Computational Physics (6810): Session 13

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6810 Endgame

Various recaps and followups

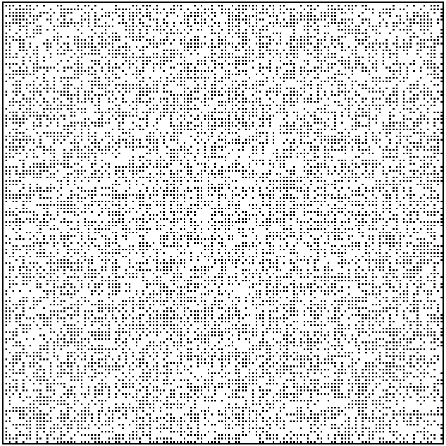
Random stuff (like RNGs :)

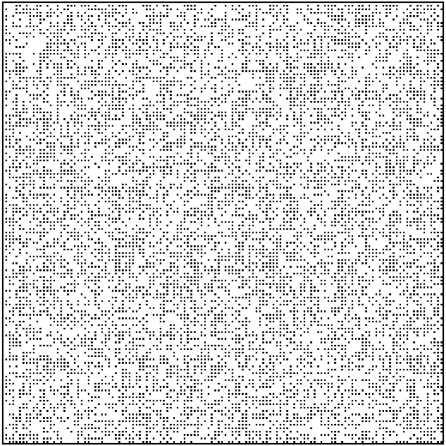
Session 13 stuff

6810 Computational Physics Endgame

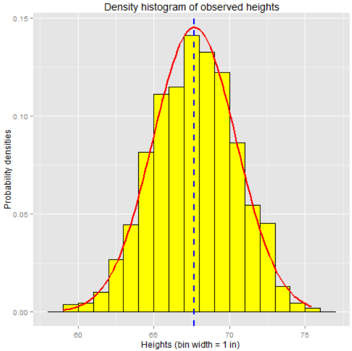
- April 21 is our last class period!
- Projects are due at the end of Monday, May 1
  - Create a `Project` subfolder of your BuckeyeBox folder
  - Include codes, makefiles, plots, etc. (like for problem sets)
  - Include an explanation of how it all fits together in a separate file or in comments of the codes.
  - It is recommended that you turn in something earlier than the due date to get feedback while there's time for iteration.
- Session guides and homework will be accepted until 5pm on Thursday, April 27
  - Remember that you can always upgrade a check
  - Get in *some* version (even if incomplete) soon!

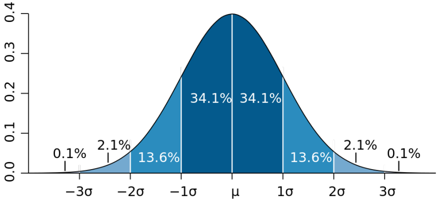
Which one is not really random?





Gaussian or Normal distributions





- Gaussian is *fully* characterized by mean μ and variance σ^2

$$p(x) = \frac{1}{2\pi\sigma^2} e^{-(x-\mu)^2/2\sigma^2}$$

  - Standard deviation σ is square root of variance
  - About 2/3 of numbers in $[-\sigma, +\sigma]$ "within 1 sigma"
  - PDG requires a "5σ signal" to declare a new particle is found

Comments on probability distribution functions (PDFs)

- Two common ones are uniform and gaussian [think histograms!]
  - Always normalized: $\int_{-\infty}^{\infty} p(x)\,dx = 1$ (total probability is one)
  - Uniform: $p(x) = \frac{1}{b-a}\theta(x-a)\theta(b-x)$

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  - PDG requires a "5σ signal" to declare a new particle is found
- 2D random walk and $\sqrt{N}$: How far away after N steps? (label by i)

