

HW TIP! https://www.monash.edu/rlo/ assignment-samples/science/ science-writing-a-lab-report

Szydagis

## VON NEUMANN'S MONTE CARLO INTEGRATION AND RELATED



## HW3 Help: Rand 3D Angles How-To

I try, but can't always predict the HW questions, so that's what Tuesday morns are for

- https://mathworld.wolfram.com/SpherePointPicking.html
- Assuming phi means polar, theta azimuthal
  - X = r cos(phi) sin(theta) where phi [0,2pi) random
  - Y = r sin(phi) sin(theta) Naming conventions change!
  - Z = r cos(theta) where theta between [0,pi] radians
- BUT, cosine of theta not theta randomized
  - Why? Has to do with uniform solid angle arguments

• Use sin^2 + cos^2 = 1 in order to derive sine from cosine

Elastic collision? (Fixed energy & angle) What to do: <u>https://en.wikipedia.org/wiki/Elastic collision</u> again is the right answer; you can ignore (complex) and do random angle, half-*E* MFP: diff types of exp. Mine v. 1/MFP (C++ default)
 While loop: do NOT stop at 0, but \*>\* it! You can use – instead of /

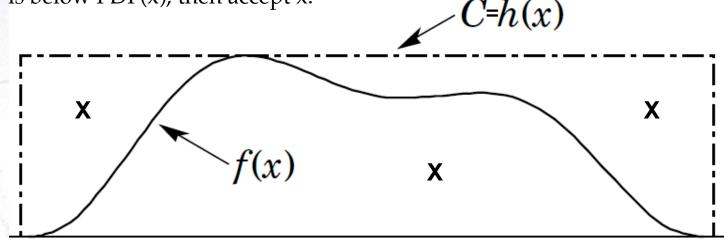
Time permitting: the C glossary doc.

# Accept-Reject method

#### (Von Neumann method)

If the PDF<sup>\*</sup>we wish to sample from is bounded both in x and y, then we can use the "Accept-Reject" method to select random numbers from it, as follows:

- Pick x and y uniformly without in the range of the PDF.
- If y is below PDF(x), then accept x.



The main advantage of this method is its **simplicity**, and given modern computers, one does not care much about efficiency. However, it requires **boundaries**!

\* PDF = Point Distribution Function

https://www.nbi.dk/~petersen/Teaching/Stat2015/ Week3/AS2015\_1130\_MonteCarlo.pdf

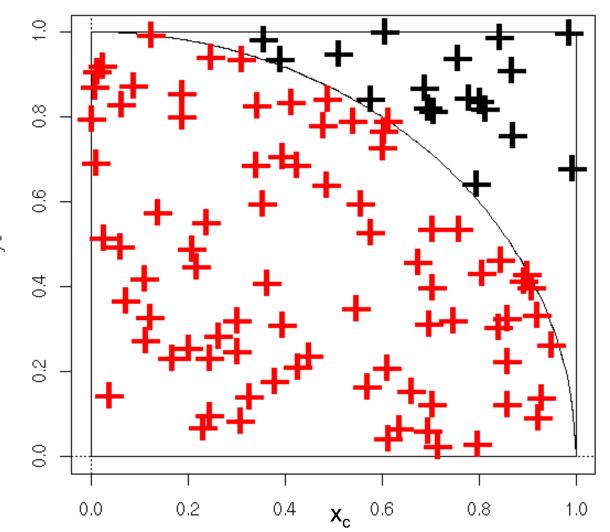
# **Calculating Pi**

Why quarter unit circle? Because then 1D \*function\* (monotonic too)

- This is called the Hit-and-Miss method (Von Neumann method):
- Find min and max in both x and y.
- Generate uniform random numbers (x,y) in these ranges.
- Accept x, if y < f(x).
- Reject x, if y > f(x). >= ?  $\leq$

It is remarkable accuracy (though not precision) for such a relatively small number of darts throws! (at right)

#### Monte Carlo Simulation: pi=3.28



Goes as 1/sqrt(N) and thus wins over all other methods (e.g. trapezoidal integration) eventually 4

