One Lattice Gauge Theorist's Perspective on Important Skills and Concepts for Computational Physics Courses

Steven Gottlieb, Indiana University

sg at indiana.edu

Abstract

Lattice Gauge Theory employs a number of numerical and statistical techniques including: sparse matrix inversion, Monte Carlo methods, higher order numerical integration schemes, resampling methods such as jackknife and bootstrap, and parameter estimation from correlated data. Many of these techniques can be taught to undergraduates in contexts more easily understood than a lattice gauge theory simulation.

Outline

- Caveats
- Monte Carlo Methods
- Correlated Data
- Jackknife and Bootstrap
- Sparse Matrix Methods
- Numerical Integration
- Concluding Remarks

Caveats I

- I have been teaching Computational Physics at IU for about 20 years.
- However, the vast majority of my students have been graduate students.
- P410 $\rightarrow$ P609
- Only recently has the course been extended to a second semester.
- `http://physics.indiana.edu/~sg/p609.html`
- Since early days, I have been using *An Introduction to Computer Simulations Methods*, by H. Gould and J. Tobochnik as required text.
- W. Christian, added as author of Third Edition

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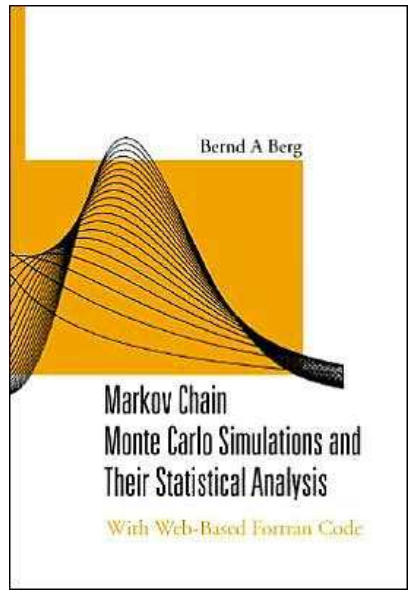
- W. Christian, added as author of Third Edition
- Don't know if my use of text had anything to do with my being invited here...

Caveats II

- Title says one person's opinion, but I used the LatticeNews mailing list to get feedback.
- 6 responses: B. Joo, B. Berg, M. Creutz, H. Markum, B. Svetitsky, U. Wolff
- Berg: Most of those topics are covered in my book.
  Markov Chain Monte Carlo Simulations and Their Statistical Analysis; With Web-Based Fortan Code



Monte Carlo Methods

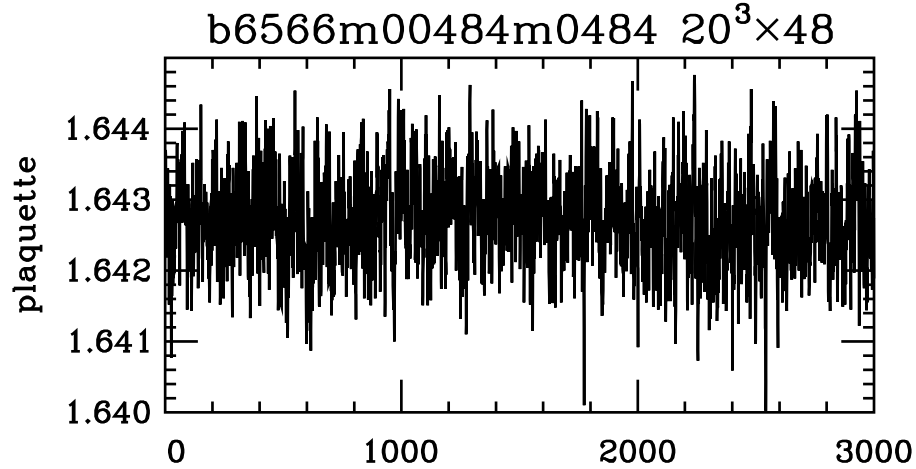
- Monte Carlo methods are just over 50 years old and are very widely used.
- Lattice QCD developed by K. Wilson in 1974, preserves essential symmetry called gauge invariance.
- Lattice QCD is not just a model, it is the theory dealt with numerically.
- Wilson was applying renormalization group method, but in 1979, Creutz, Jacobs and Rebbi introduced Monte Carlo sampling to study gauge systems.
- Current methods are dominated by ‘pseudo’ molecular dynamics approach, but may still use a Monte Carlo accept/reject step.
- Resampling methods developed by Ferrenberg and Swendson are useful.