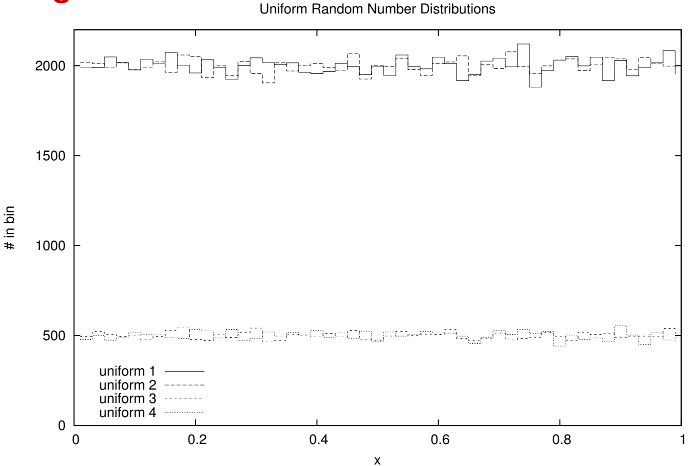
$$R_{\mathrm{avg}}^2 \approx \langle(\Delta x_1 + \Delta x_2 + \cdots + \Delta x_N)^2 + (\Delta y_1 + \Delta y_2 + \cdots + \Delta y_N)^2\rangle$$

  - This is not one walk, but the *average* of many (note $\langle\rangle$'s)
  - Δx_i and Δy_i chosen by $p(x)$ with means $\langle\Delta x_i\rangle = \langle\Delta y_i\rangle = 0$
  - Uncorrelated steps means $\langle\Delta x_i \Delta x_j\rangle = \langle\Delta y_i \Delta y_j\rangle = 0 \quad$ if $i \neq j$

$$\Longrightarrow R_{\mathrm{avg}}^2 \approx N\langle\Delta x_i^2 + \Delta y_i^2\rangle \equiv N\langle r^2\rangle \Longrightarrow R_{\mathrm{rms}} \approx \sqrt{N} r_{\mathrm{rms}}$$

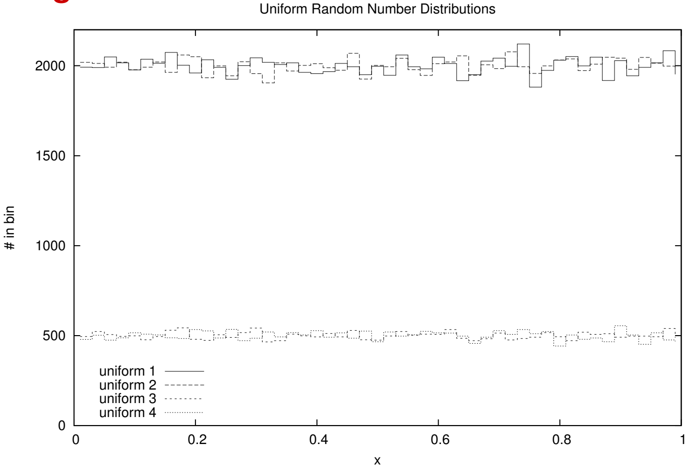
  - Applies generally to processes with combined random errors

Scaling of fluctuations with N



- Four times as many points on top. Scaling of fluctuations?

Scaling of fluctuations with N



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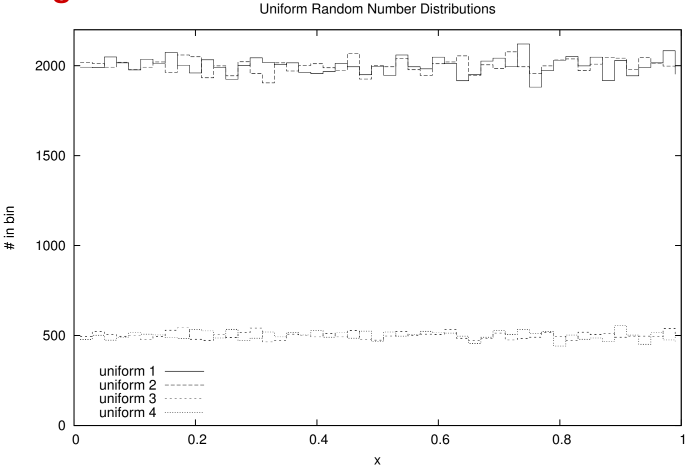
  answer: proportional to $\sqrt{N}$, so twice as large on top
- What is the *relative* scaling of the fluctuations with N?

