

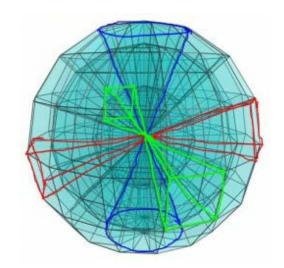
Survey of Scientific Computing (SciComp 301)

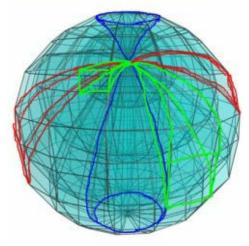
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Session 20 Monte Carlo Method

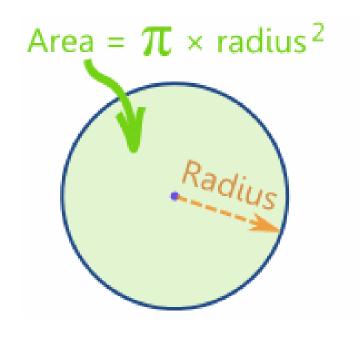
An Interesting Question

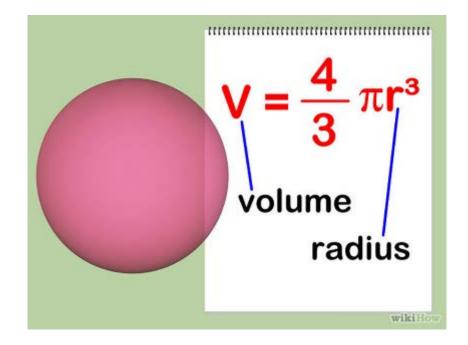
- What is the volume of a fourdimensional unit hypersphere?
 - What does a 4D sphere "look" like?
 - What is a "unit" sphere?
 - Where do I even start?
- Break down complex questions into simpler steps:
 - How can we calculate the area of a 2D circle?
 - How can we calculate the volume of a 3D sphere?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



