

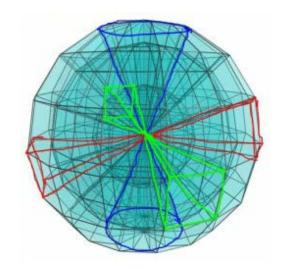
Survey of Scientific Computing (SciComp 301)

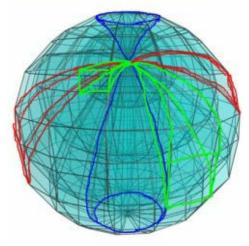
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Session 20 Monte Carlo Method

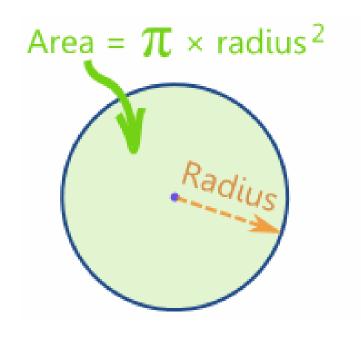
An Interesting Question

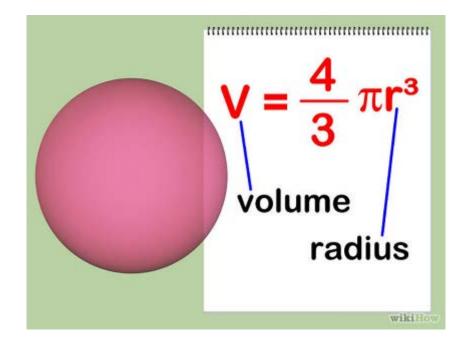
- What is the volume of a fourdimensional unit hypersphere?
 - What does a 4D sphere "look" like?
 - What is a "unit" sphere?
 - Where do I even start?
- Break down complex questions into simpler steps:
 - How can we calculate the area of a 2D circle?
 - How can we calculate the volume of a 3D sphere?
 - How do we move from 3D to 4D?



