a 3-D torus follows an even larger radius circle. That is, the lower-dimensional torus is shifted a fixed distance and rotated about a *new* axis perpendicular to the axis of the hole. The next two sections describe the process in detail.





**Figure 10:** Generating a torus: 2-D to 3-D (top row), and 3-D to 4-D (bottom row).



**Figure 11:** 2-D, 3-D, and 4-D tori with features highlighted.

### Ring Torus

A ring torus has a hole in the center of the object. It is generated recursively. A 2-D circle forms the base of the torus, which is defined by:

$$\begin{aligned} X_1 &: \cos(\theta_1) * r_1 \\ X_2 &: \sin(\theta_1) * r_1 \end{aligned}$$

using one radius and one angle. The 3-D torus is defined by:

$$\begin{aligned} X_1 &: \cos(\theta_1) * (r_1 + \cos(\theta_2) * r_2) \\ X_2 &: \sin(\theta_1) * (r_1 + \cos(\theta_2) * r_2) \\ X_3 &: \sin(\theta_2) * r_2 \\ r_1 &> r_2 \end{aligned}$$

Notice how the 3-D torus builds from the 2-D:  $r_1$  is replaced by  $(r_1 + \cos(\theta_2)r_2)$ . The 3-D torus has four parameters: two angles and two radii. The third dimension is formed entirely by the additional angle and radius. A 4-D torus will be generated with the same pattern as the 3-D torus: a new dimension will be added and material will be inserted recursively into the formulas:

$$\begin{aligned} X_1 &: \cos(\theta_1) * (r_1 + \cos(\theta_2) * (r_2 + \cos(\theta_3) * r_3)) \\ X_2 &: \sin(\theta_1) * (r_1 + \cos(\theta_2) * (r_2 + \cos(\theta_3) * r_3)) \\ X_3 &: \sin(\theta_2) * (r_2 + \cos(\theta_3) * r_3) \\ X_4 &: \sin(\theta_3) * r_3 \\ r_1 &> r_2 > r_3 \end{aligned}$$

The patterns to the higher-dimensional torus generation are:

1. add a new dimension each time.
2. insert material on the inside of each equation, except for the new dimension.
3. the newest radius will always be smaller than the previous radii.

This is not easy to recurse, though. Inserting more material inside a formula after it has been formed is not simple. By rearranging the formulas, a better method is achieved:

$$\begin{aligned}
X_1 &: ((\cos(\theta_3) * r_3 + r_2) * (\cos(\theta_2) + r_1) * \cos(\theta_1)) \\
X_2 &: ((\cos(\theta_3) * r_3 + r_2) * (\cos(\theta_2) + r_1) * \sin(\theta_1)) \\
X_3 &: (\cos(\theta_3) * r_3 + r_2) * \sin(\theta_2) \\
X_4 &: \sin(\theta_3) * r_3 \\
r_1 &> r_2 > r_3
\end{aligned}$$

Here's the first step of the recursion, starting from the last dimension.

$$\begin{aligned}
X_1 &: \cos(\theta_3) * r_3 \\
X_2 &: \cos(\theta_3) * r_3 \\
X_3 &: \cos(\theta_3) * r_3 \\
X_4 &: \sin(\theta_3) * r_3
\end{aligned}$$

which translates to this R code:

```

torus<-c(
  rep(cos(theta[p - 1]) * radius[p - 1], p - 1),
  sin(theta[p - 1]) * radius[p - 1]
)

```

From this start, we recurse backwards from  $p - 1$  to 2. A new radius is added at each iteration which is multiplied with the previous equation by the cosine of an angle. The final step adds a last radius and multiplies the result by the sine of the new angle.

```

for (i in (p - 1):2) {
  for (j in (i - 1):1) {
    torus[j] <- (torus[j] + radius[i - 1]) * cos(theta[i - 1])
  }
  torus[i] <- (torus[i] + radius[i - 1]) * sin(theta[i - 1])
}