Scaling of fluctuations with N



- Four times as many points on top. Scaling of fluctuations?
  answer: proportional to $\sqrt{N}$, so twice as large on top
- What is the *relative* scaling of the fluctuations with N?
  answer: $\frac{\sqrt{N}}{N} = \frac{1}{\sqrt{N}}$

Things to watch for in Session 12 and beyond

- For Monte Carlo methods, we need a set of random numbers
  - *uncorrelated* means we can't predict x_{i+1} given $x_1, x_2, \cdots, x_i$
- Doesn't have to be uniform
  - the histogram of random numbers will approach the shape of the corresponding probability distribution function (PDF)
- We'll use *pseudo*-random numbers from GSL random number generators (rng)
  - trade-offs between period and speed
  - see Session 12 notes for tests (e.g., using your eye) and Session 13 notes for pitfalls!
  - You need to *seed* the rng, or you'll get the same numbers!

Things to watch for in Session 12 and beyond (cont.)

- Random walks in two dimensions: N steps
  - Be able to derive standard deviation distance $R \approx \sqrt{N} r_{\rm rms}$
  - Remember how to find the average of a function in an interval:

$$\langle f \rangle = \frac{1}{b-a}\int_a^b f(x)\,dx \implies \langle r^2 \rangle = \frac{1}{(b-a)^2}\int_a^b dx \int_a^b dy\,(x^2+y^2)$$

- (Crude) approximation of an integral I

$$\langle f \rangle = \frac{1}{b-a}\int_a^b f(x)\,dx \approx \frac{1}{N}\sum_{i=1}^{N} f(x_i) \implies I = \int_a^b f(x)\,dx \approx \frac{b-a}{N}\sum_{i=1}^{N} f(x_i)$$

- Better approximation: sample according to an appropriate pdf

$$I = \int_a^b dx\, f(x) = \int_a^b dx\, w(x)\,\frac{f(x)}{w(x)} = \left\langle \frac{f}{w} \right\rangle_w \approx \frac{1}{N}\sum_{i=1}^{N}\frac{f(x_i)}{w(x_i)}$$

- $\implies$ Sample the integrand (i.e., choose points) where big or steep

Averaging functions over probability distributions

$$\langle f(x)\rangle \equiv \int f(x)P(x)\,dx \quad \text{where} \quad \int P(x)\,dx = 1 \quad \text{(usually from } -\infty \text{ to } +\infty\text{)}$$

generalizes to

$$\langle g(x,y)\rangle \equiv \iint g(x,y)P_2(x,y)\,dx\,dy \quad \text{where} \quad \iint P_2(x,y)\,dx\,dy = 1$$

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$$\langle r^2\rangle = \langle x^2 + y^2\rangle \stackrel{?}{=} \langle x^2\rangle + \langle y^2\rangle = 2\langle x^2\rangle$$

Here we have special cases of P_2 and g:

$$P_2(x,y) = P(x)P(y) \quad \text{and} \quad g(x,y) = f(x) + f(y)$$

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$$P_2(x,y) = P(x)P(y) \quad \text{and} \quad g(x,y) = f(x) + f(y)$$

$$\begin{aligned}
\langle f(x) + f(y)\rangle &= \iint [f(x) + f(y)]P(x)P(y)\,dx\,dy \\
&= \left[\int f(x)P(x)\,dx\right] \times \left[\int P(y)\,dy\right] + \left[\int P(x)\,dx\right] \times \left[\int f(y)P(y)\,dy\right] \\
&= \int f(x)P(x)\,dx + \int f(y)P(y)\,dy = \langle f(x)\rangle + \langle f(y)\rangle \checkmark
\end{aligned}$$

Ways to do *Importance Sampling*

- In general, identify a pdf $P(x)$ in your integrand:

$$\int_a^b f(x)\,dx \longrightarrow \int_a^b g(x)P(x)\,dx \approx \frac{1}{N}\sum_{i=1}^{N} g(\widetilde{x}^{(i)})$$

