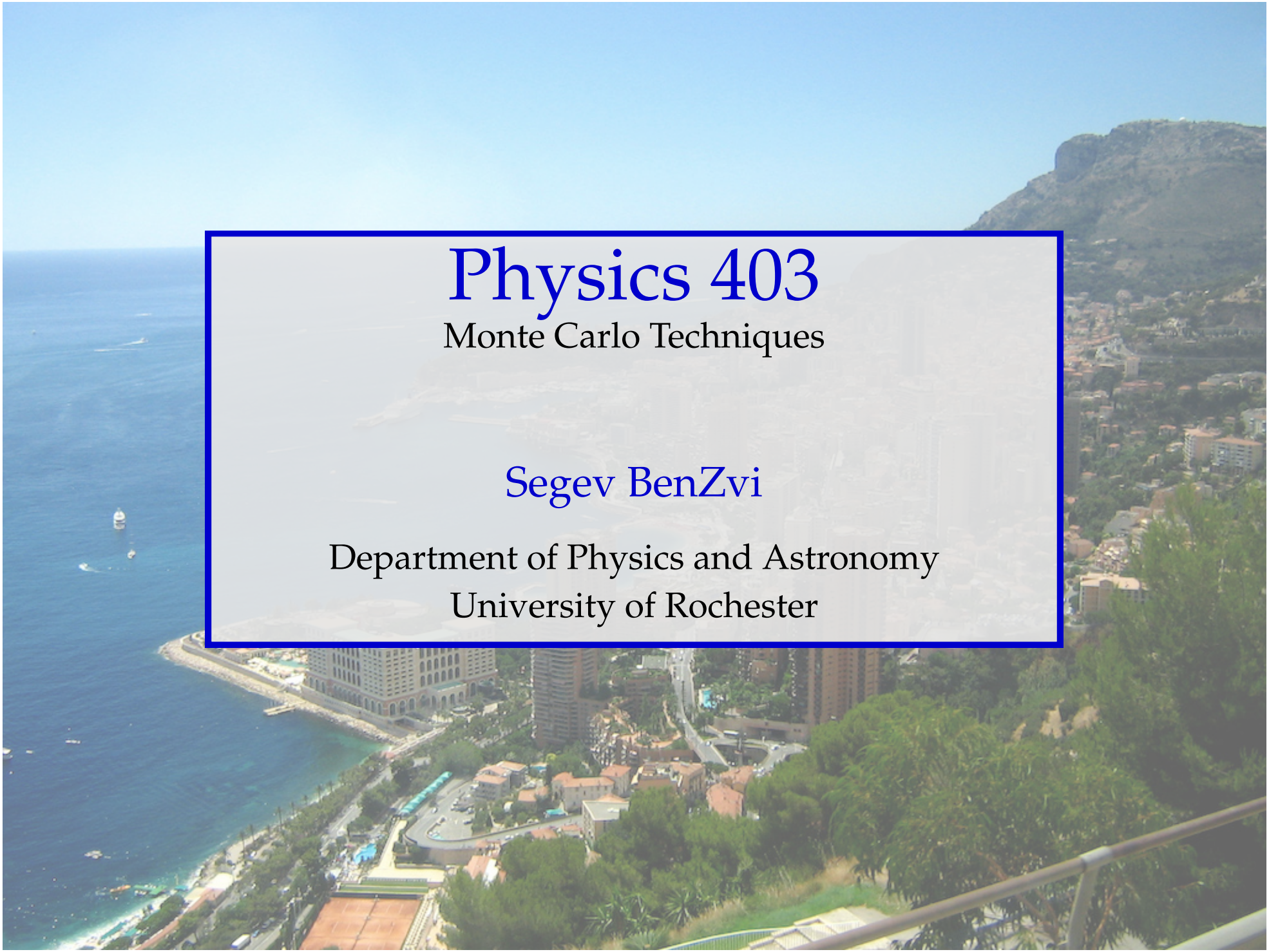

Physics 403

Monte Carlo Techniques

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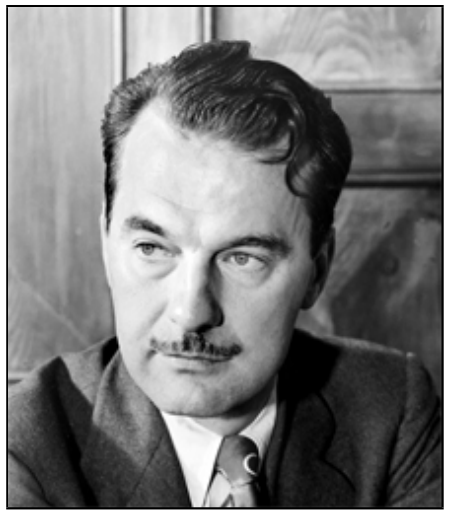
Monte Carlo Method

"Monte Carlo" methods are a broad set of techniques for calculating probabilities and related quantities using sequences of random numbers.





Developed by S. Ulam, J. von Neumann, and N. Metropolis at LANL in 1946 to model neutron diffusion in radiation shields.

Method was called "Monte Carlo" after the Casino de Monte-Carlo in Monaco.

Simulation and Random Number Generation in Physics

Some examples of problems where this technique is very popular:

- Simulate physical systems with models of noise and uncertainty
- Simulate data with known inputs to stress-test your analysis ("data challenges"). Can be quite extensive...
- Perform calculations that cannot be done analytically or with a deterministic algorithm. E.g., function minimization, or many high-dimensional integrals
- Inverse Monte Carlo: estimate best-fit parameters with uncertainties using many simulated data sets, avoiding explicit and difficult uncertainty propagation

All this depends upon the generation of (pseudo-)random numbers. This means you MUST understand how random number generators (RNGs) work!