```

Here is how the recursion builds the 4-D torus:

$$\begin{aligned}
p &= 4 \\
\text{Base} \\
X_1 &: \cos(\theta_3) * r_3 \\
X_2 &: \cos(\theta_3) * r_3 \\
X_3 &: \cos(\theta_3) * r_3 \\
X_4 &: \sin(\theta_3) * r_3 \\
\\ 
i &= p - 1 = 3 \\
j &= 2 : 1 \\
X_1 &: (\cos(\theta_3) * r_3 + r_2) * \cos(\theta_2) \\
X_2 &: (\cos(\theta_3) * r_3 + r_2) * \cos(\theta_2) \\
X_3 &: (\cos(\theta_3) * r_3 + r_2) * \sin(\theta_2) \\
X_4 &: \sin(\theta_3) * r_3 \\
\\ 
i &= 2 \\
j &= 1 : 1 \\
X_1 &: ((\cos(\theta_3) * r_3 + r_2) * \cos(\theta_2) + r_1) * \cos(\theta_1) \\
X_2 &: ((\cos(\theta_3) * r_3 + r_2) * \cos(\theta_2) + r_1) * \sin(\theta_1) \\
X_3 &: (\cos(\theta_3) * r_3 + r_2) * \sin(\theta_2) \\
X_4 &: \sin(\theta_3) * r_3
\end{aligned}$$

This code results in one row of data for one point on the 4-D torus for each value of angle. By varying the angle and binding the result we get points over the surface of the torus:

```
finished <- rbind(finished, torus.row)

or

matrix(
  do.call(rbind, as.list(
    replicate(
      n,
      torus.row(radius, p)
    )
  )),
  ncol = p, byrow = TRUE
)
```

The angles create the rings, and thus need to vary fully between 0 and  $2\pi$ :

```
theta <- runif(p - 1, min = 0, max = 2 * pi)
```

The radii for the process are fixed at the start. To produce a hole in each dimension the radii need to decrease with  $p$ . We set the hole to have a size of 1 in every dimension, and the radii are a power of 2 less than the previous dimension.

```
radius <- 2 ^ ((p - 2):0)
```

This produces points fairly evenly, but not uniformly spread on the surface of the torus. A more regular way to form a torus is to form the angles into a set of intervals, resulting in more circular patterns.

### Flat Torus

Another common hyper-torus is the flat torus. A flat torus is commonly seen expanding into infinity as a screen saver on some computers. It has multiple holes in the center. It is easy to generate.

A flat torus is formed in pairs of dimensions, defined by a sine and cosine of one angle, for example the circle is generated in 2-D by  $\cos(\theta_1)$  and  $\sin(\theta_1)$ . A flat torus in any dimension is created from multiple pairs of sine and cosine, e.g. a 1-D torus is generated by one pair, a 2-D torus by two pairs, four variables, and a 3-D torus by three pairs, six variables (Figure 12). All values of sine and cosine are generated from angles,  $(-2\pi, 2\pi)$ , separately for each pair. The flat torus has an even number of dimensions, but an effective dimension half that size. Figure 13 illustrates the construction.

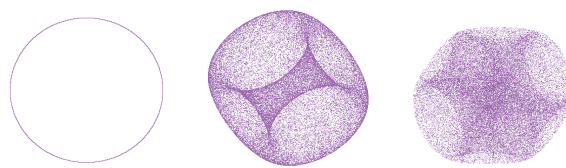


Figure 12: Flat tori in 2-D, 4-D, and 6-D.