  - where the points $\{\widetilde{x}^{(i)}\}$, $i = 1, N$, are sampled from $P(x)$
  - Note that $P(x)$ does not appear explicitly in the sum
- This is called "Importance Sampling"
  - Pick a distribution $P(x)$ that matches the integrand as best as possible (e.g., make $g(x)$ as close to constant as possible)
- Ways to determine the $\widetilde{x}$'s:
  1. Choose an explicit $P(x)$ if you know how to sample it (e.g., a Gaussian distribution)
  2. Determine $P(x)$ *adaptively*. E.g., `vegas` in GSL
  3. Build up a set of *configurations* $\{\widetilde{x}^{(i)}\}$ via a Markov chain (e.g., via the Metropolis algorithm or some variation)

First pass at statistical mechanics basics

- The state of our (approximated) system is specified by a *configuration*
  - For example, for an N-particle quantum system, it could be where each particle is located (plus other quantum #'s)
  - For the Ising model, it is whether each "spin" on the lattice (which could be in any number of dimensions) is up or down
  - Our approximation to the system is such that specifying a configuration takes a finite amount of data but the number of *possible* configurations can still be (and usually is!) enormous.
- The *partition function* tells us what we need for thermodynamics
  - E.g., the expectation value of the energy or of an observable like the pressure or magnetization
  - We can express it two equal ways (canonical ensemble here)

$$Z = \sum_i e^{-E^{(i)}/k_B T} = \sum_{E_j} (\#\text{ of } E_j\text{s}) e^{-E_j/k_B T} \equiv \sum_{E_j} \Omega(E_j) e^{-E_j/k_B T}$$

    - The first sum is over all configurations, labeled by i
    - The second sum is over all energies, labeled by j

Example of one-dimensional Ising model with N spins

- Specify a configuration by whether each of N spins is up or down:

$$\begin{array}{cccccccc} \uparrow & \downarrow & \uparrow & \uparrow & \uparrow & \downarrow & \cdots & \uparrow \\ 0 & 1 & 2 & 3 & 4 & 5 & & N-1 \end{array}$$

- Suppose the Hamiltonian specified the energy as: $-J\sum_{\langle ij\rangle} S_i S_j$
  - Here J is a constant with dimensions of energy
  - $\langle ij\rangle$ means all adjacent spins ("nearest neighbors")
  - $S_i = 1$ for $\uparrow$ and $S_i = -1$ for $\downarrow$ (e.g., so $S_i S_j = 1$ if both down)
- Consider $N = 3$ with periodic boundary conditions: states and energies

config. i	state	energy (with $J = 1$)
0	$\downarrow\downarrow\downarrow$	$E^{(0)} = -(+1+1+1) = -3$
1	$\downarrow\downarrow\uparrow$	$E^{(1)} = -(+1-1-1) = +1$
2	$\downarrow\uparrow\downarrow$	$E^{(2)} = -(+1+1+1) = +1$
3	$\downarrow\uparrow\uparrow$	$E^{(3)} = -(+1+1+1) = +1$
4	$\uparrow\downarrow\downarrow$	$E^{(4)} = -(+1+1+1) = +1$
5	$\uparrow\downarrow\uparrow$	$E^{(5)} = -(+1+1+1) = +1$
6	$\uparrow\uparrow\downarrow$	$E^{(6)} = -(+1+1+1) = +1$
7	$\uparrow\uparrow\uparrow$	$E^{(7)} = -(+1+1+1) = -3$

There are 7 different configurations but $E_0 = -3$ and $E_1 = +1$ are the only two choices for E_j.

Find Z by summing over configurations i or energies E_j

More statistical physics in a nutshell (I)

Maximizing the Free Energy (not the energy!)

- Return to partition function and probability $P(E)$ of finding energy E:

$$Z = \sum_{\text{all i}} e^{-E^{(i)}/k_B T} = \sum_{E_j} (\#\text{ of } E_j\text{s}) e^{-E_j/k_B T} \equiv \sum_{E_j} \Omega(E_j) e^{-E_j/k_B T}$$

- Here $P(E) \propto \Omega(E) e^{-E/k_B T}$. The system will maximize E. How?
  - Move $\Omega(E)$ to exponent, as $e^{-\alpha}$ maximized when α minimized
  - $\Omega = e^{\ln \Omega} \Longrightarrow P(E) \propto e^{-(E-TS)/k_B T}$ with $S = k_B \ln \Omega(E)$
  - What is the minimized quantity at fixed T? $E - TS$
  - Note the tradeoff between E and TS!