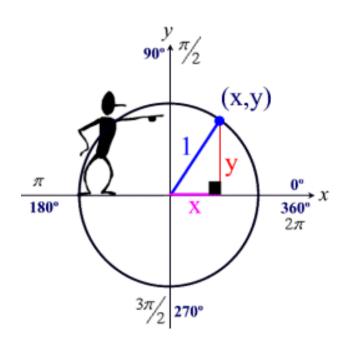


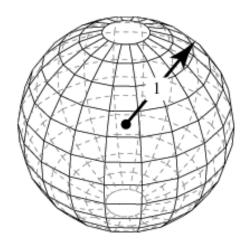
Area and Volume



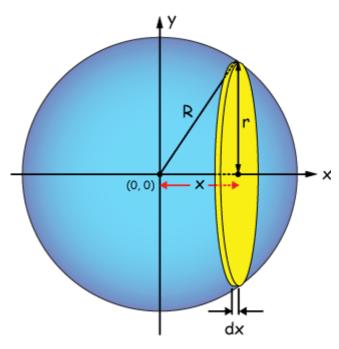


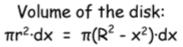
A Unit Circle and Unit Sphere

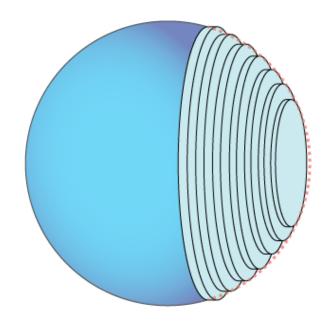




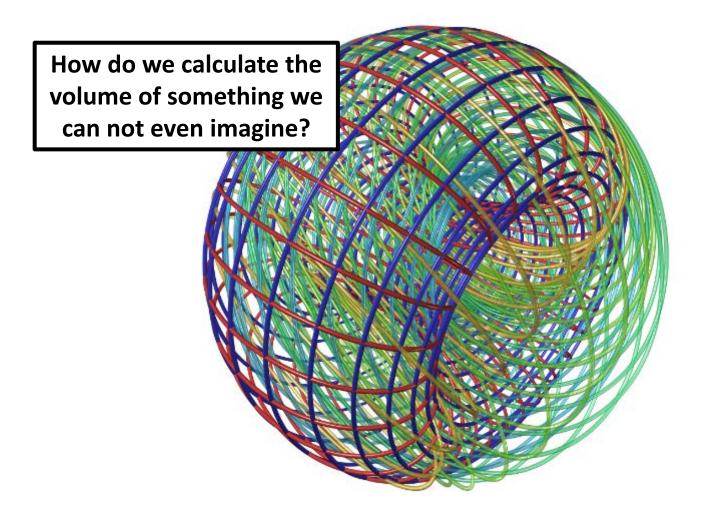
2-D Area → 3-D Volume



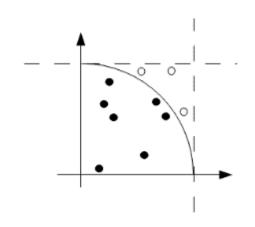


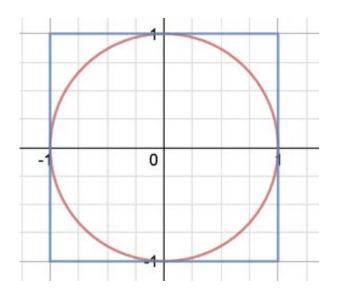


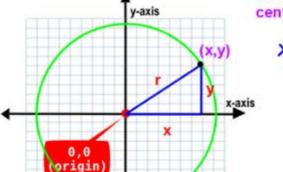
A 4-D Hypersphere



Area as a "Ratio" of Inside vs. Total Dots





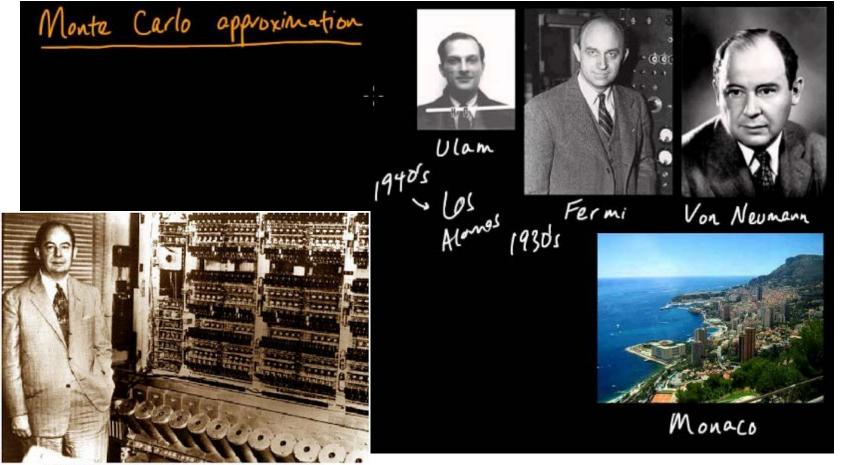


The equation of a circle centered at the origin

$$x^2 + y^2 = r^2$$

We pick a million random points and <u>count</u> how many are inside the circle

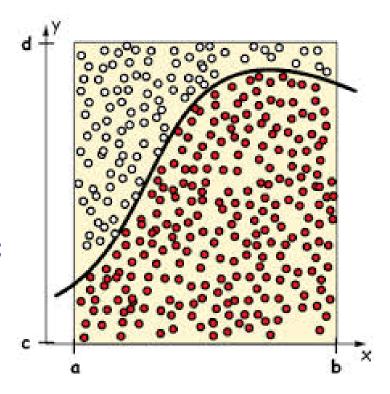
The Monte Carlo Method



Johnny von Neumann [1903-1957] alongside the Maniac computer at the Institute for Advanced Studies, Princeton.

The Monte Carlo Method

- With Monte Carlo, we randomly sample points across the entire space and count how many are below the curve
- The ratio between points below the curve to total points is an estimate of the area (integral)
- Monte Carlo is a non-deterministic approach because it uses a pseudo-random number generator



```
void draw(SimpleScreen& ss)
    ss.DrawAxes():
    ss.DrawCircle(0, 0, 1, "green", 2);
    seed seq seed{ 2017 };
    default random engine generator{ seed };
    uniform real distribution<double> distribution{ 0,
    const int iterations = 100000;
    int count{}:
    ss.LockDisplay();
    for (int i{};i < iterations;++i) {</pre>
        double x = distribution(generator) * 2.0 - 1.0;
        double y = distribution(generator) * 2.0 - 1.0;
        if (x*x + y*y \le 1.0) {
            ss.DrawPoint(x, y, "red");
            count++:
            ss.DrawPoint(x, y, "blue");
    ss.UnlockDisplay();
    double area = (double)count / iterations * 4.0;
    double err = (M PI - area) / M PI * 100;
    cout << "2D Circle Area PRNG" << endl</pre>
        << "Iterations = " << iterations << endl</pre>
        << "Est. Area = " << area << endl
        << "Act. Area = " << M PI << endl
        << "Abs. % Err = " << abs(err) << endl;</pre>
```

2-D Area as a "Ratio" of Dots

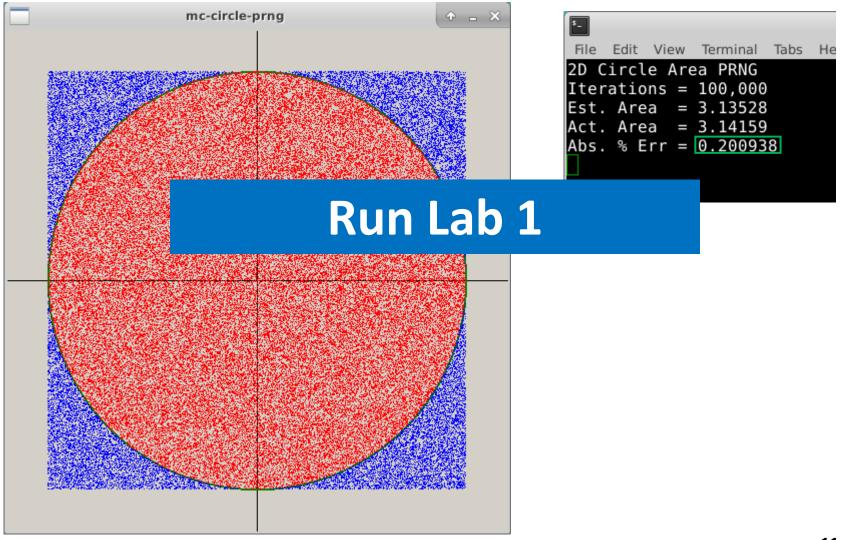
Open Lab 1

$$\frac{dots_{inside}}{dots_{total}} = \frac{area_{circle}}{area_{square}}$$

$$area_{square} = 2 \times 2 = 4$$

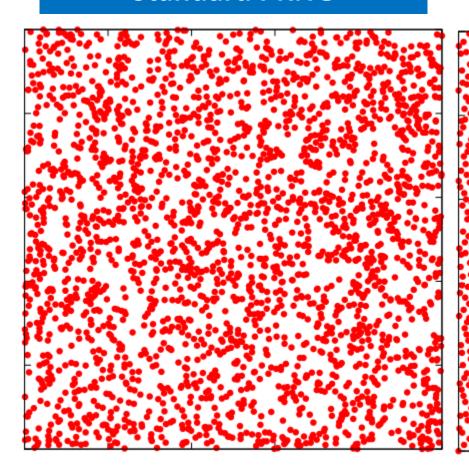
$$area_{circle} = \frac{count}{iterations} \times 4$$