Example Simulation from U of R Faculty

Physics of granular materials which become rigid with increasing density ("jamming" transition) [1]:

PRL **113,** 148002 (2014) PHYSICAL REVIEW LETTERS week ending 3 OCTOBER 2014

Universality of Jamming Criticality in Overdamped Shear-Driven Frictionless Disks

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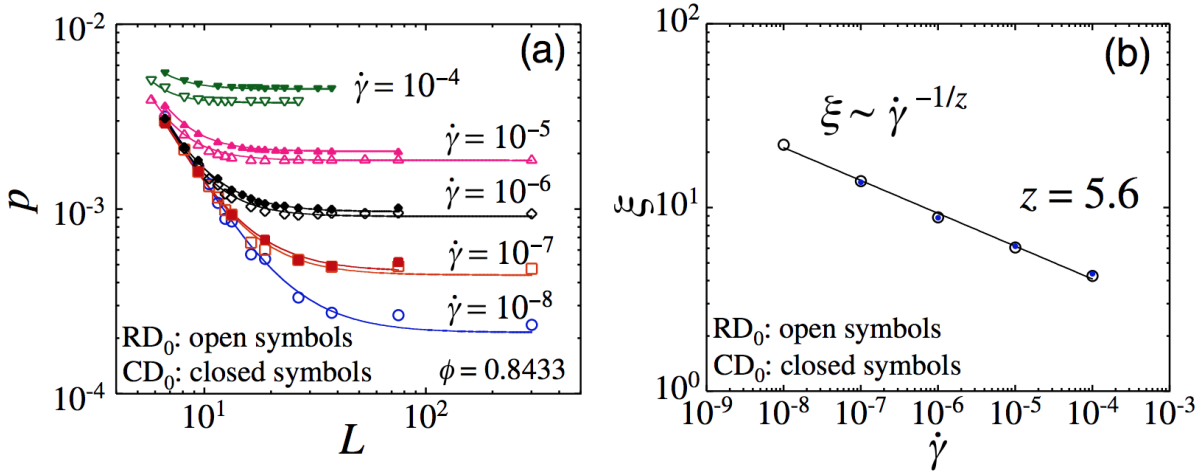
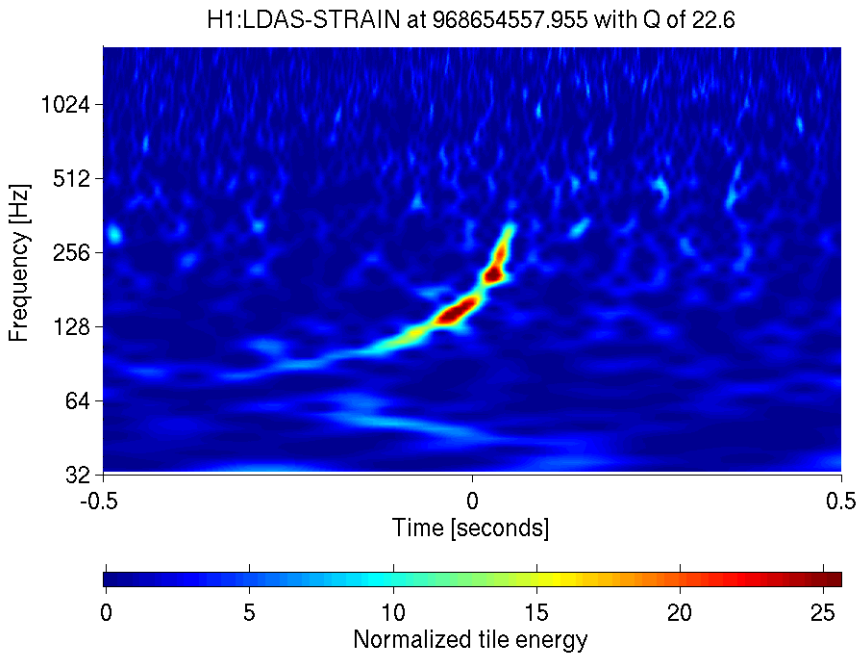
(Received 18 December 2013; revised manuscript received 4 August 2014; published 3 October 2014)

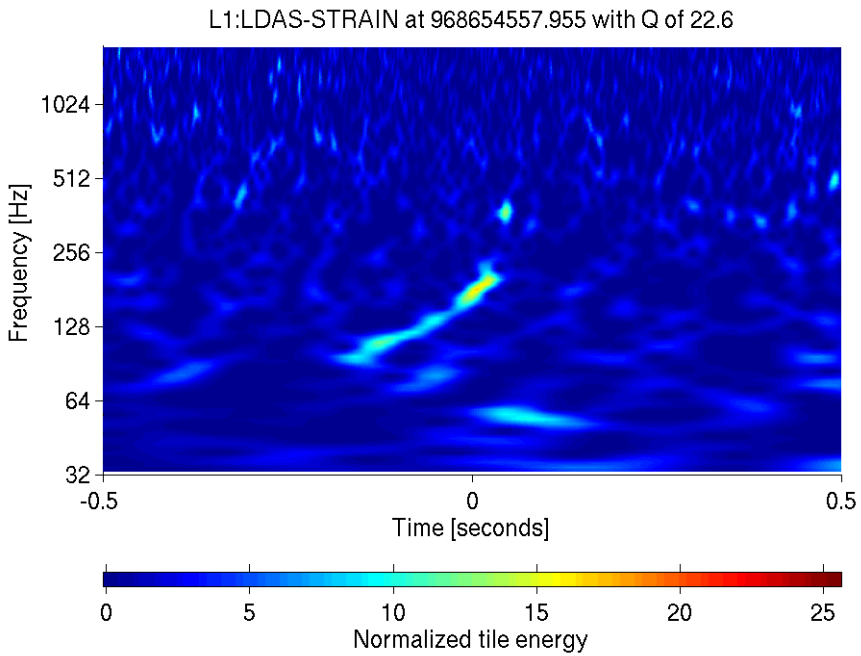
We investigate the criticality of the jamming transition for overdamped shear-driven frictionless disks in two dimensions for two different models of energy dissipation: (i) Durian's bubble model with dissipation proportional to the velocity difference of particles in contact, and (ii) Durian's "mean-field" approximation to (i), with dissipation due to the velocity difference between the particle and the average uniform shear flow velocity. By considering the finite-size behavior of pressure, the pressure analog of viscosity, and the macroscopic friction σ/p, we argue that these two models share the same critical behavior.



Example "Data Challenge"

The Laser Interferometer Gravitational Wave Observatory (LIGO) is (in)famous for carrying out extensive data challenges [2]





Very important to conduct end-to-end "stress tests" in background-dominated analyses. Above: fake binary merger injected into LIGO data stream, 2011

Generating Random Numbers

The Monte Carlo Method depends upon the generation of random numbers with a computer.

But a computer is (supposed to be) a deterministic device: given a fixed input and starting conditions, we should always get the same output.