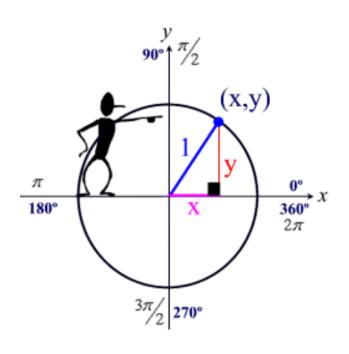


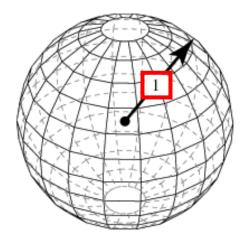
Area and Volume



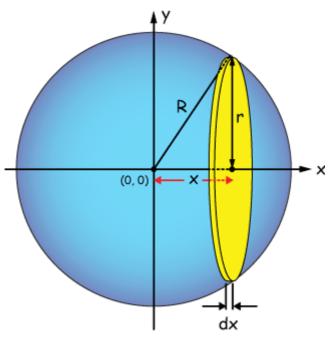


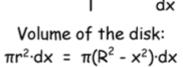
A Unit Circle and Unit Sphere

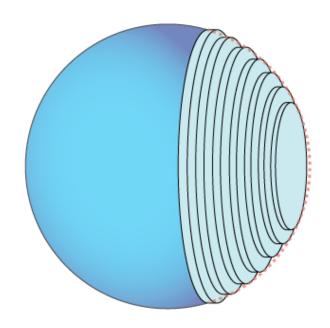




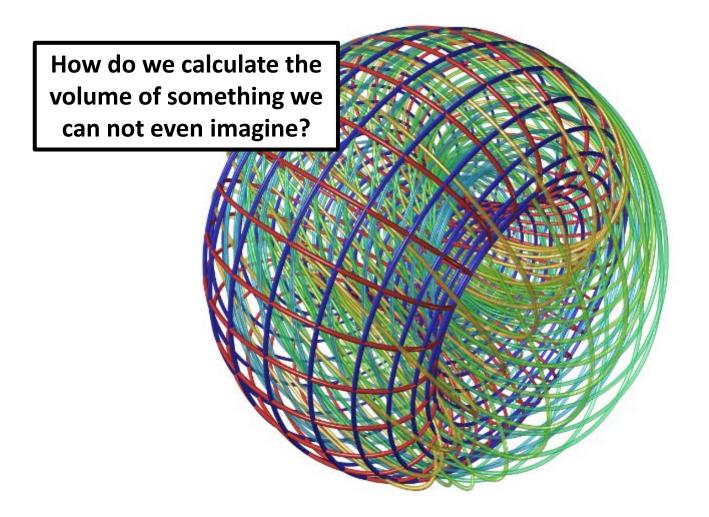
2-D Area → 3-D Volume



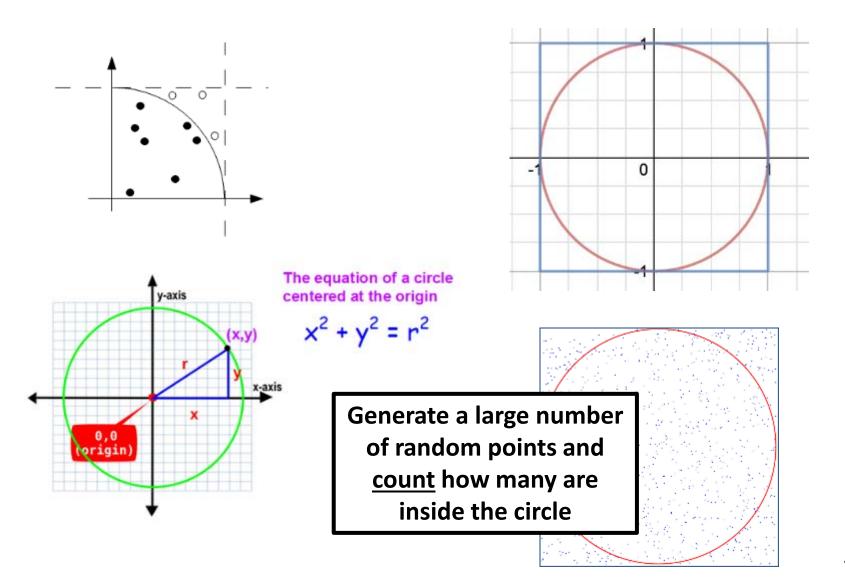


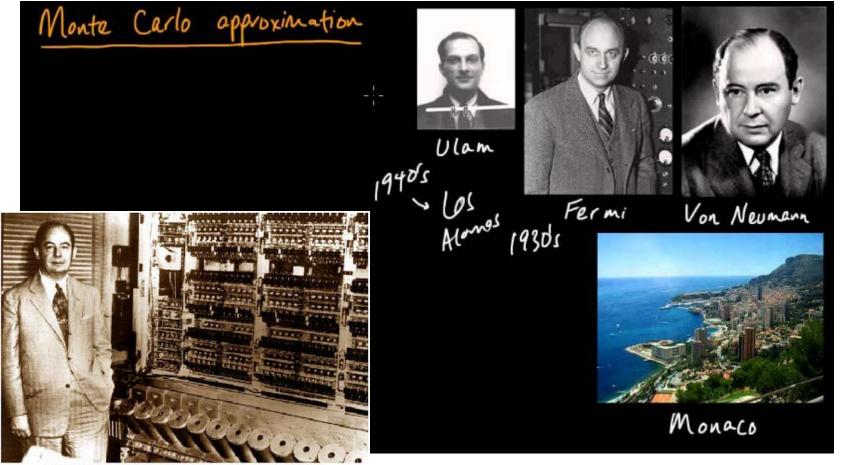


A 4-D Hypersphere



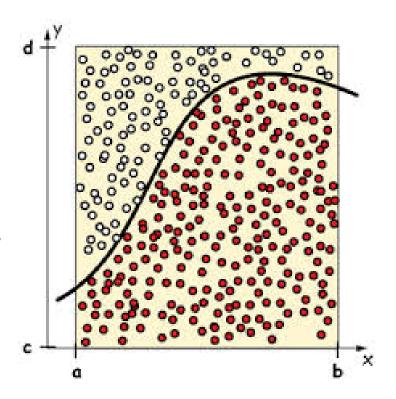
Area as a "Ratio" of Inside vs. Total Dots