2-D Area as a "Ratio" of Dots



Comparing "Random" Number Generators

Standard PRNG

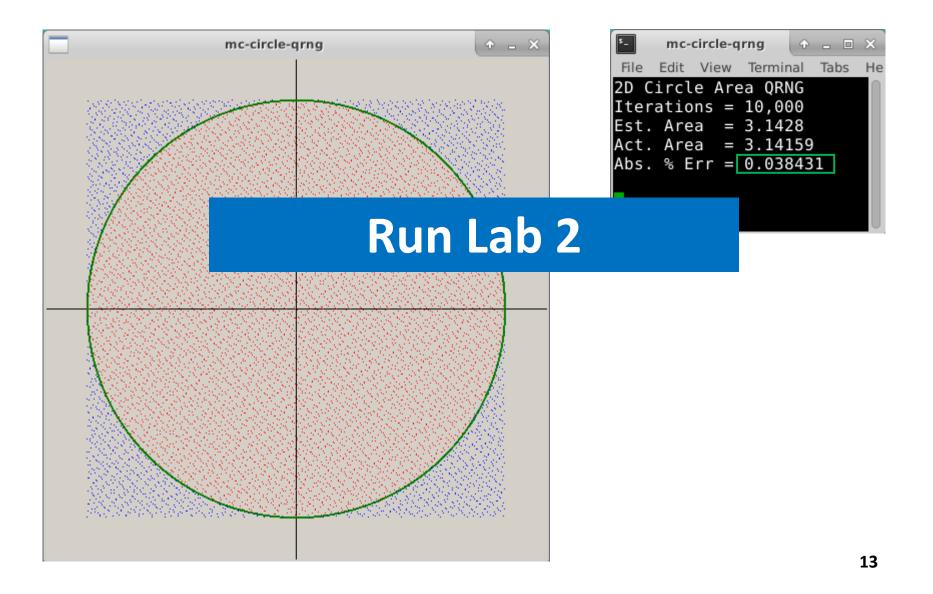


Niederreiter QRNG

The Niederreiter sequence generates a smoother distribution of "random" points

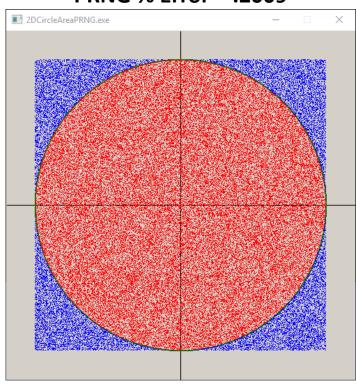


Improved 2-D Monte Carlo Estimator

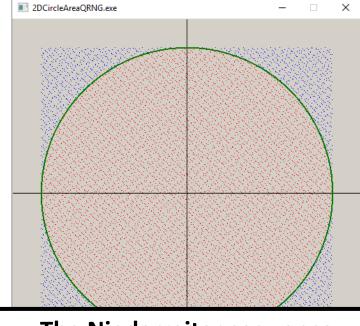


Improved 2-D Monte Carlo Estimator





QRNG % Error = .0384



The Niederreiter sequence provides a 6X increase in accuracy of the estimate using 10X fewer points!

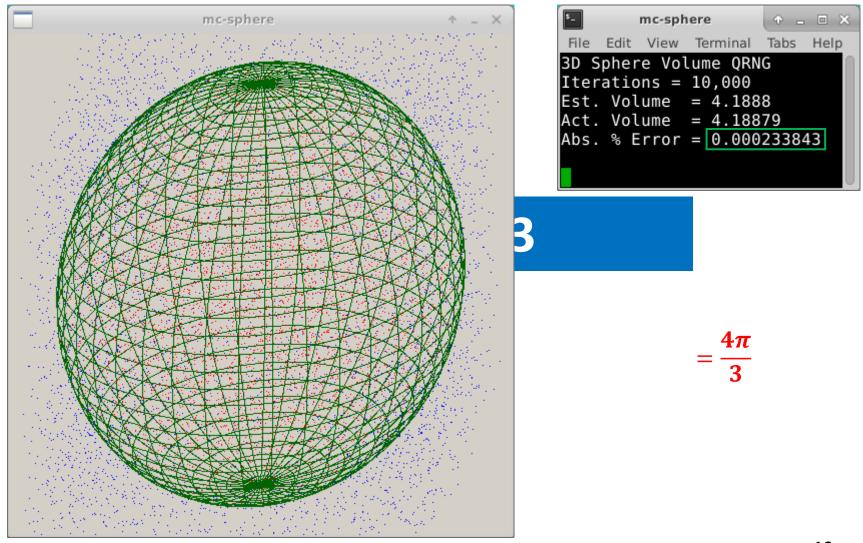
Niederreiter2 qrng; double r[3]: int seed{}; const int iterations = 10000; int count{}; ss.LockDisplay(); for (int i{};i < iterations;++i) {</pre> grng.Next(3, &seed, r); **double** x = r[0] * -2.0 **double** y = r[1] * -2.0 **double** z = r[2] * -2.0 - 1.0**if** (x*x + y*y + z*z <= 1.0)ss.DrawPoint3D(x, y, z, "red"); count++: ss.DrawPoint3D(x, y, z, "blue"); ss.UnlockDisplay(); double estVol = (double)count / iterations * 8; double actVol = 4.0 / 3.0 * M PI; double err = (actVol - estVol) / actVol * 100: cout << "3D Sphere Volume QRNG" << endl << "Iterations = " << iterations << endl</pre> << "Est. Volume = " << estVol << endl</pre> << "Act. Volume = " << actVol << endl << "Abs. % Error = " << abs(err) << endl << endl;</pre>