## **Higher Dimensions**

- Your homework #4 will be for 1-D integration (single-valued function of y versus x)
- A circle pi example (completing circle from last slide all the way around) is more 2-D
- We can extend this to 3-D: vol of (unit+) sphere
  - Bounding cube (or rectangular prism more generally) instead of a bounding box
  - Can also be used to find pi, but only if you know spherical volume formula first <sup>©</sup> And, this is slower
  - Download "sphere.cpp" sample code from site

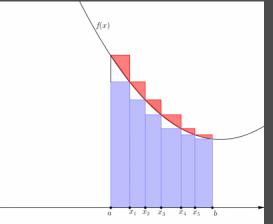
Very powerful: method will work for any shape

As #trials goes to inf, though may converge slowly

#### **Contrast: Blast From the Past**

#### Good old-fashioned Riemann integration

- Left-hand "rule"
- Right-hand
- Midpoint
- Trapezoid
- Simpson's rule



DOWNLOAD "integrator.cpp" from the course website

- 3/8-version, higher-order polynomials
- Adaptive step size
- Taylor, Maclaurin, Laurent, or similar series
  - Expand first, then integrate that (easier?)
- What does Mathematica do? Richardson extrapolation compared to Simpsons-like

#### Integrator dot CPP

- We will pick integrands that canNOT be integrated analytically
  - And pick some reasonable finite bounds 'a,' 'b' (no singularities YET)
- We will compare these different methods and pick the fastest + most accurate
  - N=? to match online answer(s)?
  - Richardson: I accidentally re-derived myself!
- If difference between convergent numerical result from the main part of our code and the right answer (or a pi or 'e' trick) differs by less than 10^-7, then we can safely call that the analytical answer (???)

#### HW #4: Integration. Due Feb. 22

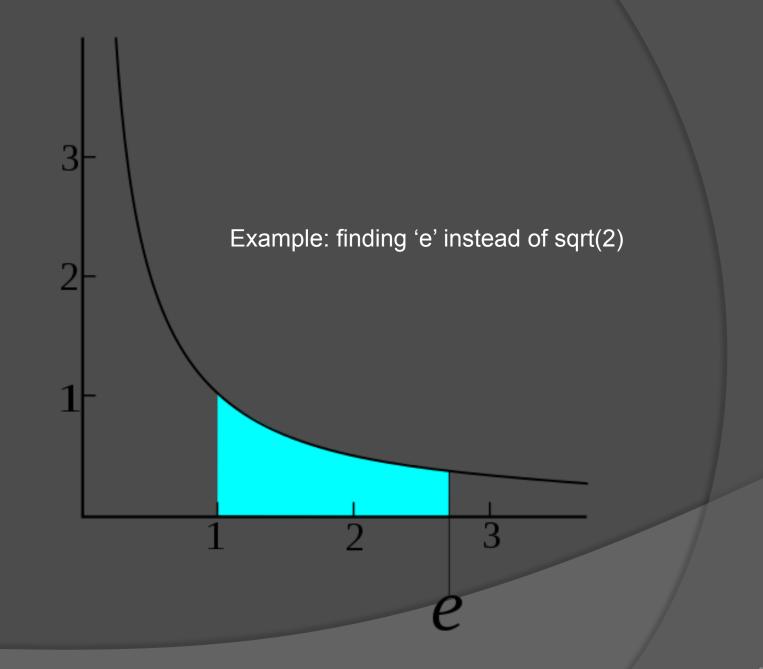
- Integrate the area (should come out to exactly root 2) under the curve 0.5/x^1.5 from 1-2 to find a precise and accurate value as fast as possible
  - The analytical answer is 1-1/sqrt(2), so manipulate it
- Use Monte Carlo integration first, but then...