> *Anyone who considers arithmetical methods of producing random digits is, of course, in a state of sin.*
> *– John von Neumann*

So we are actually talking about generating pseudorandom numbers.

To understand Monte Carlo methods, we MUST understand how pseudo random number generators (PRNGs) function.

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Pseudo-Random Numbers

- We need to generate sequences of random numbers to model noise and uncertainty.

- Computers are not random, they are deterministic. So how do we get random sequences of numbers?
- Answer: we don't. We produce *pseudo*-random sequences and try to use them in clever ways.

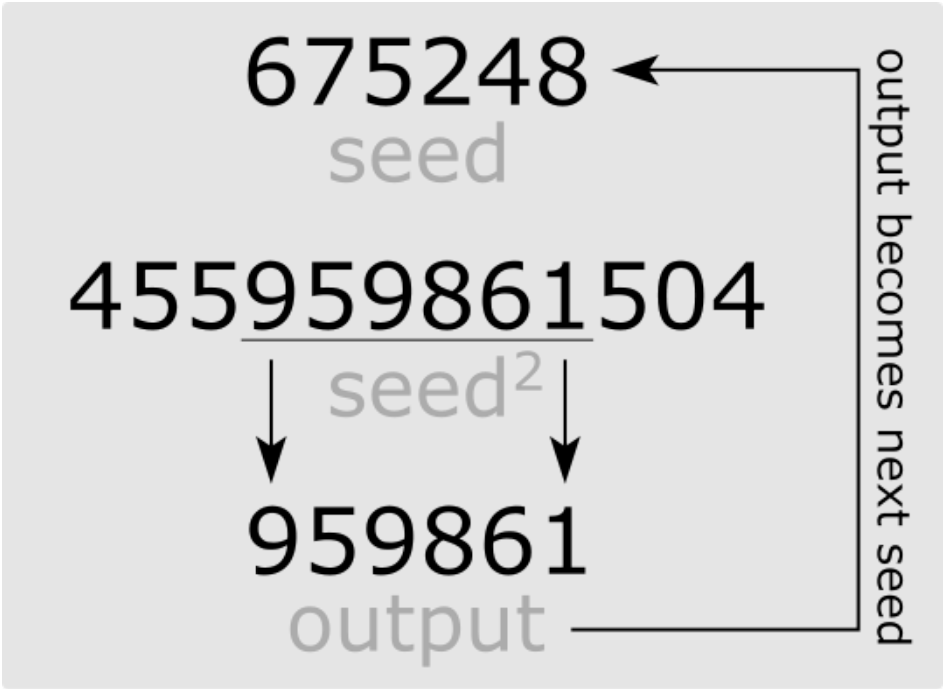
Pseudo-Random Number Generators (RNGs)

Middle-Square Method

Arithmetical approach to producing a sequence of "random" numbers:

- Start with a "seed" value containing n digits
- Square the number to get a new value with $2n$ digits; if the result has less than $2n$ digits, pad it with leading zeros
- Take the central n digits as the output
- Use the output as the next "seed" value

Note: this is just a toy example!



Pseudo-Random Number Generators (RNGs)

Linear Congruential Generator

- The pseudo-RNG used in the `rand()` function of the C standard library is a linear congruential generator (LCG)
- A sequence of values $x_i \in [0, m-1]$ is generated using the recurrence relation

$$x_{n+1} = (a x_n + c) \bmod m$$

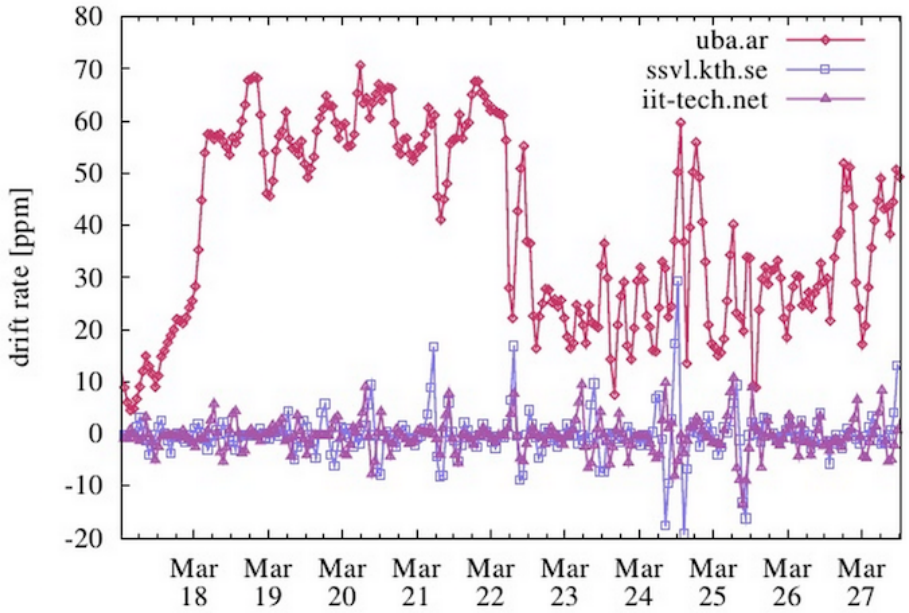
- The **period** of the RNG, defined as the longest number of steps before the sequence starts repeating, is at most 2^m.
- Note: if m is an unsigned integer (`uint32_t` on most systems) then the period will be at most $2^{32} \approx 4 \times 10^9$. (Note: $2^{64} \approx 10^{18}$)
- For many choices of m, the period will be much less than 2^m.
- **Theorem**: the full period of the LCG is achieved iff c and m are co-prime, $a-1$ is divisible by all prime factors of m, and $a-1$ is a multiple of 4 if m is a multiple of 4 [3].