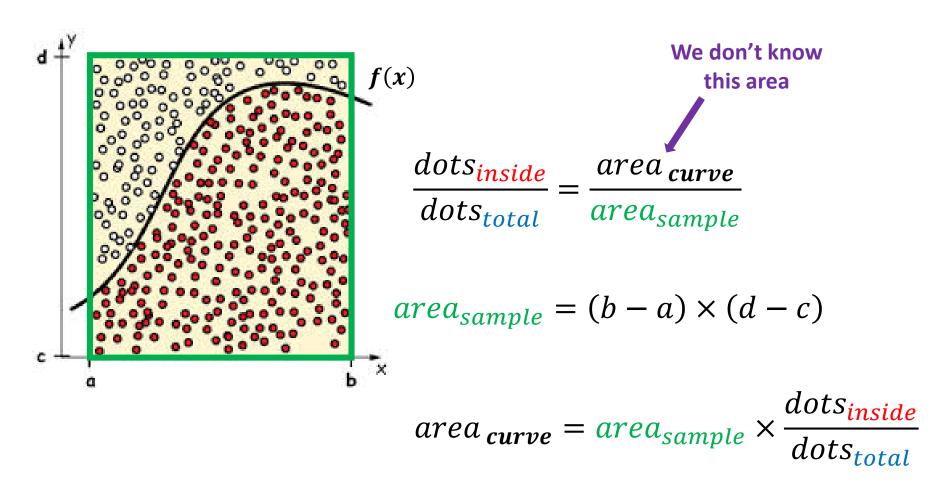


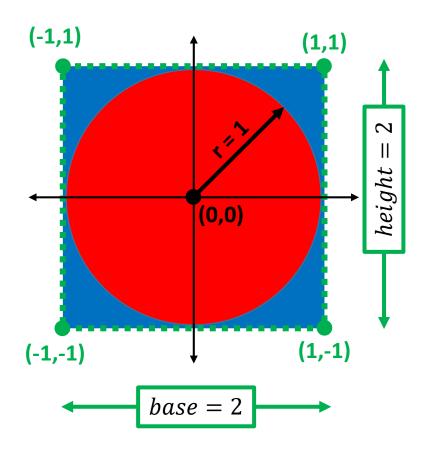


Johnny von Neumann [1903-1957] alongside the Maniac computer at the Institute for Advanced Studies, Princeton.

- With Monte Carlo, we randomly sample points within a bounded space and count how many are below the curve
- The <u>ratio</u> of <u>inside</u> dots (those under the curve) vs. <u>total</u> dots leads to an estimate of the *integral*
- Monte Carlo is non-deterministic when a random number generator is used to create the sample points







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

$$area_{sample} = base \times height$$

= 2 \times 2
= 4

$$area_{circle} = 4 \times \frac{dots_{inside}}{dots_{total}}$$

```
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{-1, 1}
   const int iterations = 100000;
   int count{};
    ss.LockDisplay();
   for (int i{}; i < iterations; ++i)</pre>
       double x = distribution(generator)
       double y = distribution(generator)
       if (x * x + y * y \le 1.0)
            ss.DrawPoint(x, y, "red");
            count++;
        else
            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</pre>
         << "Act. Area = " << M PI << endl
         << "Abs. % Err = " << abs(err) << endl:
```

2-D Area as a "Ratio" of Dots

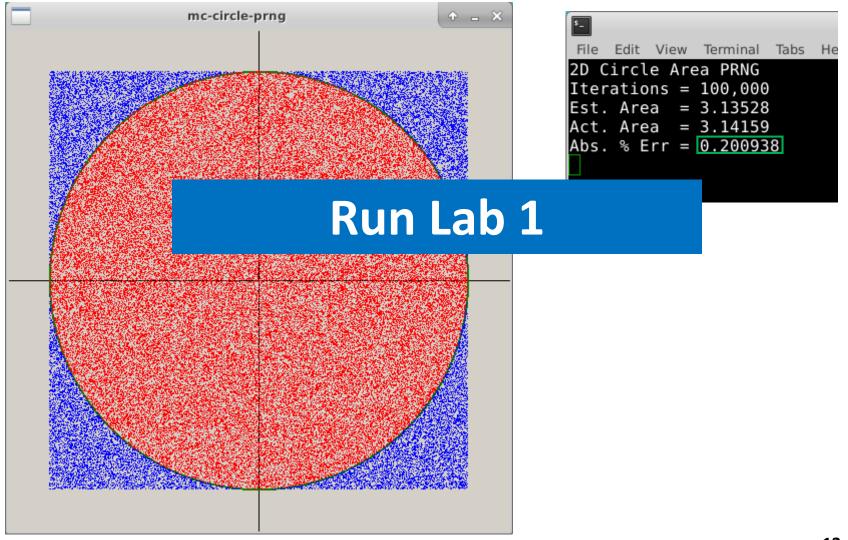
Open Lab 1

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

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

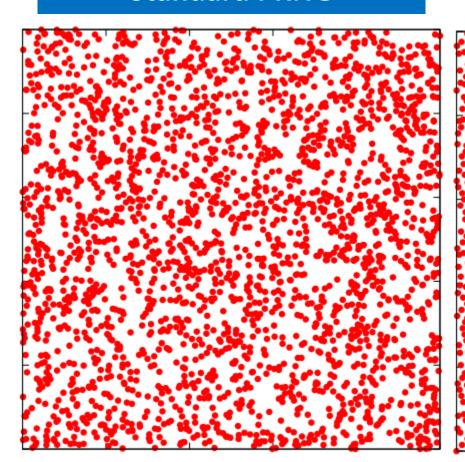
$$area_{circle} = \frac{count}{iterations} \times 4$$