Correlated Data

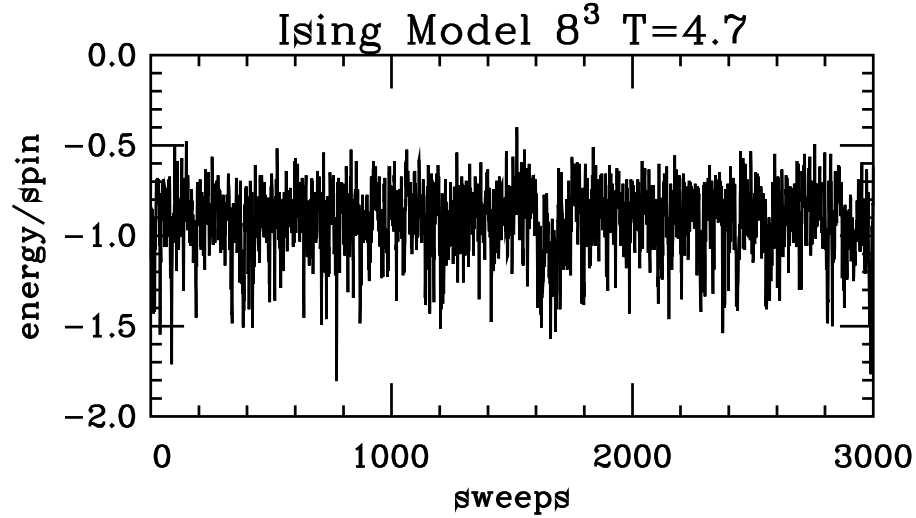
- Data generated in a typical lattice calculation is correlated in several ways:
  - Correlated in ‘simulation time’ (autocorrelation)
  - Correlated in Euclidian time and space
  - Different quantities determined in the same ensembles are correlated with each other
- Neglecting the autocorrelation underestimates the error
- Neglecting the correlations in Euclidean time means the results cannot be properly fit
  - Confidence level of fit is meaningless
  - Can’t properly estimate error in fit parameters

Autocorrelation I

Plaquette is a basic quantity in LQCD. Here is the time history of a run that took 1706 hours (71 days) on 128 cpus.



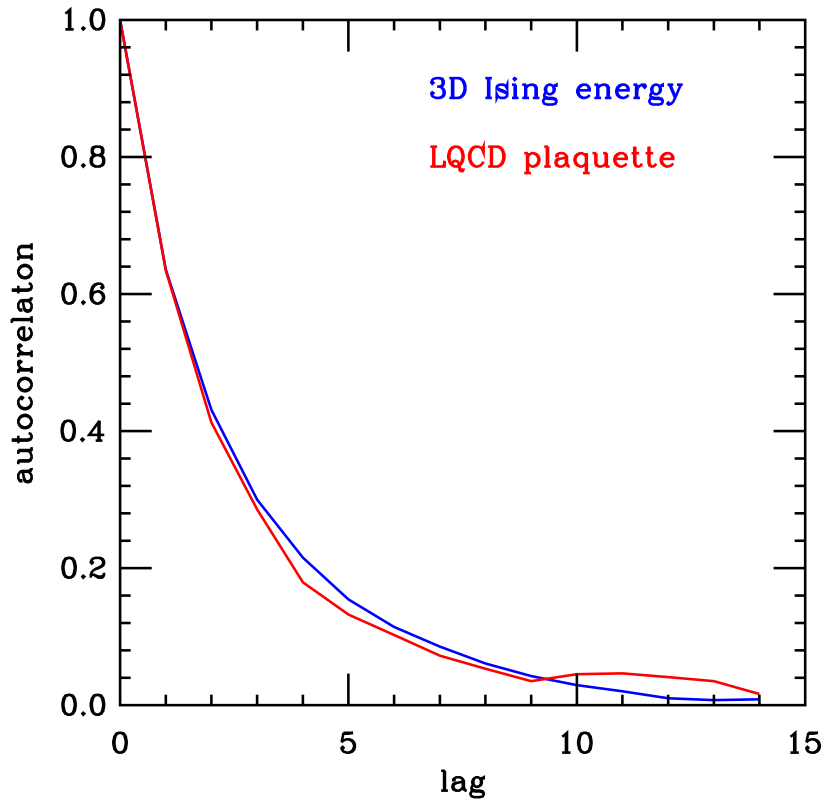
Energy/spin for 3D Ising model. Run took about 1 second on 1 cpu.