"Seeding" the RNG

- Note that pseudo-RNGs are deterministic. If you always use the same x_0, a value known as the **seed**, you always get the same sequence.
- The choice of seed can affect the performance of the LCG; i.e., a poor choice could lead to a period $\ll m$.
- Determinism is great for debugging, but if you generate the same numbers over and over you aren't getting a pseudo-random sequence
- **Common mistake 1**: accidentally hardcoding the seed into your simulation code
- **Common mistake 2**: failing to save the seed you used, which makes it hard to regenerate the sequence later for checks

Choosing the Seed

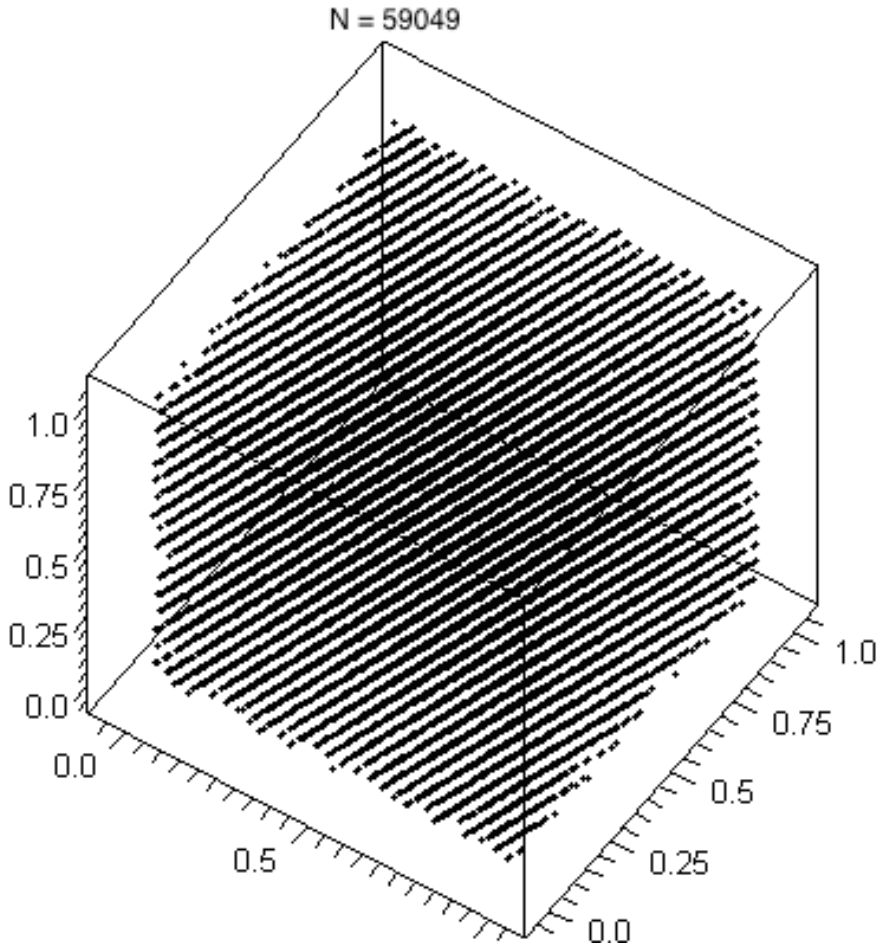
- **Solution 1**: use system clock to choose x_0. On UNIX-like machines, `time(0)` gives seconds since 00:00 UT, 1 Jan 1970 (UNIX epoch). Requires caution when running parallel jobs!



- **Solution 2**: use the reservoir of random bits in the computer's entropy pool, accessible in `/dev/random`. Could be noise measured in a resistor, or clock drift [4], or a peripheral device connected to a source of randomness (e.g., a radioactive source)

Known Issues with the LCG

- The LCG is fast but will produce subtle long-range correlations between values in the sequence.
- **Ex.**: if you generate n-dimensional points with the LCG, the points will lie on $(n!m)^{1/n}$ hyperplanes [5].
- Clearly random numbers shouldn't do that.
- Could this affect your simulation? Maybe. Depends on your application.



Alternatives to the LCG

Mersenne Twister

- A popular RNG currently in use is an algorithm called the Mersenne Twister [6], which uses the matrix linear recurrence relation

$$x_{k+n} = x_{k+m} \oplus (x_k^u \mid x_{k+1}^l)\boldsymbol{A}, \quad \text{where } \boldsymbol{A} = \begin{bmatrix} 0 & \mathbf{1}_{w-1} \\ a_{w-1} & (a_{w-2}, \ldots, a_0) \end{bmatrix},$$

  $\mid$ means bitwise OR, and $\oplus$ means bitwise XOR.

- For $n =$ degree of recurrence, $w =$ word size in bits, and $0 \leq r \leq w - 1 =$ bits in lower bitmask, the algorithm requires that the period length

$$2^{nw-r} - 1$$

  is a Mersenne prime – a prime number of the form $2^n - 1$.

- The MT implementation in Python and C++ (Boost, ROOT) has period $2^{19937} - 1 \approx 4 \times 10^{6001}$.

Aside: Basic Bit Manipulation

Bitwise OR and XOR

Bitwise OR can be understood by writing its arguments in binary notation. Example: let

$$x = 5 \xrightarrow{\text{binary}} 101 \equiv 1 \cdot 2^2 + 0 \cdot 2^1 + 1 \cdot 2^0$$

Then

$$x \mid 2 \xrightarrow{\text{binary}} 101 \mid 010 = 111 \xrightarrow{\text{decimal}} 7$$

Bitwise XOR works the same way, except that its output is *false* if two bits are set to 1:

$$x = 5 \xrightarrow{\text{binary}} 101$$

$$x \hat{} 2 \xrightarrow{\text{binary}} 101 \mid 010 = 111 \xrightarrow{\text{decimal}} 7$$

$$x \hat{} 4 \xrightarrow{\text{binary}} 101 \mid 100 = 001 \xrightarrow{\text{decimal}} 1$$

Aside: Basic Bit Manipulation

Bit Shifting

Bit shifting is equivalent to multiplication by powers of 2 (left shift) or division by powers of 2 (right shift):

$$x = 5 \xrightarrow{\text{binary}} 101$$

The statement $\texttt{x} \ll \texttt{y}$ shifts the bits of the number stored in x left by y places, **padding the least significant bits with zeros**:

$$\texttt{x} \ll 2 \xrightarrow{\text{binary}} 10100 = 2^4 + 2^2 \xrightarrow{\text{decimal}} 20 = 2^2 \cdot 5$$

The statement $\texttt{x} \gg 1$ shifts the bits of the number stored in x right by y places, **dropping the least significant bits** as needed:

$$\texttt{x} \gg 1 \xrightarrow{\text{binary}} 1010 = 2^3 + 2^1 \xrightarrow{\text{decimal}} 10 = 20/2^1$$

Alternatives to the LCG

Xorshift Algorithms

- Another class of RNG is called Xorshift ("X-OR-shift"), which depends on a combination of XOR (exclusive-OR) and bit shift operations [7].
- These are extremely fast because XOR and shifting are simple CPU instructions. Example: a $2^{128} - 1$ period algorithm

```
#include <cstdint>

// State variables; start s.t. not all = 0
uint32_t x, y, z, w;

uint32_t xorshift128() {
  uint32_t t = x ^ (x << 11);
  x = y; y = z; z = w;
  return w = w ^ (w >> 19) ^ t ^ (t >> 8);
}
```

Human-Generated Random Numbers

- How good are you at generating random numbers?

