Definition of Simulation

- What is a simulation?
  - It has an internal state "S"
    - In classical mechanics, the state = positions $\{q_i\}$ and velocities $\{p_i\}$ of the particles.
    - In Ising model, they are the spins (up or down $\{\sigma_i\}$) of the particles.
    - In any computer program, a finite number of bits
  - A rule for changing the state $S_{n+1} = T\ (S_n)$
    - In a random case, the new state is sampled from a distribution $T(S_{n+1}|S_n)$.
  - From initial state S_0, we repeat the iteration many times: $n \Rightarrow \infty$

    $S_0 \Rightarrow S_1 \Rightarrow S_2 \Rightarrow S_3 \Rightarrow S_4 \Rightarrow S_5 \Rightarrow \ldots\ldots S_n \Rightarrow S_{n+1} \Rightarrow$
- Sometimes we call the *iteration index* "n" "time."

  It could be either "real time," an iteration count, or pseudo-time, sometimes called *Monte Carlo time*.
- Simulations can be:
  - Deterministic (e.g. Newton's equations via Molecular Dynamics)
  - Stochastic (Monte Carlo, Brownian motion,…)
  - Combination of the two

  Nonetheless, you analyze the errors the same way.

  As with experiment: the rules of the simulation can be simple but output can be unpredictable.

Ergodicity

- Typically simulations are assumed to be ergodic:
  - after a certain time the system loses memory of its initial state, S_0, except possibly for certain conserved quantities such as the energy, momentum and number of particles.
  - The *correlation time* κ (which we will define soon) is the number of iterations it takes to forget.
  - If you look at (non-conserved) properties for times much longer κ, they are as unpredictable as if randomly sampled from some distribution.
  - Ergodicity can be proven within Monte Carlo but difficult for deterministic simulations. More about this next week.
  - The assumption of egodicity is used for:
    - Warm up period (equilibration) at the beginning of a simulation
    - To get independent samples for computing errors.

Equilibrium distribution

- Let $F_t(S|S_0)$ be the distribution of the state after time t.
- If the system is ergodic, no matter what the initial state was, one can characterize the state of the system for $t >> \kappa$ by a unique *probability distribution: the equilibrium state* $F^*(S)$.

$$\lim_{t\to\infty} F(S \mid S_0) = F^*(S)$$

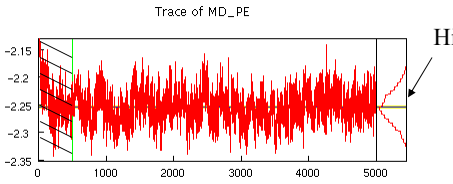
- In classical statistical systems, this is the canonical Boltzmann distribution: $F^*(S)=\exp(-V(S)/kT)/Z$
- Typically, we want to compute properties in equilibrium. e.g. the **internal energy,** as an average over the simulation**:**

$$U = \int dS F^*(S) V(S) \equiv \langle V(S) \rangle_{F^*}$$

- Another goal is to compute dynamics: for example the diffusion constant.

Estimated Errors

- In what sense do we calculate exact properties? Answer: if we average long enough the error goes to zero. Hence the error is under control.
- Next, how accurate is the estimate of the exact value?
  - Simulation results without error bars are only suggestive.
    - ***All homework exercises must include errors estimates***
    - Without error bars one has no idea of their significance.
    - **You should understand formulas and be able to make an "*eye-ball*" *estimate* of errors**
- **Error bar**: the ***estimated error*** in the ***estimated mean***.
  - Error estimates based on Gauss' ***Central Limit Theorem***.
  - **Average** of statistical processes has *normal* (Gaussian) distribution.
  - **Error bars**: square root of the variance of the distribution divided by the number of ***uncorrelated*** steps.



Histogram of E

Central Limit Theorem (Gauss)

Sample N independent values from $F^*(x)dx$: $(x_1, x_2, x_3, \ldots, x_N)$.

Calculate mean as $y = (1/N)\sum x_i$.

What is the pdf of mean? *Solve by fourier transforms*

Characteristic function: $c_x(k) = < e^{ikx} > = \int_{-\infty}^{\infty} dx\, F^*(x) e^{ikx}$ $\quad c_y(k) = c_x(k/N)^N$

$$\lim_{N\to\infty} \quad c_y(k) = e^{ik\kappa_1 - k^2\kappa_2/2N - ik^3\kappa_3/6N^2 \ldots}$$

Cumulants: Mean = κ_1 Variance= κ_2 Skewness = κ_3 Kurtosis= κ_4

The n=1 moment remains invariant but the rest get reduced by higher powers of N.