Check your answer by taking the analytic function

 And integrating that with one (your choice) of the more "regular" methods (e.g. a Riemann sum or Simpson's)

O 2 PLOTS: A v. N or step size. Show convergence

- Answer the question: which method converges faster?
- So, final answer is 1 number this time, and only 2 plots
- Sonus: Come up w/ a better bounding box shape



#### Backup Slides +Helpful Links

Can cross-check numerical answers with

- http://www.wolframalpha.com/widget/ widgetPopup.jsp?
   p=v&id=29c546473e1c796d6076bb18901b15e7&i0= 4133000%20\*%20n%5E-0.491&i1=1&i2=3000000&p odSelect=&showAssumptions=1&showWarnings=1
- Cross-check the full, analytical answers with Mathematica, or for free with
  - http://www.wolframalpha.com/widgets/view.jsp? id=a787670f0f1047d7fbe288763c55ba14
  - <u>https://www.wolframalpha.com/calculators/integral-</u> <u>calculator/</u> (Google: does not have to be Wolfram)

Can X2-check everything analytically (and/or with ~Mathematica online) but not main point.

#### Improper Integrals: Infinite Series

- Can do infinite sequences or sums, as effectively on your own as with com software
  - And with complete control and freedom to customize
- Convergence and divergence (not rigorous)
- summer.cpp (get it? Ba dum ching)
  - We will explore several different interesting infinite series to find their sums
  - Code just uses plain addition (no fancy tricks!!!)
  - Exploration: small tweaks will be able to change convergence rate, or even cause divergence!
- Let's apply to physics now, beyond "just math"

#### The Importance of Infinite Series

- Occur all of the time in physics, including in quantum mechanics, especially in QFT; string theory!
- Though examples still exist in stat mech/therm & classic mechanics
  - Consider bouncing ball problem: infinite on paper! Damped pendulum, coin spin.
  - Total gravitational force on an object in universe from all others? BHs in-spiral?
- Astronomy and astrophysics
  - Approaching edge of a finite universe in a non-trivial cosmological topology
  - Falling into a black hole from outside
- Numerical recipes for integration!

#### Let's Have Some Fun With This

Let's explore (seeing what converges fastest or not)

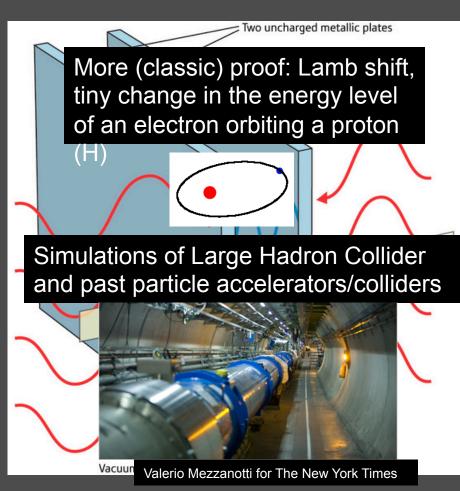
- 1/n<sup>p</sup>, where p is a positive power that is not necessarily integer. Look for pattern in convergence; n all odd, all even
- 1/n<sup>n</sup>, 1/n!, 1/log(n), 1/a<sup>n</sup> a>1, 1/exp(n), 1/sin(n). Which converge and which don't? (Same question for above)
- Same as above but with (-1)^n in numerator instead of 1.
   With (-1)^n is, naturally, known as an alternating series
- Fibonacci sequence: derive the golden ratio (of ~1.6)

Look for integer multiples or fractions of pi or e...

 Can potentially beat Mathematica in finding an analytical solution to a particularly trying (incorrigible) series that breaks our sharp, spear-tip pointed analyses repeatedly, in a non-rigorous (guess-and-check/empirical) way

• Though one that can still lead to some deep physics at some point, potentially. Integer multiples, fractions of  $\pi$ , e (e.g.,  $\pi^4/512$ ). Can use loops to automatically scan...