2-D Area as a "Ratio" of Dots



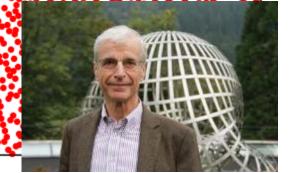
Comparing "Random" Number Generators

Standard PRNG

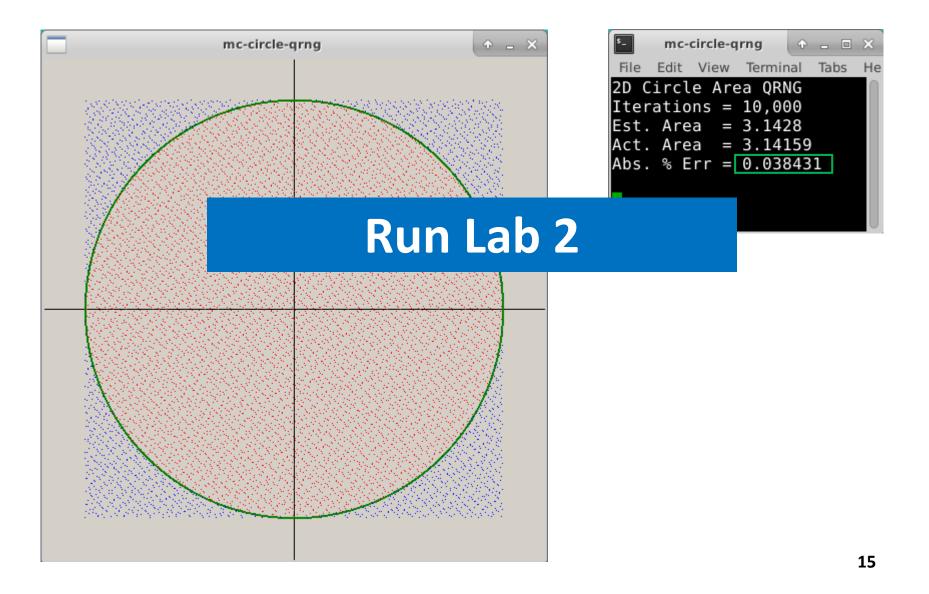


Niederreiter QRNG

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

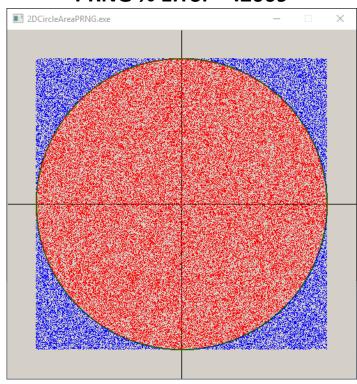


Improved 2-D Monte Carlo Estimator

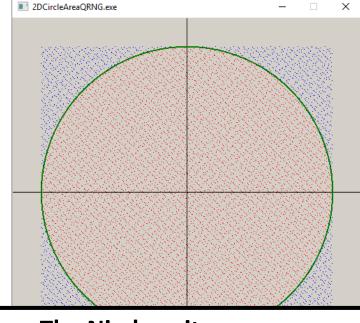


Improved 2-D Monte Carlo Estimator

PRNG % Error = .2009

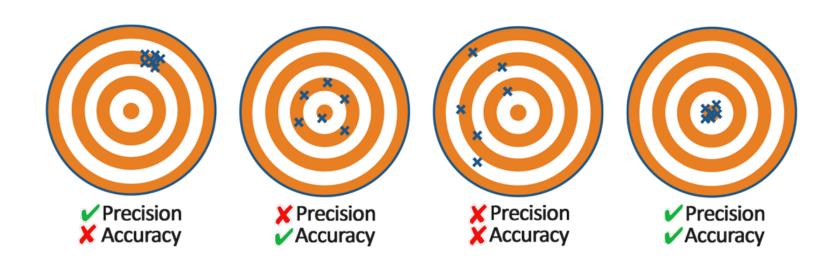


QRNG % Error = .0384



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

Accuracy vs. Precision





$\underline{\mathbf{A}}$ ccuracy = $\underline{\mathbf{A}}$ im

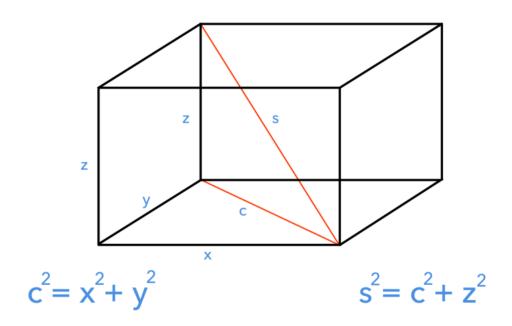
Hitting what you are pointing at

Precision = Consistency

- Digits of Precision ≠ Accuracy
- More digits → less variability

Moving to Higher Dimensions

The Pythagorean Distance is a **metric** that is true in all **orthogonal** spaces of any dimension



...
$$s^2 = x^2 + y^2 + z^2$$

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</pre> << "Iterations = " << iterations << endl</pre> << "Est. Volume = " << estVol << endl</pre> << "Act. Volume = " << actVol << endl</pre> << "Abs. % Error = " << abs(err) << endl << endl;</pre>

