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Learning to Learn

The Art of Doing Science and Engineering

Session 9: n–Dimensional Space

Overview

- **Definition of n-dimensional space.**
  - Two dimensions: Pythagoras theorem
  - Three dimensions: the length of the diagonal of a rectangular block
  - Extrapolate geometric concepts to higher dimensions
- **Volume of n-dimensional sphere**
- **The diagonal of n-dimensional cube**
- **High-dimensional spaces**

n – Dimensional Space

n – Dimensional Space is a mathematical construct which we must investigate if we are to understand what happens to us when we wander there during a design problem.

We can usefully extrapolate geometric concepts from

- 2 dimensions (2D)
- 3 dimensions (3D)

Two Dimensions

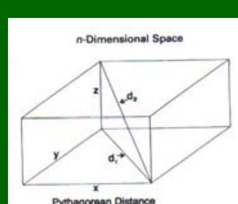
Pythagoras theorem – for a right triangle

- The square of the hypotenuse equals the sum of the squares of the other two sides.

Three Dimensions

Deriving the length of the diagonal of a rectangular block

- First, draw a diagonal on one face.
- Apply Pythagoras theorem.
- Take it as one side with the other side the third dimension, which is at right angles.
- From Pythagoras, get the square of the diagonal is the sum of the squares of the three perpendicular sides.



Three - Dimensions

As you go higher in dimensions, you still have the square of the diagonal as the sum of the squares of the individual mutually perpendicular sides:

$$D^2 = \sum_{i=1}^{n} x_i^2$$

where X_i = the length of the sides of the rectangular block in each of n dimensions

Three Dimensions

Planes in space will be simply linear combinations of X_i

A sphere about a point will be all points which are at the fixed distance (the radius) from the given central point.

Volume of n-dimensional sphere

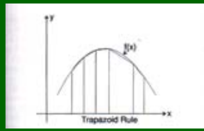
We need the Stirling approximation for n! to get an idea of the size of a piece of restricted space.

Volume of n-dimensional sphere

Derivation

- Take the log of n! $\ln n! = \sum_{k=1}^{n} \ln k$
- The sums relate to integral $\int_1^n \ln x \, dx$
- apply integration by parts $\int_1^n \ln x \, dx = \{x \ln x \, dx - x\}\big|_1^n = n \ln n - n + 1$

Volume of n-dimensional sphere



- Now apply Trapezoidal rule to the integral of ln x

$$\int_1^n \ln x \, dx \approx \frac{1}{2}\ln 1 + \ln 2 + \ln 3 + \ldots + \frac{1}{2}\ln n$$

- Since ln 1=0, adding (1/2) ln n to both terms, we get

$$\sum_{k=1}^{n} \ln k \approx n \ln n - n + 1 + \frac{1}{2}\ln n$$

- Undo the logs by taking the exponential of both sides

$$n! \approx C n^n e^{-n} \sqrt{n}$$

Volume of n-dimensional sphere

- By approximating the integral by trapezoidal rule, the error in the trapezoid approximation increases more and more slowly as n grows larger
- C is the limiting value.
- At the limit, value of the constant C is

$$c = \sqrt{2\pi} = 2.5066 \quad (e = 2.71828)$$

Volume of n-dimensional sphere

- Finally, the Stirling's formula for the factorial

$$n! \approx n^n e^{-n} \sqrt{2\pi n}$$

The table shows the quality of the Stirling approximation n!

n	Stirling	True	Stirling/true
1	0.92214	1	0.92214
2	1.91900	2	0.95950
3	5.83621	6	0.97270
4	23.50518	24	0.97942
5	118.01916	120	0.98349
6	710.07818	720	0.98622
7	4,980.3958	5,040	0.98817
8	39,902.3958	40,320	0.98964
9	359,536.87	362,880	0.99079
10	3,598,695.6	3,628,800	0.99170

Volume of n-dimensional sphere

As the numbers gets larger and larger the ratio approaches 1 but the differences get greater and greater !