Given enough averaging almost anything becomes a Gaussian distribution.

$$P(y) = (N/2\pi\kappa_2)^{1/2} \exp\left[-\frac{N(y-\kappa_1)^2}{2\kappa_2}\right] \quad \text{standard error(y)}=\sigma=\sqrt{\frac{\kappa_2}{N}}$$

Example: approach to normality

Add n random numbers together.

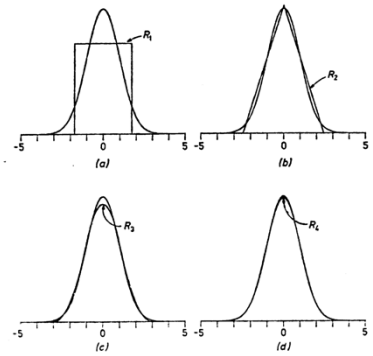


Figure 1. Distributions of sums of uniform random numbers, each compared with the normal distribution. (a) R_1, the uniform distribution. (b) R_2, the sum of two uniformly distributed numbers. (c) R_3, the sum of three uniformly distributed numbers. (d) R_{12}, the sum of twelve uniformly distributed numbers.

From Kalos and Whitlock, "Monte Carlo Methods"

Conditions on Central Limit Theorem

$$I_n = < x^n > = \int_{-\infty}^{\infty} dx\, F^*(x) x^n$$

- We need the first three moments to exist.
  - If I_0 is not defined ⇒ not a pdf
  - If I_1 does not exist ⇒ not a mathematically well-posed integral.
  - If I_2 does not exist ⇒ infinite variance. Important to know if variance is finite for simulations.
- Divergence could happen because of tails of distribution

$$I_2 = < x^2 > = \int_{-\infty}^{\infty} dx\, F^*(x) x^2$$

- We need: $\lim_{x \to \pm\infty} \quad x^3 F^*(x) \to 0$
- Or divergence because of singular behavior of F^* at certain values of x:

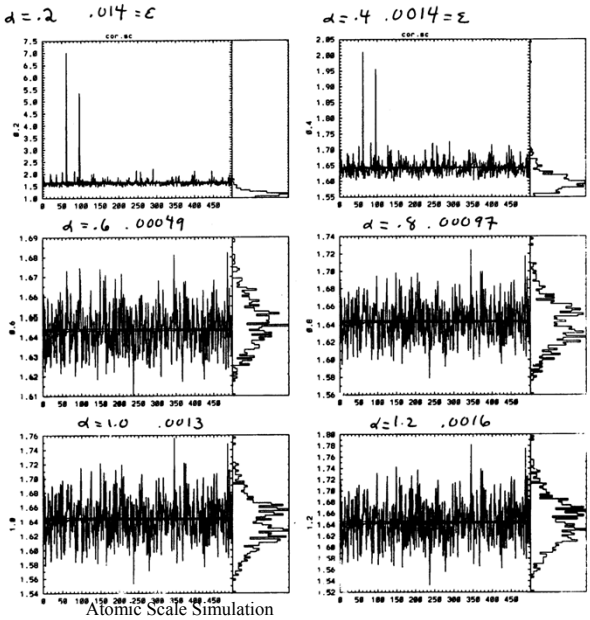
$$\lim_{x \to 0} \quad x F^*(x) \to 0$$

- We need to establish analytically that variance exists!

What does infinite variance look like?