3-D Unit Sphere Volume Estimator

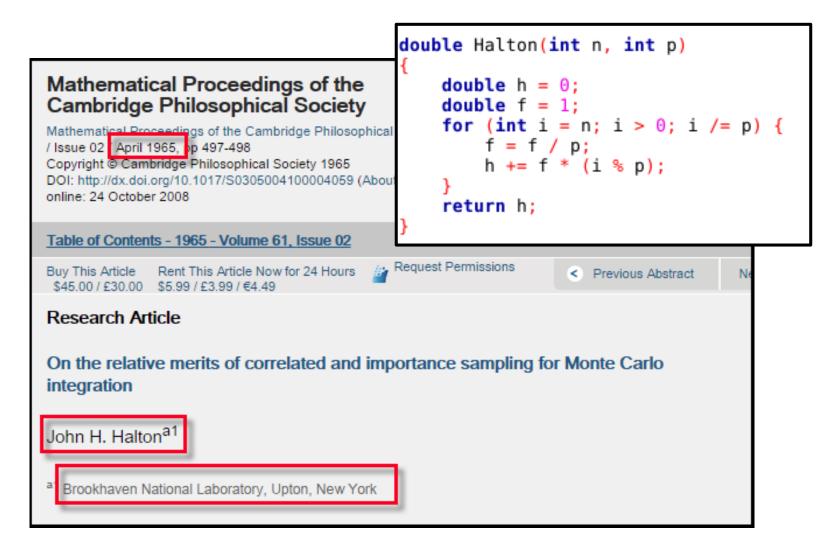
$$\frac{dots_{inside}}{dots_{total}} = \frac{volume_{sphere}}{volume_{cube}}$$
$$volume_{cube} = 2 \times 2 \times 2 = 8$$

$$volume_{sphere} = \frac{count}{iterations} \times 8$$

3-D Unit Sphere Volume Estimator



The Halton Sequence



Accommodating the 4th Dimension

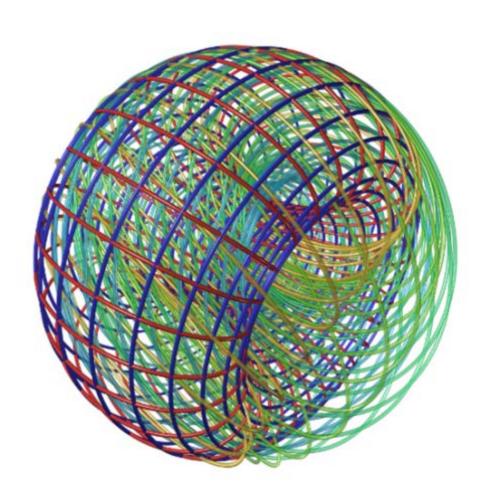
```
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43
44
        int main()
      \Box {
             int iterations = int(1e7);
                                                                                  We need to
             double count = 0;
                                                                               update this code
             for (int i = 0; i < iterations; i++) {
                                                                              to include the 4<sup>th</sup>
                  double x = Halton(i, primes[0]);
                                                                                            bn!
                         Open and edit Lab 4
                  if (distance \leftarrow 1.0)
                       count++;
             double volume = count / iterations * 8;
             cout << fixed << setprecision(4)</pre>
                  << volume << endl:
             return 0:
```

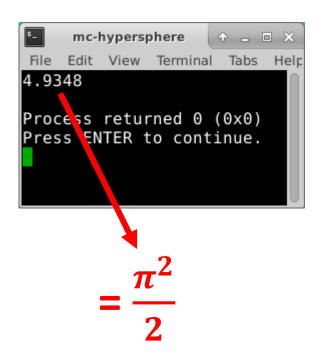
Accommodating the 4th Dimension

```
int main()
21
22
     □ {
            int iterations = int(1e7);
23
24
25
           double count = 0:
26
27
            for (int i = 0; i < iterations; i++) {
                double x = Halton(i, primes[0]);
28
29
                double y = Halton(i, primes[1]);
30
                double z = Halton(i, primes[2]);
31
                double w = Halton(i, primes[3]
32
                double distance = x * x + y * y + z * z + w * w;
33
34
35
                if (distance <= 1.0)</pre>
36
                    count++:
37
38
            double volume = count / iterations * 16;
39
40
            cout << fixed << setprecision(4)</pre>
41
42
                << volume << endl:
43
44
            return 0;
45
46
```

Add all the code in red then run the application

What is the content of a 4-D unit hypersphere?