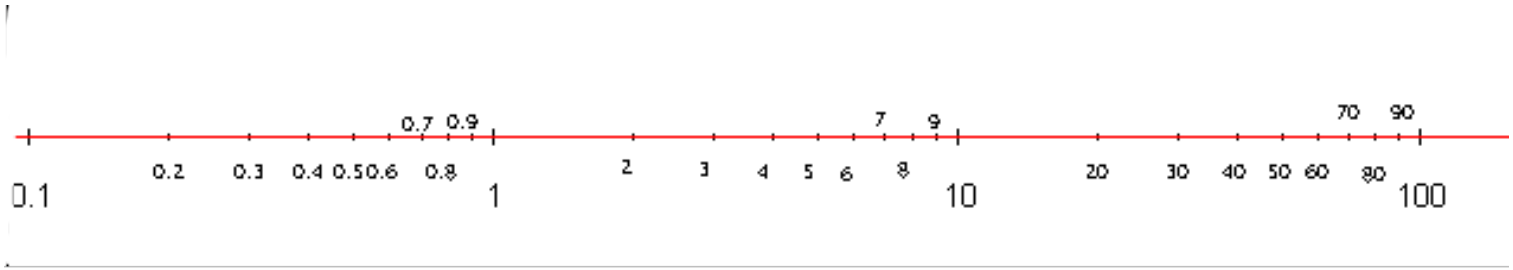
Example

Without over-thinking this, take a minute to write down as many random values between 1 and 100 as you can.

- What does the distribution of numbers look like?
- How would you tell if this is really a random sequence? Is it easy to predict parts of the sequence (auto-correlation)?
- Do we need to specify more information to answer this question?

Benford's Law

- If you are like most people, you didn't repeat numbers enough (remember the demon in the cartoon...)
- Also, your "random" sequence is probably uniform between 1 and 100
- However, in many sources of data the values follow a distribution known as Benford's Law: 1 is the leading digit 30% of the time, 2 is the leading digit 18% of the time, etc.
- If you pick a number randomly from the logarithmic number line, it will roughly follow Benford's Law



- This rule can be used to detect fraudulent numbers in elections, accounting (stock prices), and scientific papers.

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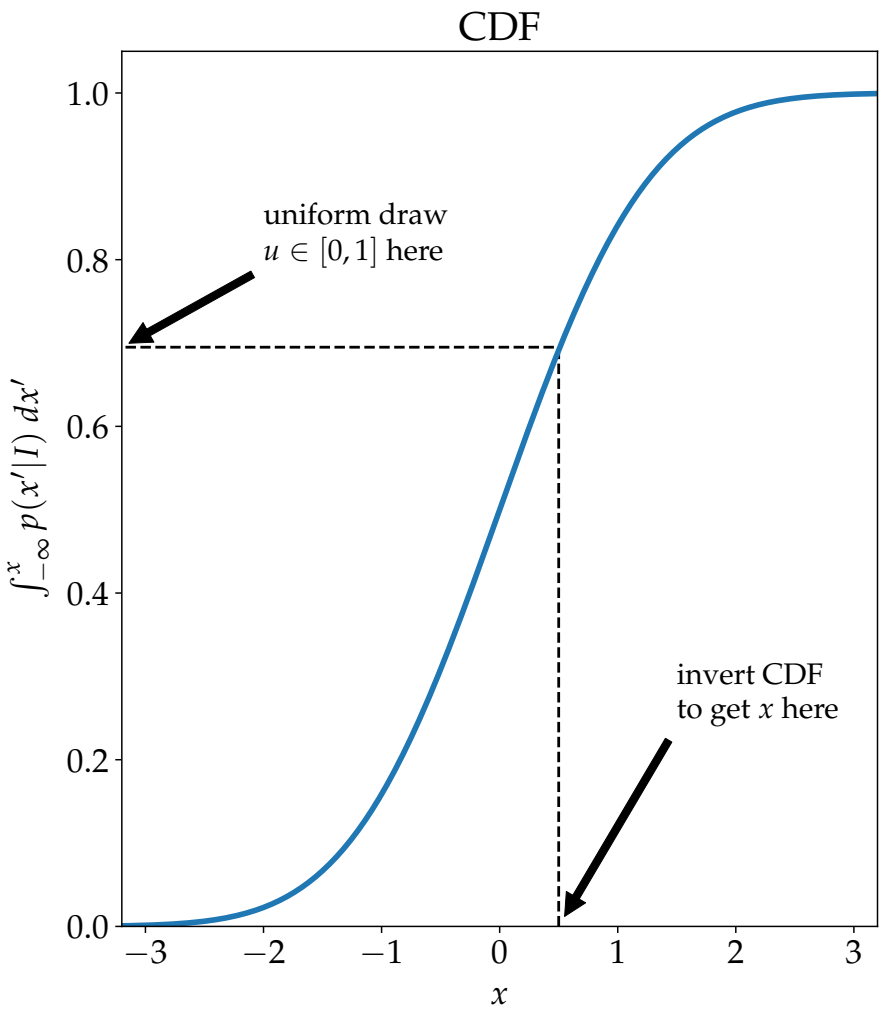
Generating Arbitrary Random Numbers

- All of the RNGs we have discussed will produce uniformly distributed random numbers:
  - LCG generates numbers between $[0, m]$
  - MT generates numbers between $[0, 1]$
- This is great for situations when you want a uniform distribution, but that does not correspond to most physical situations
- Luckily, there are several ways to convert a uniform distribution to an arbitrary distribution:
  1. Transformation or inversion method
  2. Acceptance/rejection method
- The transformation method is generally the most efficient technique, but it is only applicable in cases where the PDF is easy to integrate and the CDF can be inverted
- Acceptance/rejection is less efficient but works for any PDF you will want to use for random draws

Transformation/Inversion Method



Given a PDF $p(x|I)$ and its CDF $F(x) = \int_{-\infty}^{x} p(x'|I)\,dx'$:

1. Generate a uniform random number u between $[0, 1]$
2. Compute the value x s.t. $F(x) = u$
3. Take x to be the random draw from $p(x|I)$

In other words, from u and the invertible CDF $F(x)$, the value $x = F^{-1}(u)$ is distributed according to $p(x|I)$.