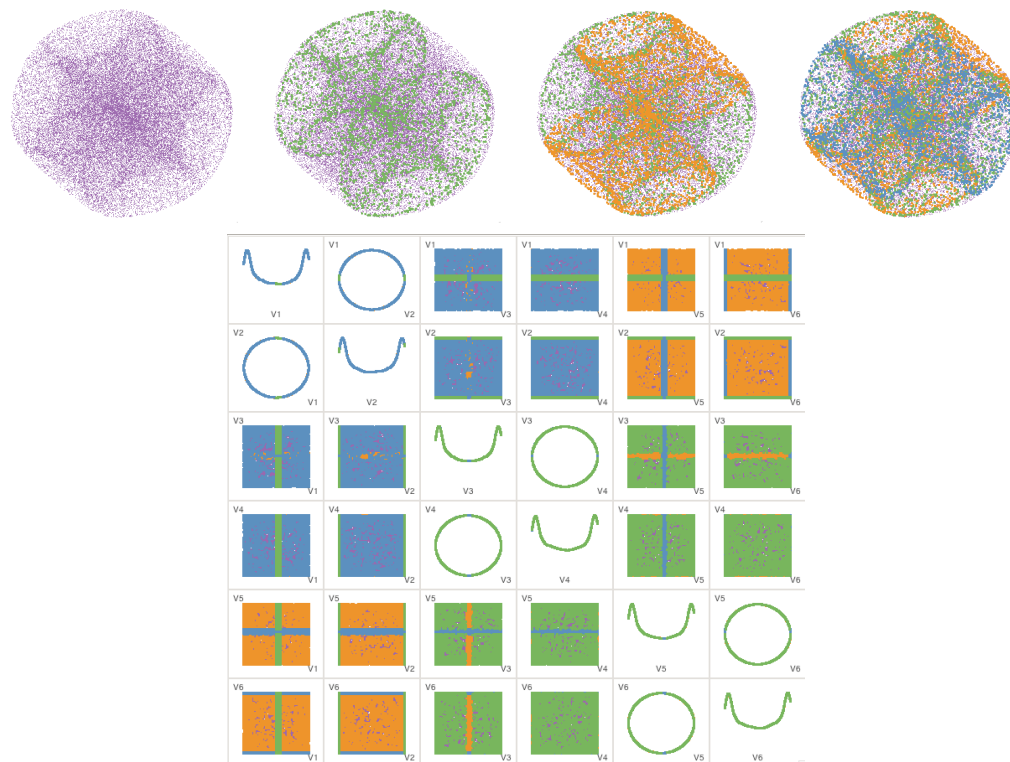
### Solid

These tori are all hollow. To create points in the interior of the tori one would randomly generate the smallest radii in the hyper-ring torus and all radii in the flat torus.

### Conclusion

This paper has described how **geozoo** generates several types of high-dimensional geometric shapes. The result is a library designed to help conceptualize objects in high-dimensional spaces. It has also led to some new geometric shape definitions.

This library, although seemingly removed from real high-dimensional data has some strong connections. Much of our data analytic methods are based in high-dimensional Euclidean space.



**Figure 13:** Views of the 6-D flat torus which illustrate its construction. The torus (top right) has its components highlighted with green, orange and blue, and the same torus is displayed as a scatterplot matrix, better revealing the construction.

Developing some visual insight into this space can help to understand the methods that operate in the space. Some data problems can be closely mapped to the geometric shapes. For example, ranked data showing preferences for a fixed set of objects, can be mapped to high-dimensional polytopes (Thompson, 1993). Values in a sample are commonly constrained to sum to a fixed number, for example, 100%, forming compositional data. This type of data lies inside a  $(p - 1)$ -D simplex. Good experimental designs commonly have a geometric structure (Hedayat et al., 1999). The ideas to examine boundaries of supervised classifiers described in Caragea et al. (2008) build on the geometric shapes described here.

We encourage the reader to look at the movies, and images, and download the data on the project web site, which is accessed at <http://schloerke.github.io/geozoo/>. The **geozoo** package contains the R code to generate the geometric shapes, is available to download from CRAN (<http://www.R-project.org>). We especially encourage readers to experiment with creating new high-dimensional geometric shapes, or contribute ideas and code back to this project.

## Acknowledgments

This work was supported by National Science Foundation grant DMS0706949. Andreas Buja provided some helpful feedback on the work. Dianne Cook thanks the Isaac Newton Institute, Cambridge, UK for support, where she was visiting while drafting this paper.