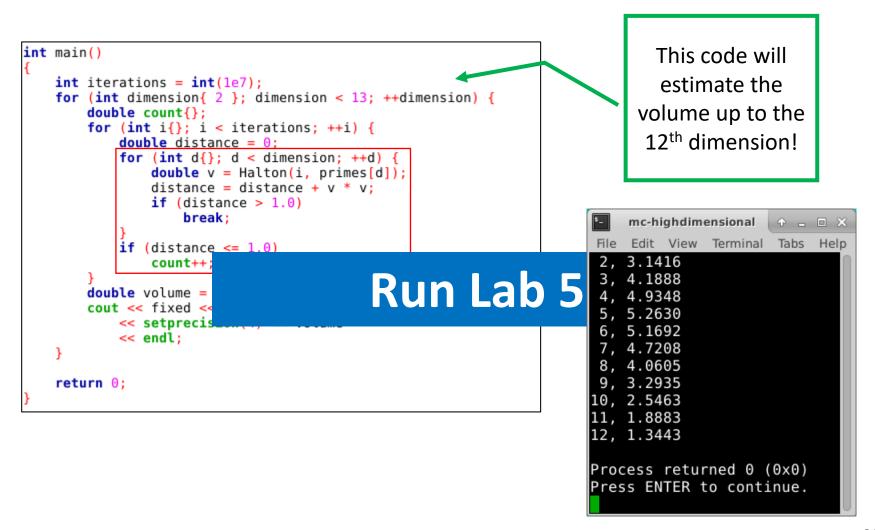




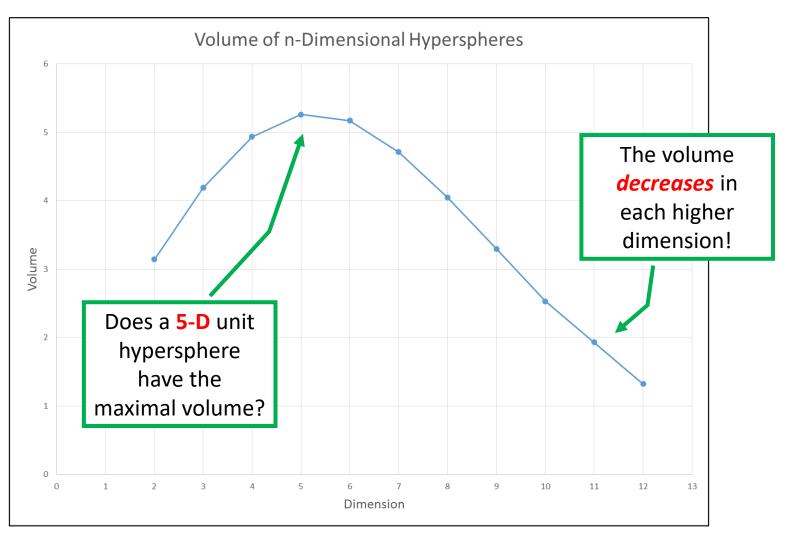
What lurks beyond the 4th dimension?

```
int main()
                                                                                    This code will
    int iterations = int(1e7);
                                                                                     estimate the
    for (int dimension{ 2 }; dimension < 13; ++dimension) {</pre>
                                                                                  volume up to the
        double count{};
        for (int i{}; i < iterations; ++i) {</pre>
                                                                                   12<sup>th</sup> dimension!
            double distance = 0;
            for (int d{}; d < dimension; ++d) {</pre>
                 double v = Halton(i, primes[d]);
                 distance = distance + v * v;
                 if (distance > 1.0)
                     break:
            if (distance <= 1.0)</pre>
                 count++:
        double volume = count / iterations * pow(2, dimension);
        cout << fixed << right << setw(2) << dimension << ", "</pre>
            << setprecision(4) << volume
            << endl;
    return 0;
                                                                             count
                                                                                         \times 2^{dimensions}
                                                   volume_{sphere} = \frac{}{iterations}
```

What lurks beyond the 4th dimension?



What lurks beyond the 4th dimension?



The Power Of Monte Carlo Integration

$$\mathbf{F}^{(n)} = \frac{\mu}{8\pi} \int_{r_1}^{r_2} \int_{s_1}^{s_2} \int_{y_1}^{y_2} \left(\frac{2}{R_a^3} + \frac{3a^2}{R_a^5}\right) \{ (\mathbf{R} \times \mathbf{b}) (\mathbf{t} \cdot \mathbf{n}) + \mathbf{t} \left[(\mathbf{R} \times \mathbf{b}) \cdot \mathbf{n} \right] \}$$

$$\times \left(\frac{r - r_1}{r_2 - r_1} \frac{s - s_1}{s_2 - s_1} \right) ds dr dy$$

$$- \frac{\mu}{4\pi (1 - \nu)} \int_{r_1}^{r_2} \int_{s_1}^{s_2} \int_{y_1}^{y_2} \left(\frac{1}{R_a^3} + \frac{3a^2}{R_a^5} \right) \left[(\mathbf{R} \times \mathbf{b}) \cdot \mathbf{t} \right] \mathbf{n} \left(\frac{r - r_1}{r_2 - r_1} \frac{s - s_1}{s_2 - s_1} \right) ds dr dy$$

$$+ \frac{\mu}{4\pi (1 - \nu)} \int_{r_1}^{r_2} \int_{s_1}^{s_2} \int_{y_1}^{y_2} \frac{1}{R_a^3} \left\{ (\mathbf{b} \times \mathbf{t}) (\mathbf{R} \cdot \mathbf{n}) + \mathbf{R} \left[(\mathbf{b} \times \mathbf{t}) \cdot \mathbf{n} \right] \right\} \left(\frac{r - r_1}{r_2 - r_1} \frac{s - s_1}{s_2 - s_1} \right) ds dr dy$$

$$- \frac{\mu}{4\pi (1 - \nu)} \int_{r_1}^{r_2} \int_{s_1}^{s_2} \int_{y_1}^{y_2} \frac{3}{R_a^5} \left[(\mathbf{R} \times \mathbf{b}) \cdot \mathbf{t} \right] (\mathbf{R} \cdot \mathbf{n}) \mathbf{R} \left(\frac{r - r_1}{r_2 - r_1} \frac{s - s_1}{s_2 - s_1} \right) ds dr dy.$$

A Functional Equation for the Factorial

Consider the classic factorial function:

$$n! = n * (n - 1) * (n - 2) * (n - 3) * \cdots * 1$$

 $5! = 5 * 4 * 3 * 2 * 1 = 120$

- We wish to find a functional equation that provides a shortcut to compute the factorial without having to iterate through the product of every term
- A closed form (analytic) Riemann Integral is the functional equation of an infinite series of diminishing rectangles under a curve within a given interval
- Can we express the factorial function as an integral?