Transformation/Inversion Method

Exponential Distribution

Example

The PDF of the exponential distribution is

$$p(x|\xi) = \frac{1}{\xi} e^{-x/\xi}$$

and the CDF is

$$F(x) = P(X \leq x|\xi) = \int_0^x \frac{1}{\xi} e^{-x'/\xi}\, dx' = 1 - e^{-x/\xi}$$

Therefore, given $u \in [0,1]$ we can generate x according to $p(x|\xi)$ by inverting the CDF:

$$u = F(x) = 1 - e^{-x/\xi}$$
$$x = F^{-1}(u) = -\xi \ln(1-u) = -\xi \ln u$$

Limits of the Inversion Method

- Inversion is very efficient and great if you can invert your CDF
- Unfortunately this condition is not fulfilled even for many basic 1D cases

Example

The CDF of the Gaussian distribution is

$$F(x) = \int_{-\infty}^{x} p(x|\mu,\sigma) = \frac{1}{2}\left[1 + \mathrm{erf}\left(\frac{x-\mu}{\sigma\sqrt{2}}\right)\right]$$

The error function cannot be expressed in closed form, though there are numerical approximations to erf and erf^{-1} in `scipy`.

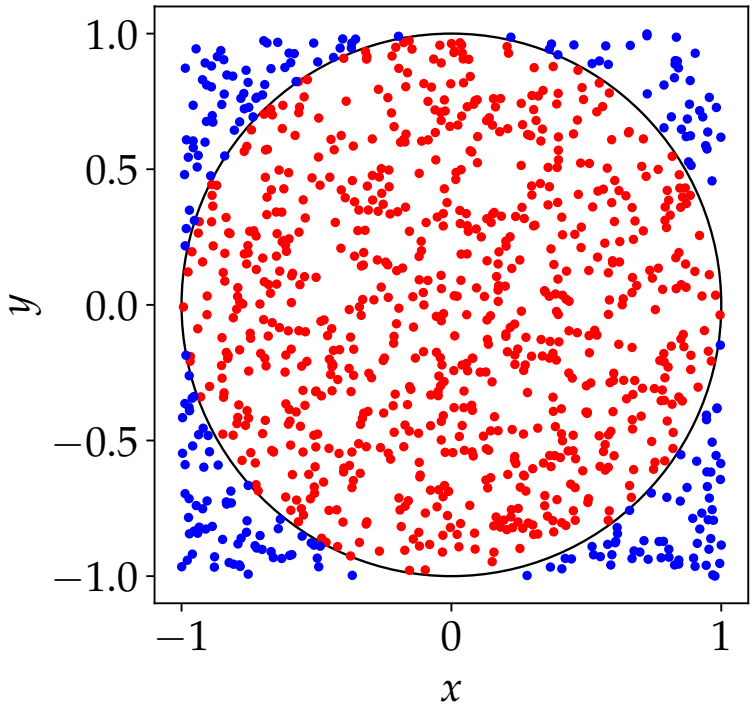
- A trick for complicated PDFs: express the CDF as a tabulated list of values $(u, F(x))$, "invert" it, and interpolate.

Acceptance/Rejection Method

Very old technique; modern form due to von Neumann. AKA "hit and miss," it generates x from an arbitrary $f(x)$ using a so-called instrumental distribution $g(x)$, where $f(x) < Mg(x)$ and $M > 1$ is a bound on $f(x)/g(x)$.

1. Sample x from $g(x)$ and $u \in [0,1]$.
2. Check if $u < f(x)/Mg(x)$
   - Yes: accept x
   - No: reject x, sample again

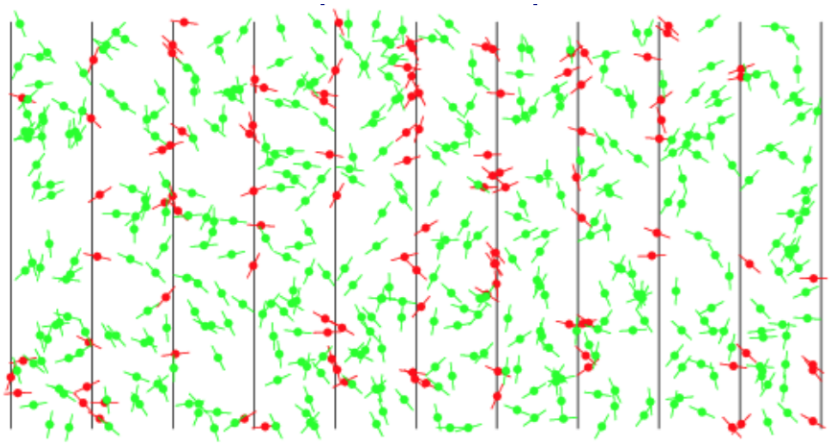
Very easy to implement, no limits on $f(x)$.

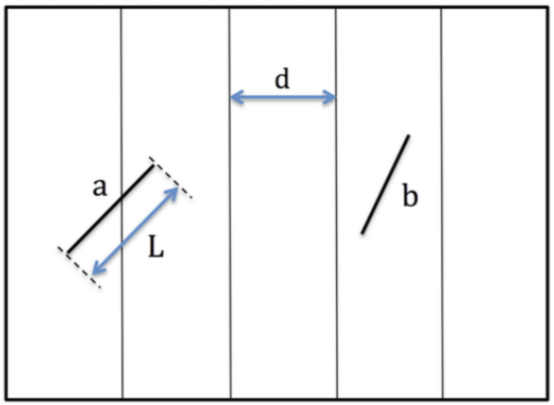


Calculation of π: uniformly generate (x,y) pairs in box, count up points inside the circle.
$\pi \approx 4N_{\text{circle}}/N_{\text{box}}$.

Buffon's Calculation of π

- An early variant of the Monte Carlo approach can be seen in Buffon's Needle (1700s), a method of calculating π





Drop a needle of length L dropped on a floor with parallel strips of width d. What is the probability the needle will cross a line if $L < d$?