Autocorrelation II

Autocorrelation of time series $M(t)$ at lag l is

$$A(l) = (\langle M(t)M(t+l)\rangle - \langle M(t)\rangle^2)/(\langle M(t)M(t)\rangle - \langle M(t)\rangle^2)$$

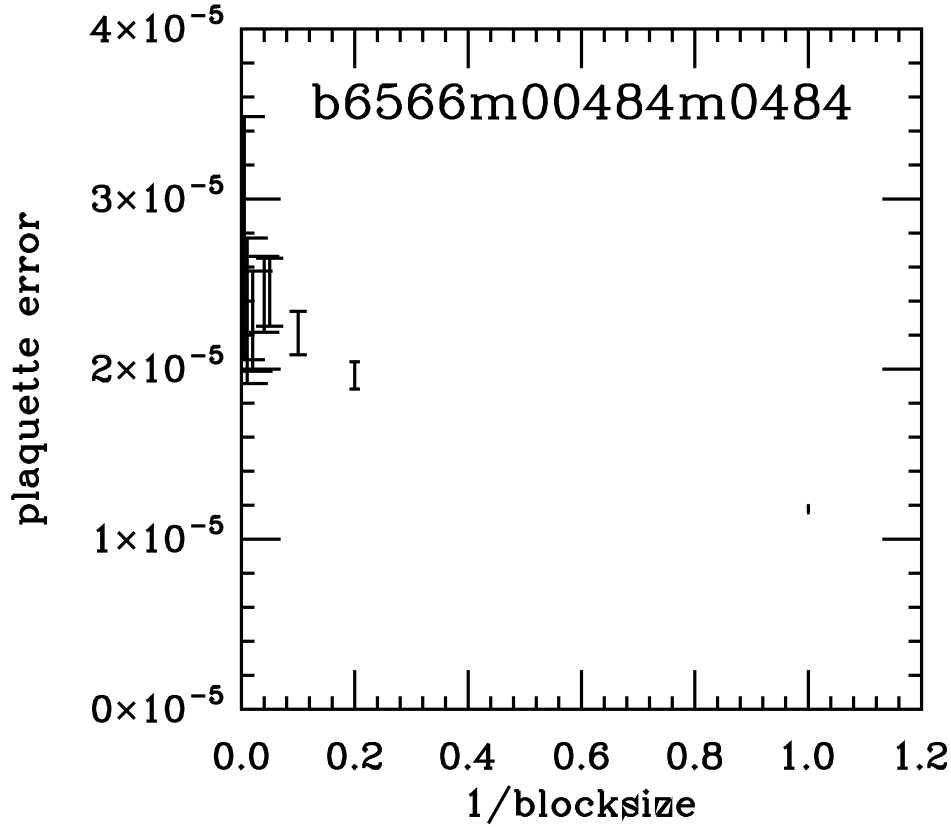


- Ising temperature was selected so that the autocorrelations are similar to the chosen QCD run.

- Using only a trivial amount of computer time, students can generate data that shares important aspects of research quality data.
- They can also generate lots more data enabling better statistical analysis.

Autocorrelation III

Let's see what happens to the plaquette error when we block data before computing standard deviation:

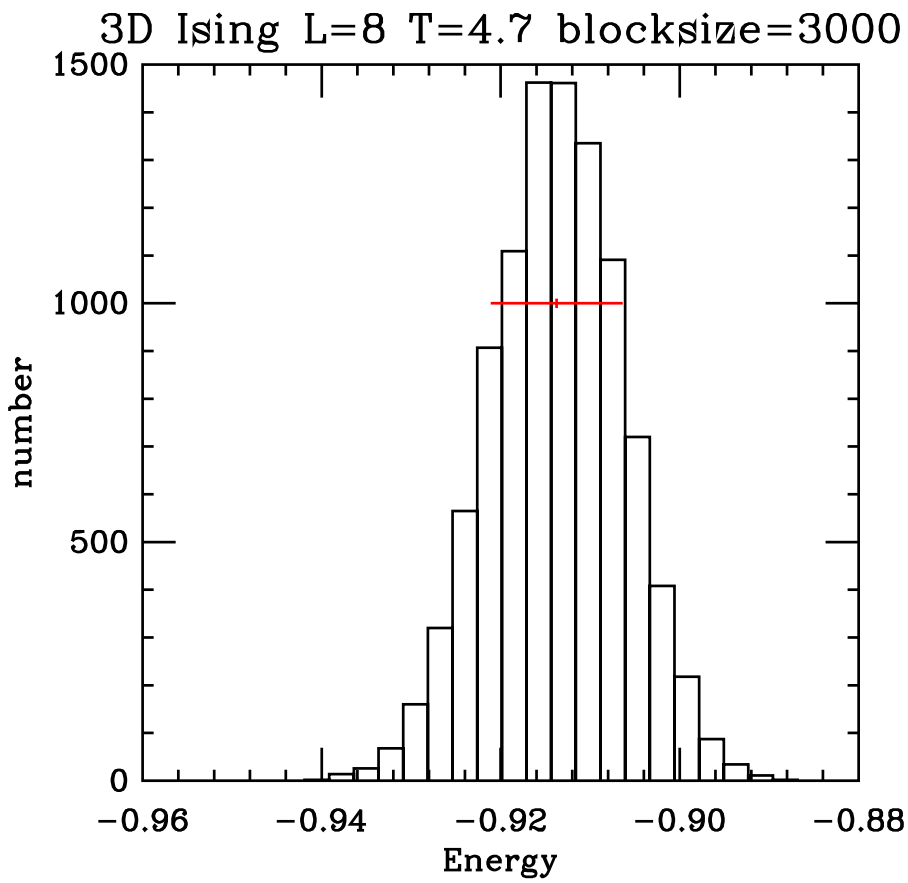


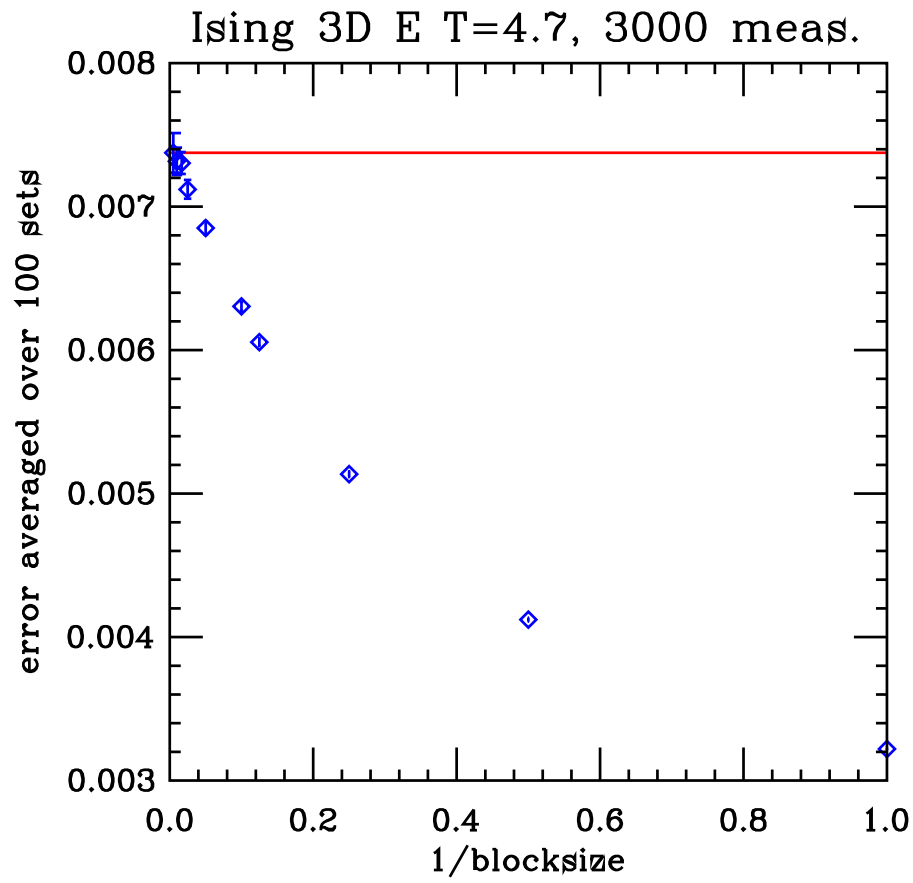
- Error seems to grow linearly with inverse blocksize.
- If we don't block, we grossly underestimate the error.
- Larger autocorrelation requires a larger blocksize.

Autocorrelation: Exercise

- If we could repeat this experiment 100 times, we could histogram the average of 3000 sweeps and see the variance. That would be the true error.
- We can't do that for LQCD, but for the Ising model, we can do so.
- Create a very long Ising model simulation and split it into blocks of 3000 sweeps.
- Histogram the average value and compute the variance to get the true error for a block of length 3000.
- On one (or each) block of 3000, employ blocking as described above to compute the error. How do the two results compare?

Autocorrelation: Solution





- On left we have a histogram based on the average of 10,000 blocks of length 3000.
- On the right we compute the error for different blocksizes on each of 100 blocks of length 3000. For each blocksize, the errors are then averaged.