Euler's Gamma Function

$$\Gamma(s) = \int_0^\infty x^{s-1} e^{-x} dx \quad \{s \in \mathbb{C}, Re(s) > 0\}$$

$$\Gamma(n) = (n-1)! \ \{n \in \mathbb{Z}^+\}$$

$$\Gamma(6) = (6-1)! = 5! = 120$$



Euler's Gamma Function

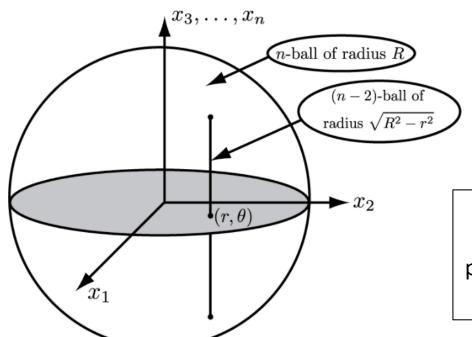
- Euler was a mathematical pathfinder he liked to bend the rules and push the boundaries of existing functions
 - He asked "what is the factorial of a fraction?"
 - He also asked "what is the factorial of a negative number?"
- Using his Gamma function, Euler proved these two gems:

$$\left(\frac{1}{2}\right)! = \frac{\sqrt{\pi}}{2} = 0.8862269 \dots$$

$$\left(-\frac{1}{2}\right)! = \sqrt{\pi} = 1.7724538 \dots$$

Analytic Solution

Observe that the intersection of the (x_1, x_2) -plane with the n-ball is a disk of radius R centered at the origin.



The perpendicular cross section of the n-ball at the point (r,θ) is an (n-2)-ball of radius $\sqrt{R^2-r^2}$

A Proportionality Relation

If a solid in n-dimensional space is scaled by a factor of k, then its volume increases by a factor of k^n

$$V_n(R) \propto R^n$$

 $V_n(R) = V_n(1)R^n$

The scaling factor is the **volume** of the **unit** sphere for that dimension

The volume of the n-ball is the integral of volumes of (n-1) balls:

$$V_n(R) = \int_{-R}^{R} V_{n-1} \left(\sqrt{R^2 - x^2} \right) dx$$

due to the inductive assumption

$$V_{n}(R) = R^{n-1} \int_{-R}^{R} V_{n-1} \left(\sqrt{1 - \left(\frac{x}{R}\right)^{2}} \right) dx$$

$$t = \frac{x}{R}$$

$$V_{1}(1) = 2$$

$$V_{n}(R) = R^{n} \int_{-1}^{1} V_{n-1} \left(\sqrt{1 - t^{2}} \right) dt$$

$$V_{2}(1) = ?$$

$$R = 1 \quad V_{1}(1) = 2 \int_{-1}^{1} \sqrt{1 - t^{2}} dt = \frac{\pi}{2}$$

$$V_{2}(1) = \frac{\pi}{2}$$

$$V_{2}(1) = \frac{\pi}{2}$$

$$V_{3}(1) = \frac{\pi}{2}$$

$$V_{1}(1) = 2 \int_{-1}^{1} \sqrt{1 - t^{2}} dt = \frac{\pi}{2}$$

$$V_{2}(1) = \frac{\pi}{2}$$

A Proportionality Relation

If a solid in n-dimensional space is scaled by a factor of k, then its volume increases by a factor of k^n

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The scaling factor is the **volume** of the **unit** sphere for that dimension

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$$V_n(R) = \int_{-R}^{R} V_{n-1} \left(\sqrt{R^2 - x^2} \right) dx$$

$$V_{n}(R) = R^{n-1} \int_{-R}^{R} V_{n-1} \left(\sqrt{1 - \left(\frac{x}{R}\right)^{2}} \right) dx$$

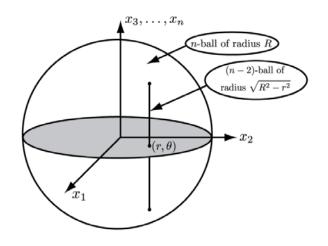
$$t = \frac{x}{R}$$

$$V_{n}(R) = R^{n} \int_{-1}^{1} V_{n-1} \left(\sqrt{1 - t^{2}} \right) dt$$

$$V_{n}(R) = V_{n}(1)R^{n}$$

A Recurrence Relationship

We can compute $V_n(R)$ by integrating $V_{n-2}(\sqrt{R^2-r^2})$ over the disk using polar coordinates:



$$V_{n}(R) = \int_{0}^{R} \int_{0}^{2\pi} V_{n-2} \left(\sqrt{R^{2} - r^{2}} \right) r \, d\theta \, dr$$

$$= \int_{0}^{R} \int_{0}^{2\pi} V_{n-2}(1) \left(\sqrt{R^{2} - r^{2}} \right)^{n-2} r \, d\theta \, dr$$

$$= V_{n-2}(1) \int_{0}^{R} r(R^{2} - r^{2})^{\frac{n-2}{2}} \theta \Big|_{0}^{2\pi} dr$$

$$= 2\pi V_{n-2}(1) \int_{0}^{R} r(R^{2} - r^{2})^{\frac{n-2}{2}} dr$$

$$= -\frac{2\pi}{n} V_{n-2}(1) \left(R^{2} - r^{2} \right)^{\frac{n}{2}} \Big|_{0}^{R}$$

$$= 2\pi V_{n-2}(1) \frac{R^{n}}{n}$$

$$V_{\mathbf{n}}(R) = \frac{2\pi R^2}{n} V_{\mathbf{n-2}}(R)$$

Volume via the Gamma Function

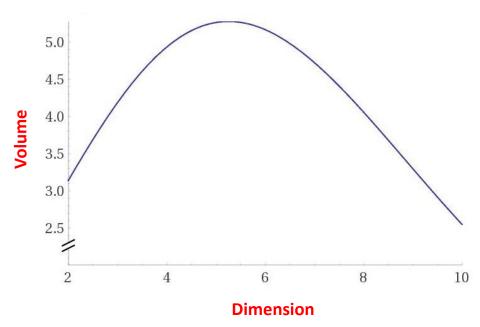
$$n_{even} \to V_n(R) = \frac{2^{\frac{n}{2}} \pi^{\frac{n}{2}} R^n}{2 \cdot 4 \cdot 6 \cdots n}$$

$$n_{odd} \to V_n(R) = \frac{2^{\frac{n+1}{2}} \pi^{\frac{n-1}{2}} R^n}{1 \cdot 3 \cdot 5 \cdots n}$$

$$V_n(R) = \frac{\pi^{\frac{n}{2}}R^n}{\Gamma(\frac{n}{2}+1)}$$

This is the key formula!