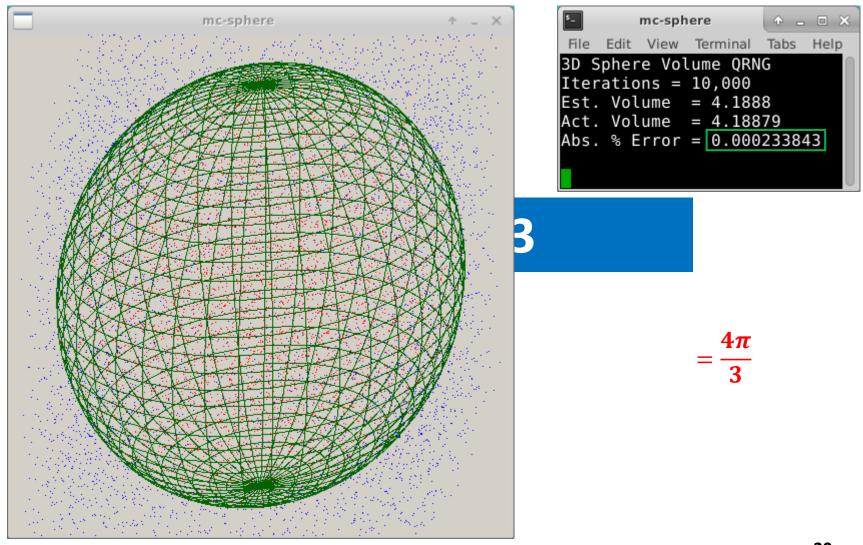
3-D Unit Sphere Volume Estimator

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

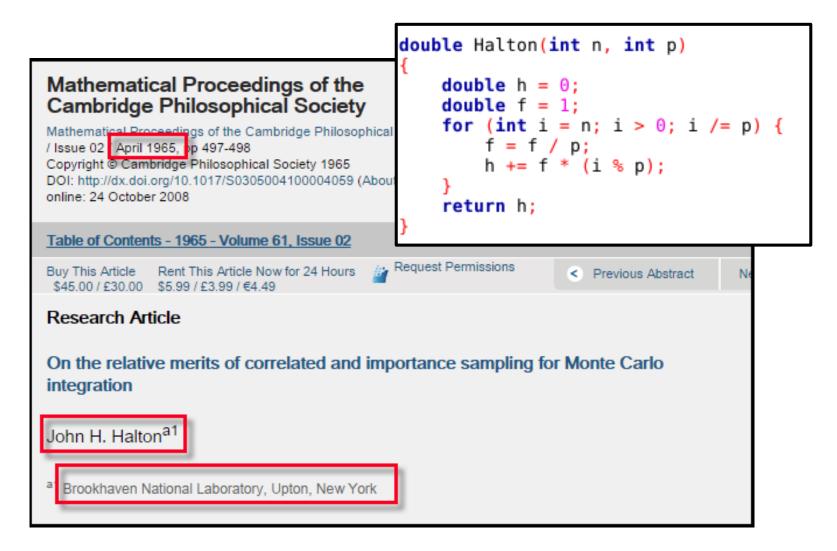
$$volume_{cube} = 2 \times 2 \times 2 = 8$$

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

3-D Unit Sphere Volume Estimator



The Halton Sequence



Accommodating the 4th Dimension

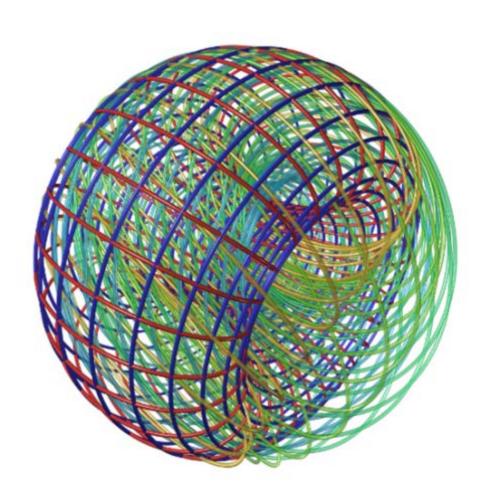
```
int main()
   int iterations = int(1e7);
   double count = 0;
                                                                      We need to
                                                                   update this code
   for (int i = 0; i < iterations; i++)</pre>
                                                                   to include the 4th
                                                                               bn!
       do
                    Open and edit Lab 4
       do
       double distance = x - x +
       if (distance <= 1.0)</pre>
           count++:
   double volume = count / iterations * 8;
   cout << fixed << setprecision(4)</pre>
        << volume << endl;</pre>
   return 0;
```