- x is center distance to nearest line; $x \sim U(0, d/2)$
- θ is angle between needle center line: $\theta \sim U(0, \pi/2)$
- Needle crosses line if $x \leq L \sin\theta/2$. Joint PDF:

$$P = \int_0^{\pi/2} d\theta \int_0^{L\sin\theta/2} dx \frac{4}{\pi d} = \frac{2L}{\pi d}$$

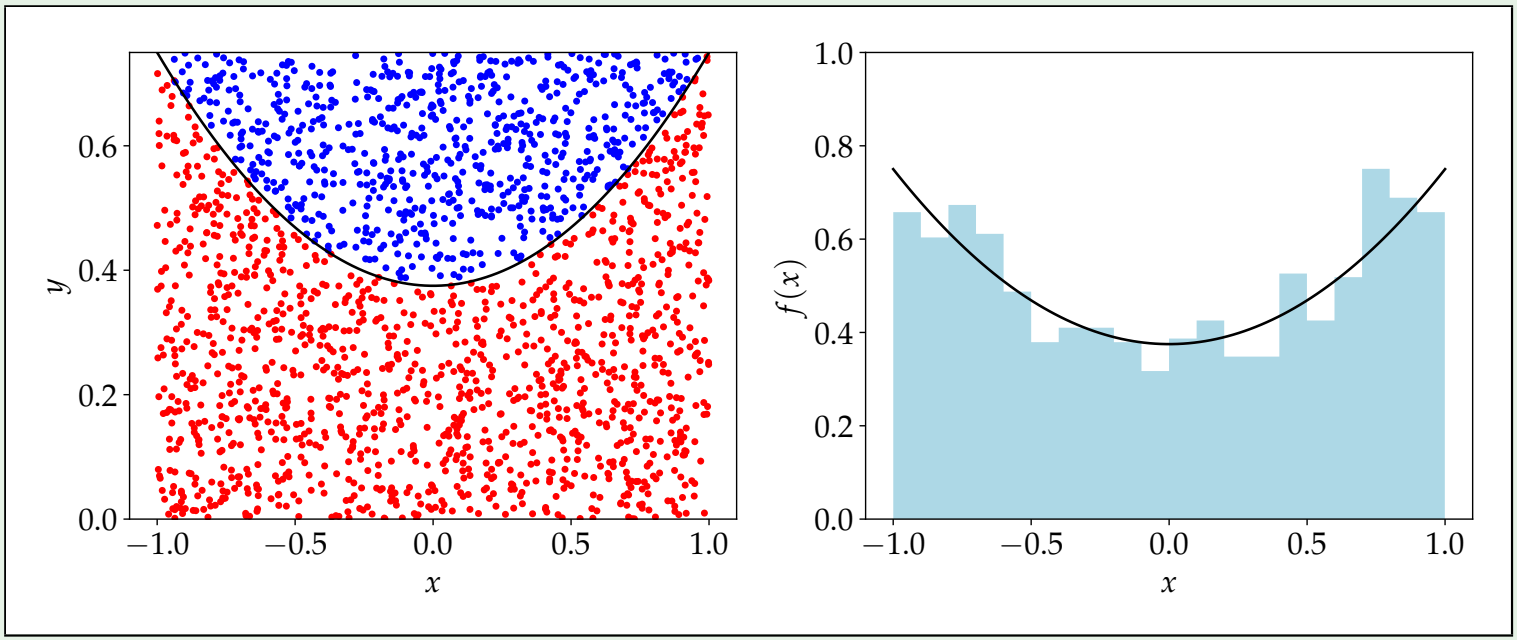
Acceptance/Rejection Method

Sampling from a 1D Distribution

Example

Suppose $f(x) = \frac{3}{8}(1+x^2)$ for $-1 \leq x \leq 1$.
(Aside: do you recognize this distribution?)

- Generate random $x \in [-1, 1]$ and $y \in [0, 0.75]$.
- If $y < f(x)$, populate the histogram with x.



Acceptance/Rejection Method

Sampling from a 2D Distribution

Example

Suppose we want to sample from the 2D angular distribution

$$\frac{1}{N}\frac{dN}{d\cos\theta d\varphi} = (1+\cos\theta)(1+\frac{1}{2}\cos 2\varphi)$$

Acceptance/Rejection Method

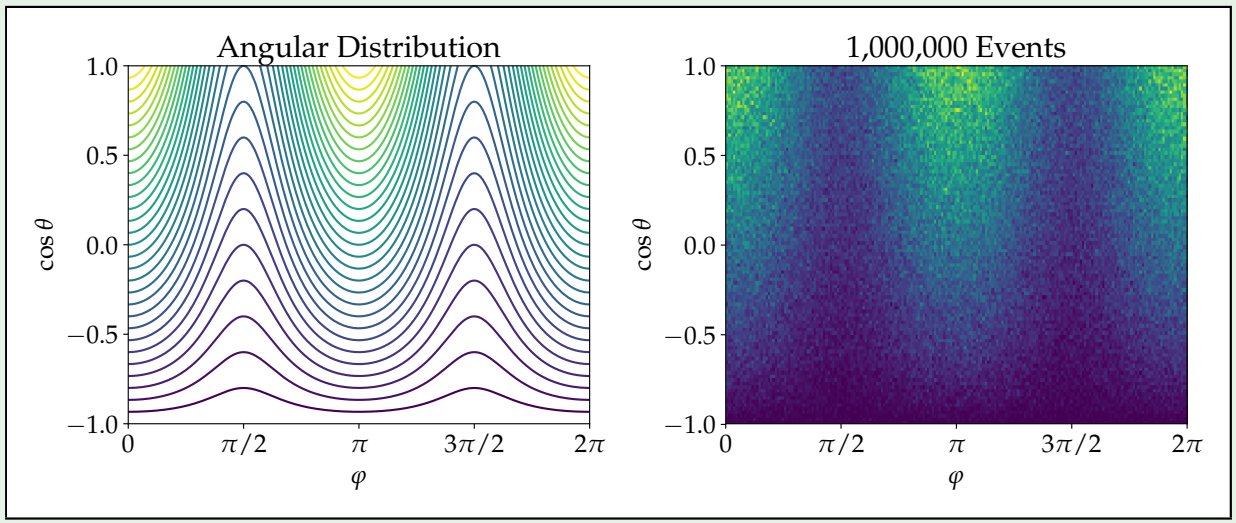
Sampling from a 2D Distribution

Example

Suppose we want to sample from the 2D angular distribution

$$\frac{1}{N}\frac{dN}{d\cos\theta d\varphi} = (1+\cos\theta)(1+\frac{1}{2}\cos 2\varphi)$$

Generate triplets (x,y,z), where $x = \varphi \in [0, 2\pi]$, $y = \cos\theta \in [-1,1]$, and $z \in [0,3]$, keeping (x,y) if $z < f(x,y)$:



Limitations of Acceptance/Rejection

Ideally you know $f_{\max}$ or normalize $f(x) = p(x|I)$ to have a maximum of 1.