Consider two functions

$f(n) = n + \sqrt{n}$ $\quad g(n) = n$

Then, the ratio f(n)/g(n), as n approaches infinity, is 1

…. but as in the table, the difference

$$f(n) - g(n) = \sqrt{n}$$

grows larger and larger as n increases.

Volume of n-dimensional sphere

Need to extend the factorial function to all positive real numbers, by introducing the *gamma function* in the form of an integral

$$\Gamma(n) = \int_0^\infty x^{n-1} e^{-x}\, dx$$

which converges for all n > 0

Volume of n-dimensional sphere

- For n >1 , again integrate by parts using

$$u = x^{n-1},\ dv = e^{-x}\, dx$$

- we have the reduction formula

$$\Gamma(n) = (n-1)\Gamma(n-1),\ with\ \Gamma(1) = 1$$

- The gamma function takes on the values (n-1)! at the positive integers n, and it provides a natural way of extending the factorial to all positive real numbers since the integral exists whenever n>0.

Volume of n-dimensional sphere

- we will need

$$\Gamma(1/2) = \int_0^\infty x^{-1/2} e^{-x}\, dx$$

- set $x=t^2$, hence dx=2tdt

$$\Gamma(1/2) = 2\int_0^\infty e^{-t^2}\, dt = \int_{-\infty}^\infty e^{-t^2}\, dt$$

- then take the product of two of the integrals

$$\Gamma^2(1/2) = \int_0^\infty \int_0^\infty e^{-(x^2+y^2)}\, dx\, dy$$

Volume of n-dimensional sphere

The $(x^2 + y^2)$ quantity suggests polar coordinates, so we convert

$$\Gamma^2(1/2) = \int_0^{2\pi}\int_0^\infty e^{-r^2} r\, dr\, d\theta = -\frac{e^{-r^2}}{2}\Big|_0^\infty 2\pi = \pi$$

Finally we obtain

$$\Gamma^2(1/2) = \pi,$$
$$Thus\quad \Gamma(1/2) = \sqrt{\pi} = 1.77245$$

Volume of n-dimensional sphere

- The volume of a cube in n – dimensions and of side X is X^n.
- The formula for the volume of an n–dimensional sphere must therefore be of the form

$$Volume = C_n r^n$$

where C is a constant

Volume of n-dimensional sphere

- for n = 2 dimensions, the constant C is pi.
- In 3 dimensions, we have

$$C_3 = \frac{4\pi}{3}$$

- Consider the volume of sphere
  - It is the sum of shells, and each element of the sum has a volume which is the corresponding shell area multiplied by the thickness, dr.

Volume of n-dimensional sphere

Surface area of a sphere can be obtained by differentiating the volume of the sphere with respect to the radius r

$$Surface = \frac{dV_n(r)}{dr} = n\,C_n\,r^{n-1}$$

Hence the elements of volume are

$$\left\{\frac{dV_n(r)}{dr}\right\} dr = n\,C_n\,r^{n-1}\,dr$$

Setting $r^2 = t$

$$\Gamma^2(1/2) = \pi^{n/2} = \int_0^\infty e^{-r^2}\left\{\frac{dV_n(r)}{dr}\right\} dr = \frac{n C_n}{2}\int_0^\infty e^{-t}\,t^{\left(\frac{n}{2}-1\right)}\,dt$$

and we obtain

$$= \frac{n C_n}{2}\,\Gamma\left(\frac{n}{2}\right) = C_n\,\Gamma\left(\frac{n}{2}+1\right)$$

Volume of n-dimensional sphere

From which we get

$$C_n = \left(\frac{\pi^{n/2}}{\Gamma\left(\frac{1}{2}n + 1\right)}\right)$$

It is easy to see it in a table representation

$$C_n = \left(\frac{2\pi}{n}\right) C_{n-2}$$

Volume of n-dimensional sphere

Thus, the coefficient Cn increases up to n = 5 and then decreases toward 0.