More statistical physics in a nutshell (II)

Temperature and Entropy

- Consider two subsystems with energies E and E' and fixed $E_{\text{tot}} = E + E'$
- Exchange energy back and forth, reach equilibrium. Meaning what? Static?
- Define $\Omega(E)$ and $\Omega(E')$ to be the number of configurations with E and E' (i.e., "microstates"). How many total ways? $\Omega(E) \times \Omega(E') = \Omega(E)\Omega(E_{\text{tot}} - E)$
- Basic principle: any accessible state (satisfies $E + E' = E_{\text{tot}}$) is equally likely. $\Longrightarrow$ probability of particular E is total number with that E divided by grand total
- So maximize $\Omega(E)\Omega(E')$ to maximize probability $\Longrightarrow$ Why is this equilibrium?
- Because $\Omega(E) = e^{S(E)/k_B}$, maximize $S(E) + S(E')$. 2nd Law of thermo?
- Set derivative to zero and use chain rule with $dE'/dE = -1$ (why?):

$$\frac{d}{dE}(S(E) + S(E')) = 0 = \frac{dS(E)}{dE} + \frac{dS(E')}{dE'}\frac{dE'}{dE}$$

- So equilibrium means $\frac{dS(E)}{dE} = \frac{dS(E')}{dE'}$
- We use this to *define* the temperature $T = \frac{dS(E)}{dE}$!

More statistical physics in a nutshell (III)

Probability and Boltzmann factors

- Find the probability of energy $P(E)$ for one of two subsystems that is very much smaller than the other, so $E \ll E_{\text{tot}}$
- Ratio of probabilities is ratio of total number of possible states

$$\frac{P(E_1)}{P(E_2)} = \frac{[\Omega(E_1)\Omega(E_{\text{tot}} - E_1)]}{[\Omega(E_2)\Omega(E_{\text{tot}} - E_2)]} = \frac{\Omega(E_1)e^{\frac{1}{k_B}S(E_{\text{tot}}-E_1)}}{\Omega(E_2)e^{\frac{1}{k_B}S(E_{\text{tot}}-E_2)}}$$

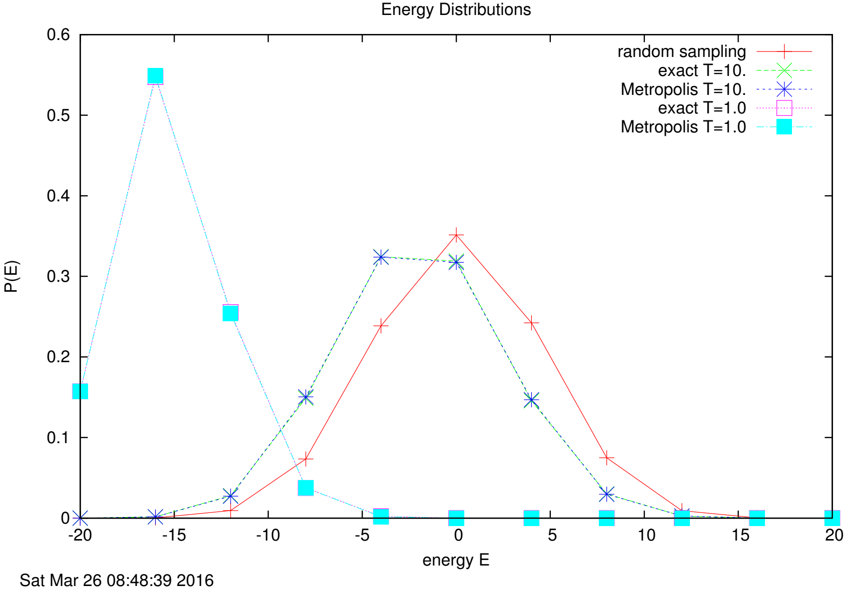
- Now Taylor expand (of course!): $S(E_{\text{tot}} - E_1) \approx S(E_{\text{tot}}) - E_1 \left.\frac{dS}{dE}\right|_{E_{\text{tot}}}$
- But $\frac{dS}{dE} = \frac{1}{T}$ and $e^{S(E_{\text{tot}})/k_B}$ factors cancel, leaving

$$\frac{P(E_1)}{P(E_2)} \approx \frac{\Omega(E_1)e^{-E_1/k_B T}}{\Omega(E_2)e^{-E_2/k_B T}}$$