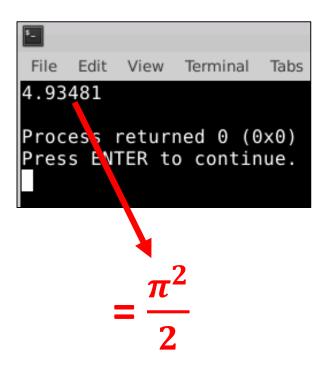
Accommodating the 4th Dimension

```
int main()
    int iterations = int(1e7);
    double count = 0;
    for (int i = 0; i < iterations; i++)</pre>
        double x = Halton(i, primes[0]);
        double y = Halton(i, primes[1]);
        double z = Halton(i, primes[2]);
        double w = Halton(i, primes[3])
        double distance = x * x + y * y + z * z + w * w;
        if (distance <= 1.0)</pre>
            count++;
    double volume = count / iterations * 16;
    cout << volume << endl;</pre>
    return 0;
```

Add all the code in red then run the application

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





We <u>can</u> calculate the volume of something we can not even *imagine!*

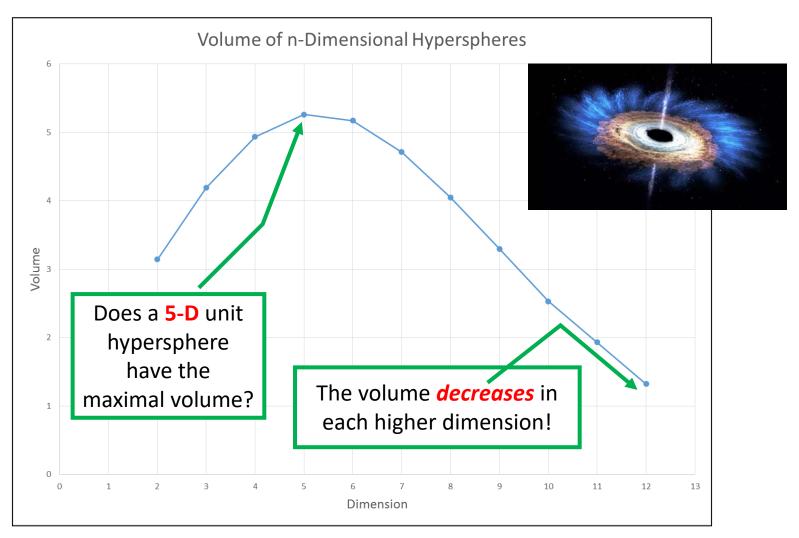
What lurks beyond the 4th dimension?

```
int main()
    int iterations = int(1e7);
                                                                                      This code will
    for (int dimension{2}; dimension < 13; ++dimension)</pre>
                                                                                       estimate the
        double count{};
        for (int i{}; i < iterations; ++i)</pre>
                                                                                    volume up to the
                                                                                     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?

```
int main()
    int iterations = int(1e7):
    for (int dimension{ 2 }; dimension < 13; ++dimension) {</pre>
        double count{};
        for (int i{}; i < iterations; ++i) {</pre>
            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:
                                                                            mc-highdimensional
                                                                            Edit View Terminal Tabs Help
            if (distance <= 1.0)</pre>
                                                                        2, 3, 1416
                count++
                                            Run Lab 5
                                                                        3, 4.1888
        double volume =
                                                                        4, 4.9348
        cout << fixed <<
                                                                        5, 5.2630
            << setprecis
                                                                         6, 5.1692
            << endl;
                                                                         7, 4.7208
                                                                         8, 4.0605
                                                                         9, 3.2935
    return 0;
                                                                        10, 2.5463
                                                                       11, 1.8883
                                                                       12, 1.3443
                                                                       Process returned 0 (0x0)
                                                                       Press ENTER to continue.
```

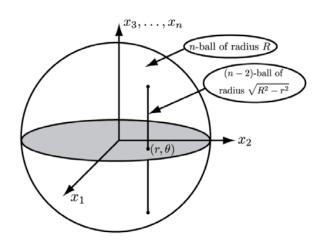
What lurks beyond the 4th dimension?



A Recurrence Relation

The **volume** of an **n-ball** is proportional to the <u>unit</u> ball for that dimension

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



We can compute $V_n(1)$ by integrating the n-2 ball over a unit disk using polar coordinates

$$V_n(1) = \int_0^1 \int_0^{2\pi} V_{n-2}(1) \left(\sqrt{1 - r^2} \right)^{n-2} r \, d\theta \, dr$$

$$= V_{n-2}(1) \int_0^1 r(1 - r^2)^{\frac{n-2}{2}} \theta \Big|_0^{2\pi} \, dr$$

$$= 2\pi V_{n-2}(1) \int_0^1 r(1 - r^2)^{\frac{n-2}{2}} \, dr$$

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

A Recurrence Relation

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

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

By definition

$$V_o(1) = 1$$

$$V_o(R) = 1$$

$$1 - (-1) = 2$$

$$V_1(1) = 2$$

$$V_1(R) = 2R$$

$$V_2(1) = \frac{2\pi}{2}(1) = \pi$$

$$V_2(R) = \pi R^2$$

$$V_3(1) = \frac{2\pi}{3}(2) = \frac{4}{3}\pi$$

$$V_3(R) = \frac{4}{3}\pi R^3$$

$$V_4(1) = \frac{2\pi}{4}(\pi) = \frac{\pi^2}{2}$$

$$V_4(R) = \frac{\pi^2}{2}R^4$$

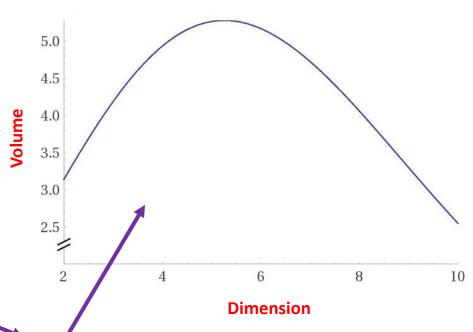
Volume via the Gamma Function

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

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

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

Volume of Unit Hypersphere



Because we can evaluate $\Gamma(x)$ at every point in \mathbb{R} we can now determine the volume of a unit hypersphere in *any* dimension

Volume via the Gamma Function

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

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

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

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

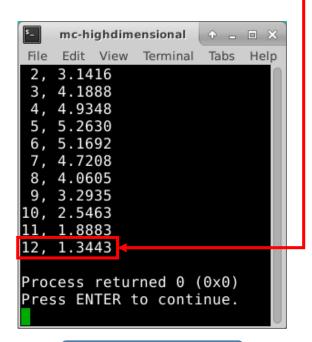
$$V_3(R) = \frac{\pi^{\frac{3}{2}}R^3}{\Gamma(\frac{3}{2}+1)} = \frac{\pi R^3}{\Gamma(\frac{5}{3})} = \frac{\pi^{\frac{3}{2}}R^3}{(\frac{3\sqrt{\pi}}{4})} = \pi^{\frac{3}{2}}R^3(\frac{4}{3\sqrt{\pi}}) = \frac{4}{3}\pi R^3$$

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

Challenges of Numerical Analysis

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

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.

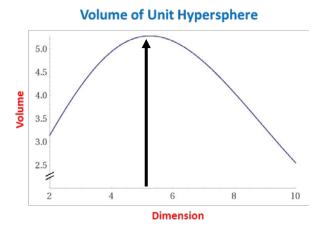
Volume via the Gamma Function

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

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