dimension n	coefficient C_n	
1	2	= 2.00000...
2	π	= 3.14159...
3	4π/3	= 4.11879...
4	$\pi^2/2$	= 4.93480...
5	$8\pi^2/15$	= 5.26379...
6	$\pi^3/6$	= 5.16771...
7	$16\pi^3/105$	= 4.72477...
8	$\pi^4/24$	= 4.05871...
9	$32\pi^4/945$	= 3.29850...
10	$\pi^5/120$	= 2.55010...
2k	$\pi^k/k!$	--> 0

For sphere of unit radius, the volume approaches 0 as n increases.

$$\frac{C_n r^n - C_n r^n (1-\varepsilon)^n}{C_n r^n} = 1 - (1-\varepsilon)^n$$

Volume of n-dimensional sphere

- If r is radius, then using n = 2 K for the volume

$$C_n r^n = \frac{(\pi r^2)^k}{k!} \to 0 \quad as \quad k \to \infty$$

- Thus no matter how large the radius, r, increasing the number of dimensions, n, will ultimately produce a sphere of arbitrarily small volume.

Volume of n-dimensional sphere

- Now look at the relative amount of the volume close to the surface of n-dimensional sphere
  - Let r = radius of the sphere, and inner radius of the shell is

$$r(1-\varepsilon)$$

then the relative volume of the shell is

$$\frac{C_n r^n - C_n r^n (1-\varepsilon)^n}{C_n r^n} = 1 - (1-\varepsilon)^n$$

- For large n, no matter how thin the shell is (relative to the radius), almost all the volume is in the shell and there is almost nothing inside.
- Apparently the volume is almost all near the surface.

Volume of n-dimensional sphere

- This has importance in design; it means almost always the optimal design will be on the surface of the design space (i.e. near endpoint values) and will not be inside as you might think.
- The best design is pushing one or more of the parameters to their extreme – obviously you are on the surface of the feasible region of design!

The diagonal of n-dimensional cube

- A vector from the origin to the point (1,1,…,1).
- The cosine of angle between this line and any axis is given as:
  - The ratio of the component along the axis, which is 1, to the length of the line, which is sqrt(n), hence

$$\cos\theta = \frac{1}{\sqrt{n}} \to 0 \quad and \quad \theta = \frac{\pi}{2}$$

Therefore, for large n, the diagonal of a cube is *almost perpendicular* to every coordinate.

The diagonal of n-dimensional cube

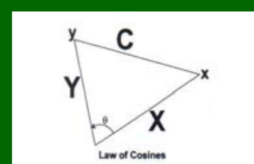
- "I have found it very valuable in important situations to review *all the basic derivations involved* so I have a firm feeling for what is going on."
- Now w will estimate the angle between two lines – vector dot product.

The diagonal of n-dimensional cube

- Take two points X and Y with their corresponding coordinates Xi and Yi.
- Apply the law of cosines in the plane of the three points X, Y, and the origin we have:

$$C^2 = X^2 + Y^2 - 2\,X\,Y\cos\theta$$

  - where X and Y are the lengths of the lines from origin to the two points x and y.



The diagonal of n-dimensional cube

- But note that the C comes from using the differences of the coordinates in each direction

$$C^2 = \sum_{k=1}^{n}(x_k - y_k)^2 = X^2 + Y^2 - 2\sum_{k=1}^{n} x_k y_k$$

- Comparing the two expressions, we have

$$\cos\theta = \frac{\sum_{k=1}^{n} x_k y_k}{x\,y}$$

- Now if we apply this formula to two lines draw from the origin to random points of the form:

$$(\pm 1, \pm 1, \ldots, \pm 1)$$

The diagonal of n-dimensional cube

- The dot product of these factors, taken at random, is again random ± 1's and these are to be added n times, while the length of each is again sqrt(n), hence

$$\cos\theta = \frac{\sum_{k=1}^{n}(\pm 1)}{n}$$

- By the weak law of large numbers this approaches zero for increasing n. But there are 2^n different random vectors, and given any one fixed vector then any other of these 2^n random vectors is *almost surely perpendicular* to it !