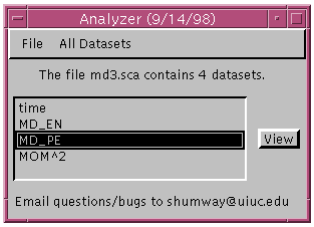
Spikes

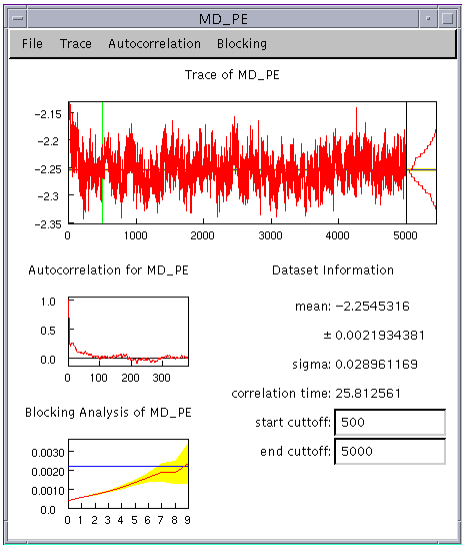
Long tails on the distributions



DataSpork

Interactive code to perform statistical analysis of data





Estimating Errors

- Uncorrelated data

$$\{a_t\} \qquad 0 < t \le N$$

$$\langle a_t \rangle \approx \bar{a} = \frac{1}{N}\sum_t a_t$$

$$error(\bar{a}) = \left\langle \left(\bar{a} - \langle a \rangle\right)^2 \right\rangle^{1/2} \approx \left[\frac{\sum_t \delta a_t^{\,2}}{N(N-1)}\right]^{1/2}$$

$$\delta a_t \equiv a_t - \bar{a}$$

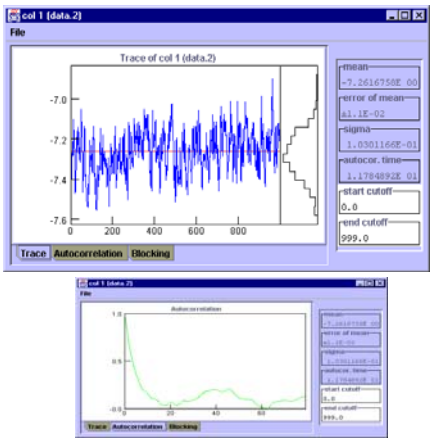
- Correlated data

$$error(\bar{a}) = \left\langle \left(\bar{a} - \langle a \rangle\right)^2 \right\rangle^{1/2} \approx \left\langle \frac{\kappa \sum_t (a_t - \bar{a})^2}{N(N-1)} \right\rangle^{1/2}$$

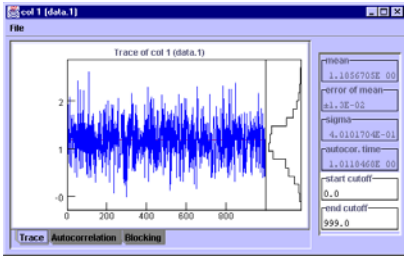
$$\kappa = 1 + 2\sum_{t=1}^{\infty} \frac{\langle \delta a_t \delta a_0 \rangle}{\langle \delta a^2 \rangle} = \text{correlation time}$$

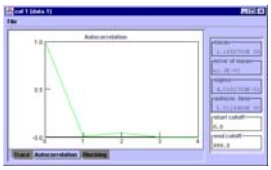
- Problem: how to cut off the summation for κ.
- Bining method: average together data in bins longer than the correlation time until it is uncorrelated.

Correlated data



Uncorrelated data





Estimate of errors: how to deal with correlation

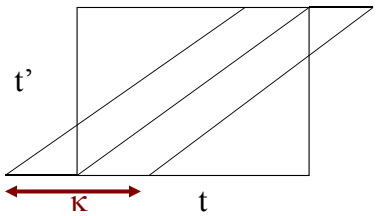
$$error(\bar{a}) = \left\langle \left(\bar{a} - \langle a \rangle\right)^2 \right\rangle^{1/2} \approx \left\langle \frac{\kappa \sum_t (a_t - \bar{a})^2}{N(N-1)} \right\rangle^{1/2}$$

$$\boxed{\bar{a} = \frac{1}{N}\sum_t a_t}$$

$$\kappa = 1 + 2\sum_{t=1}^{\infty} C(t) = \text{correlation time} \approx 2\int_0^{\infty} \frac{dt}{\delta t} \mathrm{C(t)}$$

$$C(t,t') \equiv \frac{\langle \delta a_t \delta a_{t'} \rangle}{\langle \delta a^2 \rangle} = C\left(|t-t'|\right) = \text{autocorrelation function}$$

$$\left\langle \left(\bar{a} - \langle a \rangle\right)^2 \right\rangle = \left\langle \frac{1}{N^2} \sum_{t,t'}^{N} \delta a_t \delta a_{t'} \right\rangle = \frac{\langle \delta a^2 \rangle}{N^2} \sum_{t,t'}^{N} C_{|t-t'|} < \frac{\langle \delta a^2 \rangle}{N^2} \sum_{t'=1}^{N} \sum_{t=-\infty}^{\infty} C_t = \langle \delta a^2 \rangle \frac{\kappa}{N}$$