```
Euler's Gamma integrand
inline double f(double x, double s)
    return pow(x, s - 1) * exp(-x)
// Find Gamma using Simpson's integration
double gamma(double s)
    double a{0};
    double b{1e3};
    int intervals = 1e5;
    double dx{(b - a) / intervals};
    double sum{f(a, s) + f(b, s)};
    a += dx;
    for (int i{1}; i < intervals; ++i, a += dx)</pre>
        sum += f(a, s) * (2 * (i % 2 + 1));
    return (dx / 3) * sum;
// Find volume of unit ball
// See https://en.wikipedia.org/wiki/N-sphere
double v(double x)
    double halfx = x / 2.0;
    return pow(M PI, halfx) / gamma(halfx + 1)
```

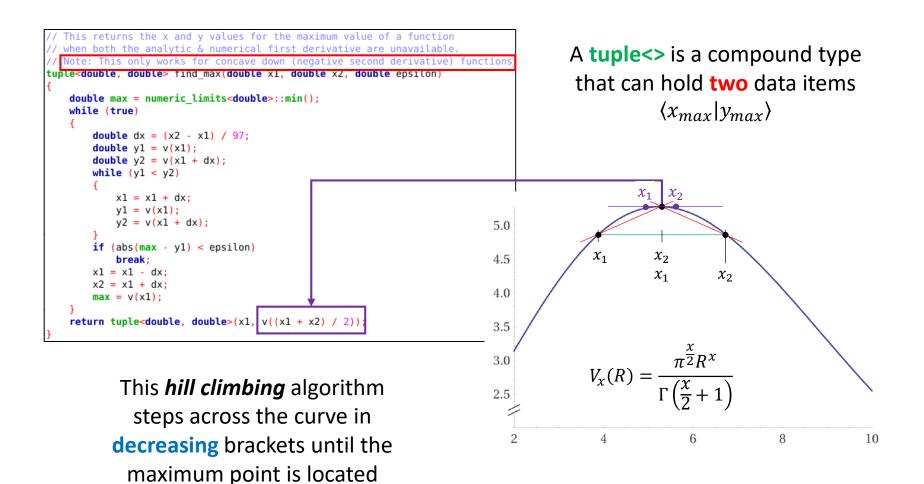
 This code uses Simpson's Rule to calculate Euler's Gamma function:

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

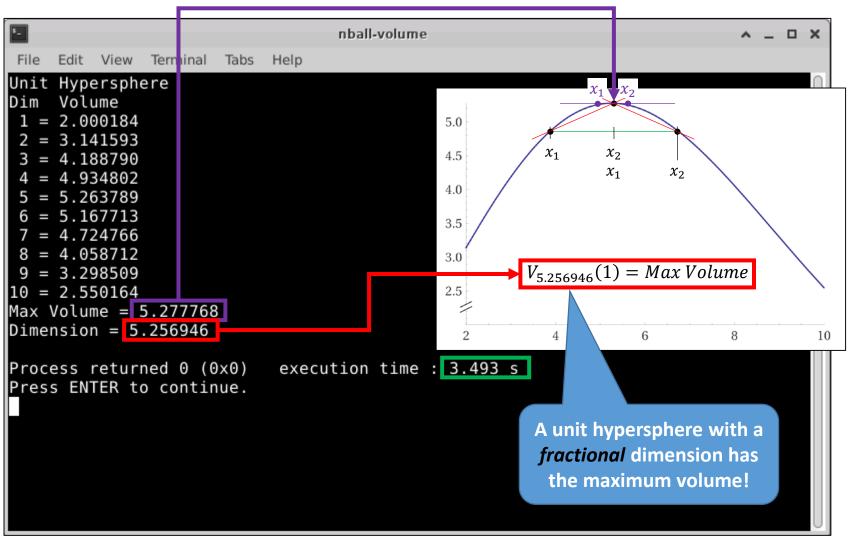
 The code uses Gamma to find the volume of unit hyperspheres with fractional dimensions

$$V_{x}(1) = \frac{\pi^{\frac{x}{2}}}{\Gamma(\frac{x}{2} + 1)}$$

View Lab 6 – nball-volume



Run Lab 6 – nball-volume



Edit Lab 6 – nball-volume