Volume of Unit Hypersphere



Volume via the Gamma Function

$$V_n(R) = \frac{\pi^{\frac{n}{2}}R^n}{\Gamma(\frac{n}{2}+1)}$$

$$\Gamma(n) = (n-1)!$$

$$n! = \Gamma(n+1)$$

$$V_2(R) = \frac{\pi R^2}{\Gamma(\frac{2}{2} + 1)} = \frac{\pi R^2}{\Gamma(2)} = \frac{\pi R^2}{(2 - 1)!} = \pi R^2$$

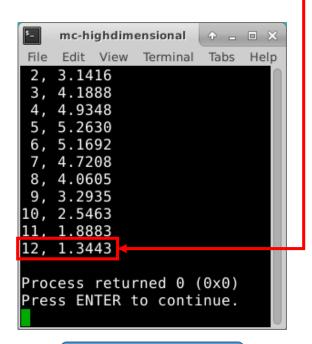
$$V_3(R) = \frac{\pi^{\frac{3}{2}}R^3}{\Gamma(\frac{3}{2}+1)} = \frac{\pi R^3}{\Gamma(\frac{5}{3})} = \frac{\pi^{\frac{3}{2}}R^3}{(\frac{3\sqrt{\pi}}{4})} = \pi^{\frac{3}{2}}R^3(\frac{4}{3\sqrt{\pi}}) = \boxed{\frac{4}{3}\pi R^3}$$

$$V_4(R) = \frac{\pi^{\frac{4}{2}}R^4}{\Gamma(\frac{4}{2}+1)} = \frac{\pi^2R^2}{\Gamma(3)} = \frac{\pi^2R^2}{(3-1)!} = \boxed{\frac{\pi^2R^2}{2}}$$

Challenges of Numerical Analysis

 $V_{12}(1) = \frac{\pi^{\frac{12}{2}} 1^{12}}{\Gamma(\frac{12}{2} + 1)} = \boxed{1.335262}$

Did we use enough dots?



From Lab 5

Curse of dimensionality

The curse of dimensionality refers to various phenomena that arise when analyzing and organizing data in high-dimensional spaces (often with hundreds or thousands of dimensions) that do not occur in low-dimensional settings such as the three-dimensional physical space of everyday experience. The expression was coined by Richard E. Bellman when considering problems in dynamic optimization.^{[1][2]}

There are multiple phenomena referred to by this name in domains such as numerical analysis, sampling, combinatorics, machine learning, data mining, and databases. The common theme of these problems is that when the dimensionality increases, the volume of the space increases so fast that the available data become sparse. This sparsity is problematic for any method that requires statistical significance. In order to obtain a statistically sound and reliable result, the amount of data needed to support the result often grows exponentially with the dimensionality.

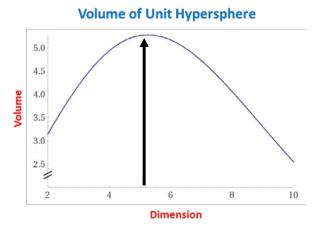
Volume via the Gamma Function

$$V_n(R) = \frac{\pi^{\frac{n}{2}}R^n}{\Gamma(\frac{n}{2}+1)}$$

As the Gamma function can extends its domain to include $n \in \mathbb{R}$, we can use this analytic solution to compute the volume of hyperspheres having fractional (non-integer) dimensions!

$$V_{7.89}(5.12) = \frac{\pi^{\frac{7.89}{2}}5.12^{7.89}}{\Gamma(\frac{7.89}{2}+1)} = 1,633,106.2809$$

It appears $V_n(1)$ has a maximum somewhere between **4** and **6** dimensions. Does a <u>fractional</u> dimension contain the largest unit hypersphere?



Open Lab 6 – nball-volume

```
nball-volume.cpp 💥
          // nball-volume.cpp
          #include "stdafx.h"
         using namespace std;
          // Euler's Gamma kernel
          inline double f(double x, double n)
   10
              return pow(x,n-1) * exp(-x)
   11
   12
   13
          // Find Gamma using Simpson's integration
   14
          double gamma(double n)
   15
   16
              double a{ 0 };
   17
              double b{ 1e3 };
   18
              int intervals = 1e5;
   19
   20
              double dx{ (b - a) / intervals };
   21
              double sum{ f(a,n) + f(b,n) };
   22
   23
              for (int i{ 1 }; i < intervals; ++i, a += dx)</pre>
   24
                  sum += f(a, n)*(2 * (i % 2 + 1));
   25
              return (dx / 3)*sum;
   26
   27
   28
          // Find volume of unit ball
   29
          // See https://en.wikipedia.org/wiki/N-sphere
   30
          double v(double x)
   31
   32
              double halfx = x / 2.0;
              return pow(M PI, halfx) / gamma(halfx + 1)
   33
   34
   35
```