- If not, you'll have to pre-scan the parameter space in advance.

If $f(x)$ ranges over many orders of magnitude, acceptance/rejection can be very inefficient as you'll waste lots of time in low-probability regions. Possible approaches:

- Subdivide x into ranges with different $f_{\max}$.
- Use importance sampling, where you generate random numbers according to a function that evelopes the PDF you really want to sample

Example implementation: `vegas` package in Python, an implementation of the adaptive Monte Carlo VEGAS multi-dimensional integration algorithm [8]

Generating a Gaussian Random Number

How would you generate a Gaussian random number?

1. You can use inversion if you can numerically estimate erf^{-1}.
2. You can use the acceptance/rejection method if you don't mind wasting some calculations.
3. You can exploit the Central Limit Theorem. Sum 12 uniform variables, which approximates a Gaussian of mean $12 \times 0.5 = 6$ and a variance of $12 \times (1/12) = 1$. Subtract 6 to get a mean of zero. This takes even more calculation and isn't exact.
4. Use the polar form of the binormal distribution

$$p(x, y|I) = \frac{1}{2\pi} \exp\left\{-\frac{1}{2}\left(x^2 + y^2\right)\right\}$$

to generate two Gaussian random numbers at once.

Box-Müller Algorithm

Re-express the 2D Gaussian PDF in polar coordinates:

$$p(x,y|I)\,dx\,dy = \frac{1}{2\pi}\exp\left\{-\frac{1}{2}\left(x^2+y^2\right)\right\}dx\,dy$$
$$= \frac{1}{2\pi}\exp -\frac{r^2}{2} r\,dr\,d\varphi$$

Then generate an exponential variable $z = r^2/2$, change variables to r, and generate a uniform polar angle φ:

- $z = -\ln u_1$ for $u_1 \sim U(0,1)$
- $r = \sqrt{2z}$
- $\varphi = 2\pi u_2$ for $u_2 \sim U(0,1)$

Then $x = r\cos\varphi$ and $y = r\sin\varphi$ are two normally-distributed random numbers. Very elegant! But due to the calls to trascendental functions (`sqrt`, `log`, `cos`, etc.), numerical approaches could be faster in practice...

Generating a Poisson Random Variable

The best way to generate a Poisson random variable is to use inverse transform sampling of the cumulative distribution.

- Generate $u \sim U(0,1)$
- Sum up the Poisson PDF $p(n|\lambda)$ with increasing values of n until the cumulative sum exceeds u:

$$s_n = \sum_{k=0}^{n} \frac{\lambda^k e^{-\lambda}}{k!}, \quad \text{while } s_n < u$$

- Return the largest n for which $s_n < u$.

This will work quite well until λ gets large, at which point you may start experiencing floating-point round-off errors due to the factor of $e^{-\lambda}$. But for large λ you an start to use the Gaussian approximation.

Monte Carlo Integration

- We can also solve integrals (esp. in several dimensions) with Monte Carlo. Mathematically, we approximate the integral by the average of the function of the interval of integration:

$$I = \int_a^b f(x)\,dx \approx (b-a)\,\mathrm{E}\left(f(x)\right)$$

- We take discrete samples of f and let the MC estimate converge to the true integral as the number of samples gets large:

$$\mathrm{E}\left(f(x)\right) = \frac{1}{N}\sum_{i=1}^{N} f(u_i) \to \frac{1}{b-a}\int_a^b f(u)\,du$$

$$I = I_{\mathrm{MC}} = \frac{b-a}{N}\sum_{i=1}^{N} f(x_i)$$

- Error on the result given by the Central Limit Theorem:

$$\sigma = \sqrt{\mathrm{var}\left(f\right)}/\sqrt{N} \propto 1/\sqrt{N}.$$

References I

[1] D. Vågberg, P. Olsson, and S. Teitel. "Universality of Jamming Criticality in Overdamped Shear-Driven Frictionless Disks". In: *Phys. Rev. Lett.* 113 (14 Oct. 2014), p. 148002. URL: http://link.aps.org/doi/10.1103/PhysRevLett.113.148002.

[2] J. Abadie et al. "Search for Gravitational Waves from Compact Binary Coalescence in LIGO and Virgo Data from S5 and VSR1". In: *Phys.Rev.* D82 (2010), p. 102001. arXiv: 1005.4655 [gr-qc].

[3] T.E. Hull and A.R. Dobell. "Random Number Generators". In: *SIAM Rev.* 4 (1962), pp. 230–254.

[4] Z. Jerzak. *Clock Synchronization in Distributed Systems*. Sept. 2009. URL: http://www.slideshare.net/zbigniew.jerzak/clock-synchronization-in-distributed-systems.

References II

[5] George Marsaglia. "Random Numbers Fall Mainly in the Planes". In: *PNAS* 61 (1968), pp. 25–28. URL: http://www.jstor.org/stable/58853.

[6] M. Matsumoto and T. Nishimura. "Mersenne Twister: A 623-dimensionally Equidistributed Uniform Pseudo-random Number Generator". In: *ACM Trans. Model. Comput. Simul.* 8.1 (Jan. 1998), pp. 3–30. URL: http://doi.acm.org/10.1145/272991.272995.

[7] George Marsaglia. "Xorshift RNGs". In: *Journal of Statistical Software* 8.14 (July 4, 2003), pp. 1–6. URL: http://www.jstatsoft.org/v08/i14.

[8] G. Peter Lepage. "A New Algorithm for Adaptive Multidimensional Integration". In: *J. Comp. Phys* 27 (2 May 1978), p. 192. URL: http://dx.doi.org/10.1016/0021-9991(78)90004-9.