## A Different Kind of Force: Casimir



Copyright © 2008 Yampol'skii and Nori

#### The Casimir Effect

- Can borrow a little energy from vacuum, and it doesn't even have to be a temporary loan (think short distance scales)
  - "Virtual" particles have real effects (can carry a force)
- Plates initially uncharged develop calculable electrical potential difference & then attract each other (diff electric charges, – and + or +/-)
  - Very small effect, difficult to measure, but we've done it

### 1 + 2 + 3 + 4 + ... = -1 / 12 ?!

- Riemann zeta function (but this is only \*one\* of a great many but, remarkably, *consistent* ways of "proving" this "fact" to be true
- Analytical continuation (other examples include factorial and gamma function, as well as scale factor vs. time in an empty anti-de Sitter space in cosmology)
- Casimir force: nature knows about the infinite energy and SUBTRACTS it out

#### Proofs

$$\zeta(n) = \sum_{k=1}^{\infty} \frac{1}{k^n},$$

• 
$$\zeta(2n) = \sum_{k=1}^{\infty} \frac{1}{k^{2n}} = (-1)^{n+1} \frac{B_{2n}(2\pi)^{2n}}{2(2n)!}$$

The first few values are:

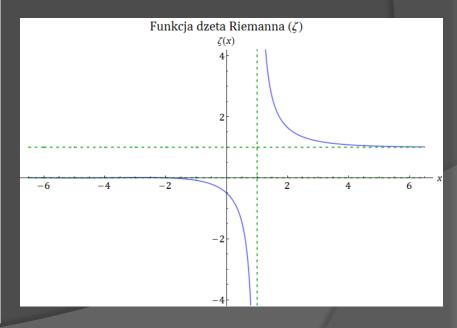
$$\zeta(2) = \sum_{k=1}^{\infty} \frac{1}{k^2} = \frac{\pi^2}{6} \text{ (the Basel problem)}$$
  

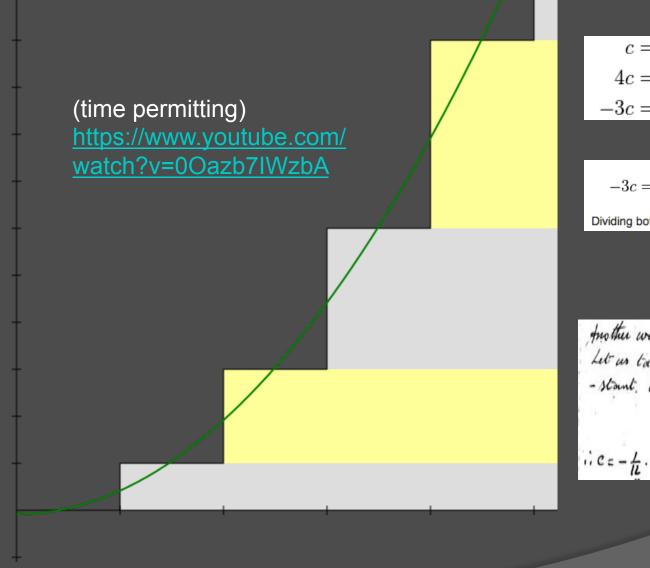
$$\zeta(4) = \sum_{k=1}^{\infty} \frac{1}{k^4} = \frac{\pi^4}{90}$$
  

$$\zeta(6) = \sum_{k=1}^{\infty} \frac{1}{k^6} = \frac{\pi^6}{945}$$

Via analytic continuation, one can show that  $\zeta(-1) = -\frac{1}{12}$ 

$$\zeta(0) = -\frac{1}{2};$$
  
 $\zeta(1/2) \approx -1.4603545$ 





$$c = 1 + 2 + 3 + 4 + 5 + 6 + \cdots$$
  

$$4c = 4 + 8 + 12 + \cdots$$
  

$$-3c = 1 - 2 + 3 - 4 + 5 - 6 + \cdots$$

$$-3c = 1 - 2 + 3 - 4 + \dots = \frac{1}{(1+1)^2} = \frac{1}{4}$$

Dividing both sides by -3, one gets c = -1/12.

Another way of Linding the constant is as follows \_41 Let us take the scile 1+2+3+4+5+&c. Let Cheils con - stant. Then C = 1+2+3+4+ &c ...+c = 4 + F + &c ...-3C = 1-2+3-4+ &c = (1+1) = 4 ic=-1.