- So $P(E) \propto \Omega(E)e^{-E/k_B T}$. How to normalize $P(E)$?

$$\sum_i \Omega(E_i)e^{-E_i/k_B T} = 1 \quad \Longrightarrow \quad P(E) = \frac{1}{Z}\Omega(E)e^{-E/k_B T}$$

Example of one-dimensional Ising model with 20 spins



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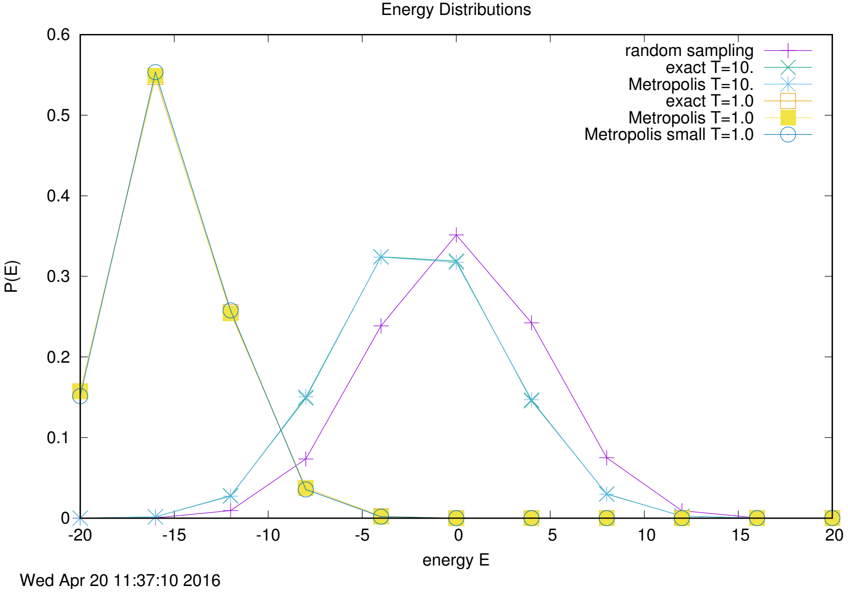

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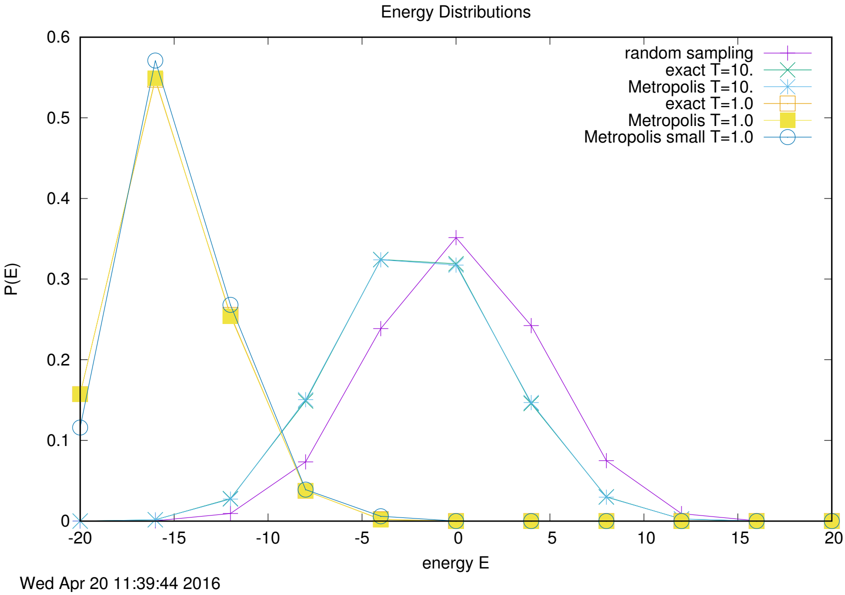

Two-D Ising model: Equilibration and cooling