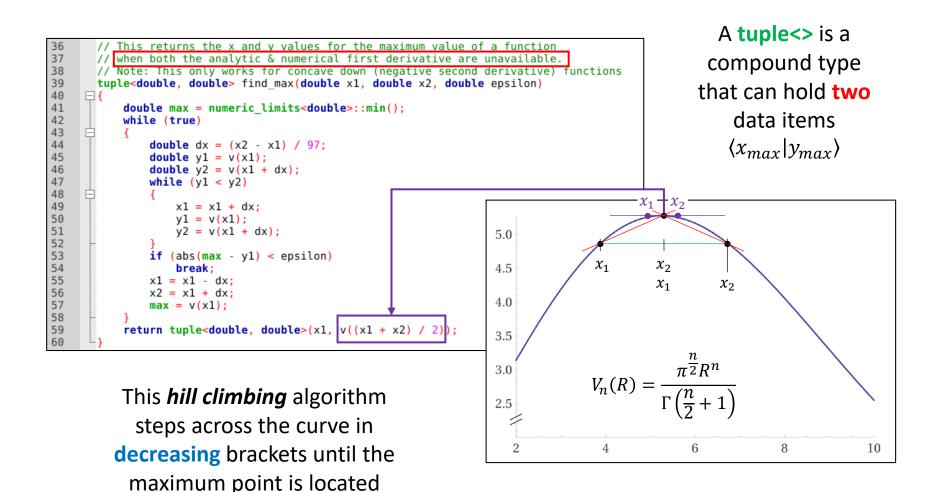
The code currently uses
 Simpson's Rule to calculate
 Euler's Gamma function:

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

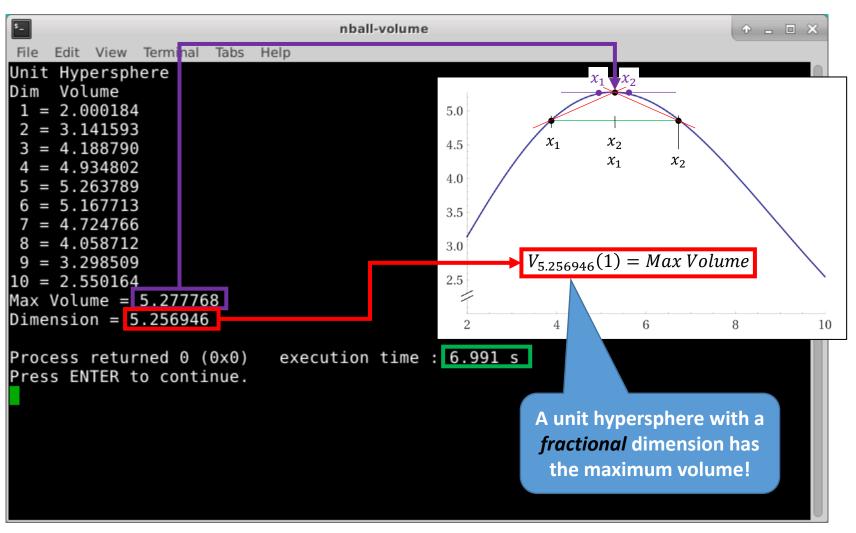
 From there, it uses Gamma to find the volume of unit hyperspheres with integer dimensions

$$V_n(1) = \frac{\pi^{\frac{n}{2}}}{\Gamma(\frac{n}{2} + 1)}$$

View Lab 6 – nball-volume



Run Lab 6 – nball-volume



Edit Lab 6 – nball-volume

```
nball-volume
     Edit View Terminal Tabs
                           Help
Unit Hypersphere
Dim Volume
 1 = 2.000000
                                 28
                                       // Find volume of unit ball
 2 = 3.141593
                                 29
                                       // See https://en.wikipedia.org/wiki/N-sphere
                                 30
                                       double v(double x)
 3 = 4.188790
                                 31
                                     □ {
 4 = 4.934802
                                 32
                                           double halfx = x / 2.0;
 5 = 5.263789
                                 33
                                                                  t_{namma}(halfx + 1):
                                           return pow(M PI, halfx)
 6 = 5.167713
                                 34
 7 = 4.724766
 8 = 4.058712
 9 = 3.298509
10 = 2.550164
Max Volume = 5.277768
Dimension = 5.256946
                                                                    Edit line # 33 to call the
                                                                    C++ tgamma() function
                              execution time : 0.015 s
Process returned 0 (0x0)
                                                                      "the true gamma"
Press ENTER to continue.
                                The built-in tgamma() is
                                46,000% faster than our
                                 Simpson's integration!
```

Now you know...

https://dlmf.nist.gov/5

Gamma gets its own chapter!



Chapter 5 Gamma Function

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Notation

5.1 Special Notation

Properties

- 5.2 Definitions
- 5.3 Graphics
- 5.4 Special Values and Extrema
- 5.5 Functional Relations
- 5.6 Inequalities
- 5.7 Series Expansions
- 5.8 Infinite Products
- 5.9 Integral Representations
- 5.10 Continued Fractions
- 5.11 Asymptotic Expansions
- 5.12 Beta Function
- 5.13 Integrals
- 5.14 Multidimensional Integrals
- 5.15 Polygamma Functions
- 5.16 Sums
- 5.17 Barnes' *G*-Function (Double Gamma Function)
- 5.18 $\it q$ -Gamma and $\it q$ -Beta Functions

Applications

- 5.19 Mathematical Applications
- 5.20 Physical Applications

Computation

- 5.21 Methods of Computation
- 5.22 Tables
- 5.23 Approximations
- 5.24 Software

In C++ use tgamma()

Now you know...

- Monte Carlo integration uses random sampling
 - The method calculates the ratio of the points below the curve to the total number of points **the final ratio is the "area"**
 - It requires <u>millions/billions of samples</u> to provide a few decimal points in accuracy
 - It may be the *only way* to take the integral of a very complex function
- We can calculate volume of any solid via the ratio of points that fall within a solid versus the total number of points
 - The volume of a 4-D unit hypersphere = $\frac{\pi^2}{2}$
 - A fractional 5-dimensional unit sphere has <u>maximum</u> volume
 - In ever increasing dimensions the volume of **all** hyperspheres approaches zero!