Bias

- Bias is a *systematic error* caused by using a random number in a non-linear expression.
- You will get a result that is systematically too high or low.
- Suppose $Z' = \bar{Z} + \delta Z$ is the result of MC sampling but we want F(Z). *Example:* F=-kT ln(Z).
- What is the statistical error and bias of F(Z')?
- Expand Z in power series about <Z>

$$F(Z') = F(\bar{Z}) + \left.\frac{dF}{dZ}\right|_{\bar{Z}} \delta Z + \frac{1}{2}\left.\frac{d^2F}{dZ^2}\right|_{\bar{Z}} \delta Z^2 + \mathrm{L}$$

$$bias(F) = < F(Z) - F(\bar{Z}) > = \frac{1}{2}\left.\frac{d^2F}{dZ^2}\right|_{\bar{Z}} < \delta Z^2 > + \mathrm{L} = \frac{1}{2}\left.\frac{d^2F}{dZ^2}\right|_{\bar{Z}} err(Z)^2 \qquad \mathbf{O(N^{-1})}$$

$$error(F) = [< (F(Z') - \langle F(Z)\rangle)^2 >]^{1/2} = \left|\left.\frac{dF}{dZ}\right|_{\bar{Z}}\right| < \delta Z^2 >^{1/2} + \mathrm{L} = \left|\left.\frac{dF}{dZ}\right|_{\bar{Z}}\right| err(Z) \qquad \mathbf{O(N^{-1/2})}$$

You may need to correct for the bias unless N is very large.

Statistical vs. Systematic Errors

- What are statistical errors?
  - Statistical error measures the distribution of the averages about their avg.
  - ***Statistical error can be reduced by extending or repeating runs***, increase N.

$$\text{standard error(y)} = \sigma = \sqrt{\frac{\kappa_2}{N}}$$

- The efficiency is how we measure the rate of convergence of the statistical errors.

$$\boxed{\zeta = \frac{1}{T\sigma^2}}$$

  - It depends on the computer, the algorithm, the property etc. But not on the length of the run.
- What are systematic errors ?
  - Systematic error refers to other types of errors, not sampling error. Even if you sample forever you do not get rid of systematic errors.
  - Systematic error can be caused by round-off error, non-linearities, bugs, non-equilibrium, etc.

Recap: problems with estimating errors

- Any good simulation quotes *systematic and statistical* errors for anything important.
- The *error and mean* are simultaneously determined from the same data.
- Central limit theorem: the distribution of an average approaches a normal distribution (*if the variance is finite*).
  - One *standard deviation* means ~2/3 of the time the correct answer is within σ of the sample average.
- Problem in simulations is that *data is correlated in time*.
  - It takes a "correlation" time κ to be "ergodic"
  - We need to correct for correlation-**this is a problem we can solve**.
  - Throw away the initial transient.
- We need about 20 *independent* data points to estimate errors. (so that the error of the error is only 20%)

Statistical Vocabulary

- **Trace of A(t)**:
- **Equilibration time**.
- **Histogram** of values of A (P(A)).
- **Mean** of A (a).
- **Variance** of A (v).
- **Bias** of A
- **estimate of the mean:** $\Sigma A(t)/N$
- **estimate of the variance**
- **Autocorrelation** of A (C(t)).
- **Correlation time** κ .
- The (estimated) **error** of the (estimated) **mean** (σ).
- **Efficiency** [= 1/(CPU time * error ^{2})]

Statistical thinking is slippery: be careful

- "Shouldn't the energy settle down to a constant"
  - NO. It fluctuates forever. It is the overall mean which converges.
- "The cumulative energy has converged".
  - BEWARE. Even pathological cases have smooth cumulative energy curves.
- "Data set A differs from B by 2 error bars. Therefore it must be different".
  - This is normal in 1 out of 10 cases. If things agree too well, something is wrong!
- "My procedure is too complicated to compute errors"
  - NO! NEVER! Run your whole code 10 times and compute the mean and variance from the different runs. If a quantity is important, you MUST estimate its errors.

Homework

- On computing error bars, using dataspork and writing Python script to compute errors.
- See the web site for the assignment.
- We will review python on Friday
- Homework due Monday, Jan 28th.