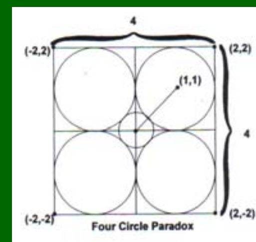
The diagonal of n-dimensional cube

- In linear algebra you learned to find the set of perpendicular axes then represent everything in terms of these coordinates.
- But you see in n-dimensions there are, after you find the n mutually perpendicular coordinate directions, 2^n other directions which *almost perpendicular* to those you have found !
- The theory and practice of linear algebra are quite different !

High dimensional spaces

- Four circle paradox.
- Begin with 4x4 square and divide it into 4 unit squares in each of which we draw a unit circle.
- Next we draw a circle about the center of the square with radius just touching the four circles on their insides. Its radius must be

$$r_2 = \sqrt{2} - 1 = 0.414$$



High dimensional spaces

- In three dimensions, this setup produces a 4x4x4 cube, along with 8 spheres of unit radius.
- The inner sphere will touch each outer sphere along the line to their center will have a radius of

$$r_3 = \sqrt{3} - 1 = 0.732$$

- Going to n dimensions, you have 4x4x…x4 cube, and 2^n spheres, one in each of the corners, and with each touching its n adjacent neighbors.
- The inner sphere, touching on the inside all of the spheres, will have a radius of

$$r_n = \sqrt{n} - 1$$

High dimensional spaces

- Let's apply it to the case of n =10 dimensions. Then consider the radius of the inner sphere

$$r_{10} = \sqrt{10} - 1 > 2$$

- Following this formula, we see that in 10 dimensions the inner sphere reaches outside the surrounding cube !
  - The sphere is convex, it touches each of the 1024 packed spheres on the inside, yet it reaches outside the cube !

High dimensional spaces

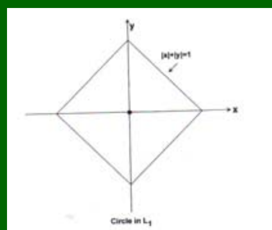
- The n-dimensional space is where the design of complex objects generally takes place. Therefore it is important and may yield design insight to determine the implications of geometrical properties in these higher dimensions.
- I did all this in the classical Euclidean space using the Pythagorean distance where the sum of the squares of the differences of the coordinates is the distance between the points squared. Mathematicians call this distance L2.

High dimensional spaces

- The space L1 uses not the sum of the squares, but rather the sum of the distances, much as you do in traveling in a city with a rectangular grid of streets.
- It is the sum of the differences between the two locations that tells you how far you must go.
- In the computing field this metric is often called the "Hamming distance."

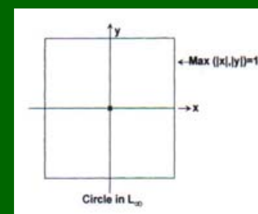
High dimensional spaces

- In Hamming space L1 a circle with unit radius (radius of 1 is equivalent to sum of x and y absolute values) in two dimensions looks like a square standing on a point.
- In three dimensions, it is like a cube standing on a point.
- Now you can better see how it is in the circle paradox above the inner sphere can get outside the cube.



High dimensional spaces

- There is a third commonly used metric called Linfinity, or *Chebyshev distance.*
- In this metric, the distance is the maximum coordinate difference, regardless of any other differences.
- In this space a circle is a square, a three dimensional sphere is a cube, and the inner circle in the circle paradox has 0 radius in all dimensions.



High dimensional spaces

- These are all examples of a *metric*, a measure of distance.
- The conventional conditions on a metric D(x, y) between two points x and y are:
  - D(x, y) >= 0 (non-negative),
  - D(x, y) = 0 if and only if x = y (identity),
  - D(x, y) = D(y, x) (symmetry),
  - D(x, y) + D(y, z) >= D(x,z) (triangle inequality).

Conclusion

- After this exposure, you should be better prepared than you were for complex design and for carefully examining the space in which the design occurs, as I have tried to do here.
- Messy as it is, fundamentally it is where the design occurs and where you must search for an acceptable design.