## Bibliography

- E. Abbott. *Flatland: A Romance of Many Dimensions*. Dover Publications, 1884. [p]
- D. Asimov. The Grand Tour: A Tool for Viewing Multidimensional Data. *SIAM Journal of Scientific and Statistical Computing*, 6(1):128–143, 1985. [p]
- P. Bourke. The Torus and Supertoroid. [http://local.wasp.uwa.edu.au/~pbourke/surfaces\\_curves/torus/](http://local.wasp.uwa.edu.au/~pbourke/surfaces_curves/torus/), 1990. [p]

- P. Bourke. Surfaces and Curves. [http://local.wasp.uwa.edu.au/~pbourke/surfaces\\_curves/](http://local.wasp.uwa.edu.au/~pbourke/surfaces_curves/), 1996. [p]
- P. Bourke. Regular Polytopes (Platonic Solids) in 4D. <http://local.wasp.uwa.edu.au/~pbourke/geometry/platonic4d/>, 2003. [p]
- A. Buja, D. Cook, D. Asimov, and C. Hurley. Computational Methods for High-Dimensional Rotations in Data Visualization. In C. R. Rao, E. J. Wegman, and J. L. Solka, editors, *Handbook of Statistics: Data Mining and Visualization*, pages 391–413. Elsevier/North Holland, <http://www.elsevier.com>, 2005. [p]
- D. Caragea, D. Cook, H. Wickham, and V. Honavar. Visual Methods for Examining SVM Classifiers. In S. Simonoff, M. Böhlen, and A. Mazeika, editors, *Visual Data Mining: Theory, Techniques and Tools for Visual Analytics*, pages 136–153. Springer-Verlag, Berlin, 2008. [p]
- D. Cook. Calibrate Your Eyes to Recognize High-Dimensional Shapes from Their Low-Dimensional Projections. *Journal of Statistical Software*, 2(6), 1997. <http://www.stat.ucla.edu/journals/jss/> and <http://www.public.iastate.edu/~dicook/JSS/paper/paper.html>. [p]
- D. Cook, E. K. Lee, A. Buja, and H. Wickham. Grand Tours, Projection Pursuit Guided Tours and Manual Controls. In C.-H. Chen and A. U. W. Härdle, W., editors, *Handbook of Computational Statistics (Volume III) Data Visualization*. Springer, New York, NY, 2007. URL <http://www.springer.com>. [p]
- P. Diaconis and D. Freedman. Asymptotics of Graphical Projection Pursuit. *Annals of Statistics*, 12(3): 793–815, 1984. [p]
- G. Hart. Virtual Polyhedra. <http://www.georgehart.com/virtual-polyhedra/vp.html>, 2000. [p]
- A. S. Hedayat, N. J. A. Sloane, and J. Stufken, editors. *Orthogonal Arrays: Theory and Applications*. Springer, <http://www.springer.com>, 1999. [p]
- E. Martin. Flatland. <http://www.der.org/films/flatland.html>, 1965. [p]
- R Development Core Team. *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria, 2003. URL <http://www.R-project.org>. ISBN 3-900051-00-3. [p]
- D. F. Swayne, D. Temple Lang, A. Buja, and D. Cook. GGobi: Evolving from XGobi into an Extensible Framework for Interactive Data Visualization. *Journal of Computational Statistics and Data Analysis*, 43:423–444, 2003. URL <http://authors.elsevier.com/sd/article/S0167947302002864>. [p]
- G. L. Thompson. Generalized permutation polytopes and exploratory graphical methods for ranked data. *The Annals of Statistics*, 21(3):1401–1403, 1993. [p]
- H. Wickham, D. Cook, H. Hofmann, and A. Buja. tourr: An R package for exploring multivariate data with projections. *Journal of Statistical Software*, 40(2):1–18, 2011. <http://www.jstatsoft.org/v40/i02/>. [p]

Barret Schloerke  
Department of Statistics  
Purdue University  
250 N. University Street  
West Lafayette, IN 47907  
USA  
[schloerke@gmail.com](mailto:schloerke@gmail.com)

Hadley Wickham  
RStudio Inc  
[hadley@rstudio.com](mailto:hadley@rstudio.com)

Dianne Cook  
Department of Econometrics and Business Statistics  
Monash University  
Wellington Road  
Clayton, Victoria 3800  
Australia  
[dicook@monash.edu](mailto:dicook@monash.edu)

*Heike Hofmann*  
*Department of Statistics*  
*Iowa State University*  
*Snedecor Hall*  
*Ames, Iowa 50011*  
*USA*  
[hofmann@iastate.edu](mailto:hofmann@iastate.edu)