```
// Find volume of unit ball
// See https://en.wikipedia.org/wiki/N-sphere
double v(double x)

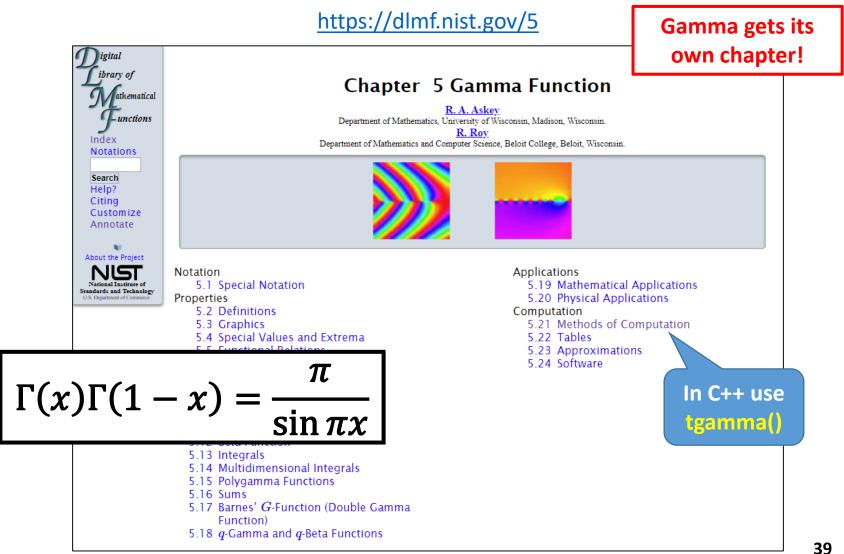
{
    double halfx = x / 2.0;
    return pow(M_PI, halfx) / tpamma(halfx + 1);
}

Edit line # 33 to call the
C++ tgamma() function
"the true gamma"
```

Run Lab 6 – nball-volume

```
nball-volume
     Edit View
               Terminal Tabs
                             Help
Unit Hypersphere
Dim Volume
                                 26
                                       // Find volume of unit ball
 1 = 2.000000
                                 27
                                       // See https://en.wikipedia.org/wiki/N-sphere
 2 = 3.141593
                                 28
                                       double v(double x)
 3 = 4.188790
                                 29
                                 30
 4 = 4.934802
                                          double halfx = x / 2.0;
 5 = 5.263789
                                 31
                                           return pow(M PI, halfx)
                                                                  t_{namma}(halfx + 1);
 6 = 5.167713
 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 : 0.030 s
Process returned 0 (0x0)
                                                                      "the true gamma"
Press ENTER to continue.
                                The built-in tgamma() is
                                11,500% faster than our
                                 Simpson's integration!
```

Euler's Gamma Function



The Power Of Monte Carlo Integration

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

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

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

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

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

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 may require <u>billions of samples</u> to provide a reasonable estimate
 - It may be the *only way* to take the integral of a very complex function
- What you are taught cannot be the limit of your knowledge
 - The volume of a 4-D unit hypersphere = $\frac{\pi^2}{2}$
 - In infinite dimensions the volume of **all** hyperspheres is zero!
 - A <u>fractional</u> 5-dimensional unit sphere has maximum volume
 - Mother Nature never said dimensions have to be integers!