Fitting Correlated Data I

- Students usually learn about least squares fitting or χ^2 for uncorrelated data.

$$\chi^2 = \sum_i \frac{(y_M(x_i, \lambda) - y_i)^2}{\sigma_i^2}$$

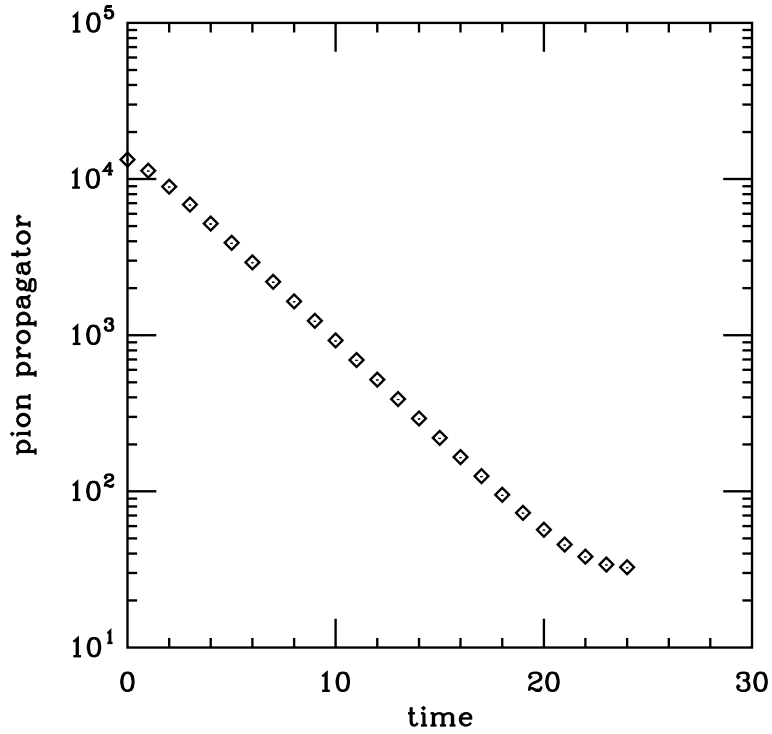
- When the data is correlated, let $C_{ij} = Cov(y_i, y_j)$ and then

$$\chi^2 = \sum_i (y_M(x_i, \lambda) - y_i) C_{ij}^{-1} (y_M(x_j, \lambda) - y_j)$$

- Uncorrelated data reduces to $C_{ij} = \delta_{ij}\sigma_i^2$.
- If the covariance matrix has positive entries, the data will look smoother than it should.

Fitting Correlated Data II

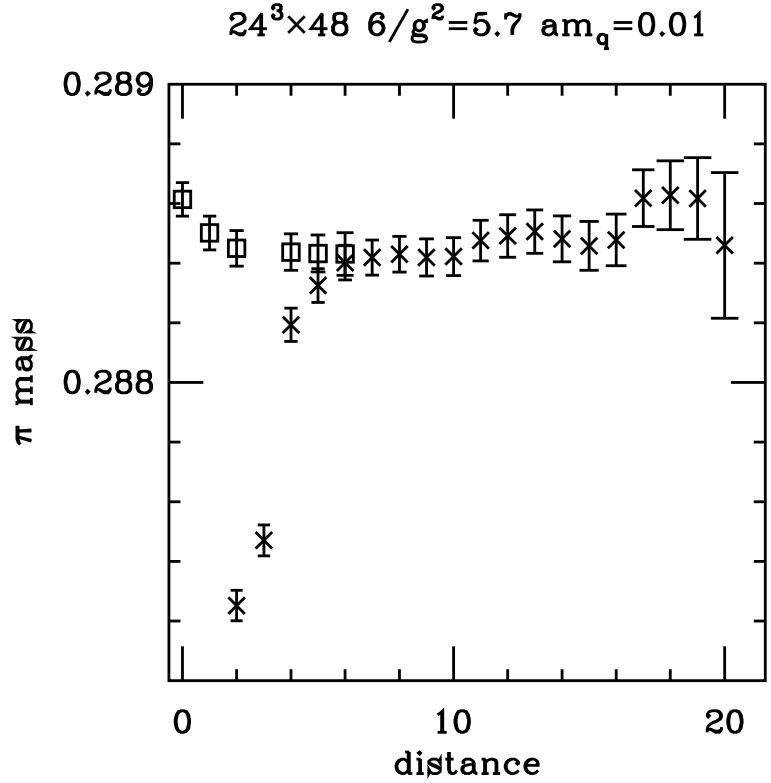
- Here we have some data for a pion propagating in Euclidean time.



- It is hard to see the errors, because they are so small.
- The propagator is supposed to fall of exponentially for long times, but there are periodic boundary conditions in time. For short times, there may be contributions from a heavier particle.

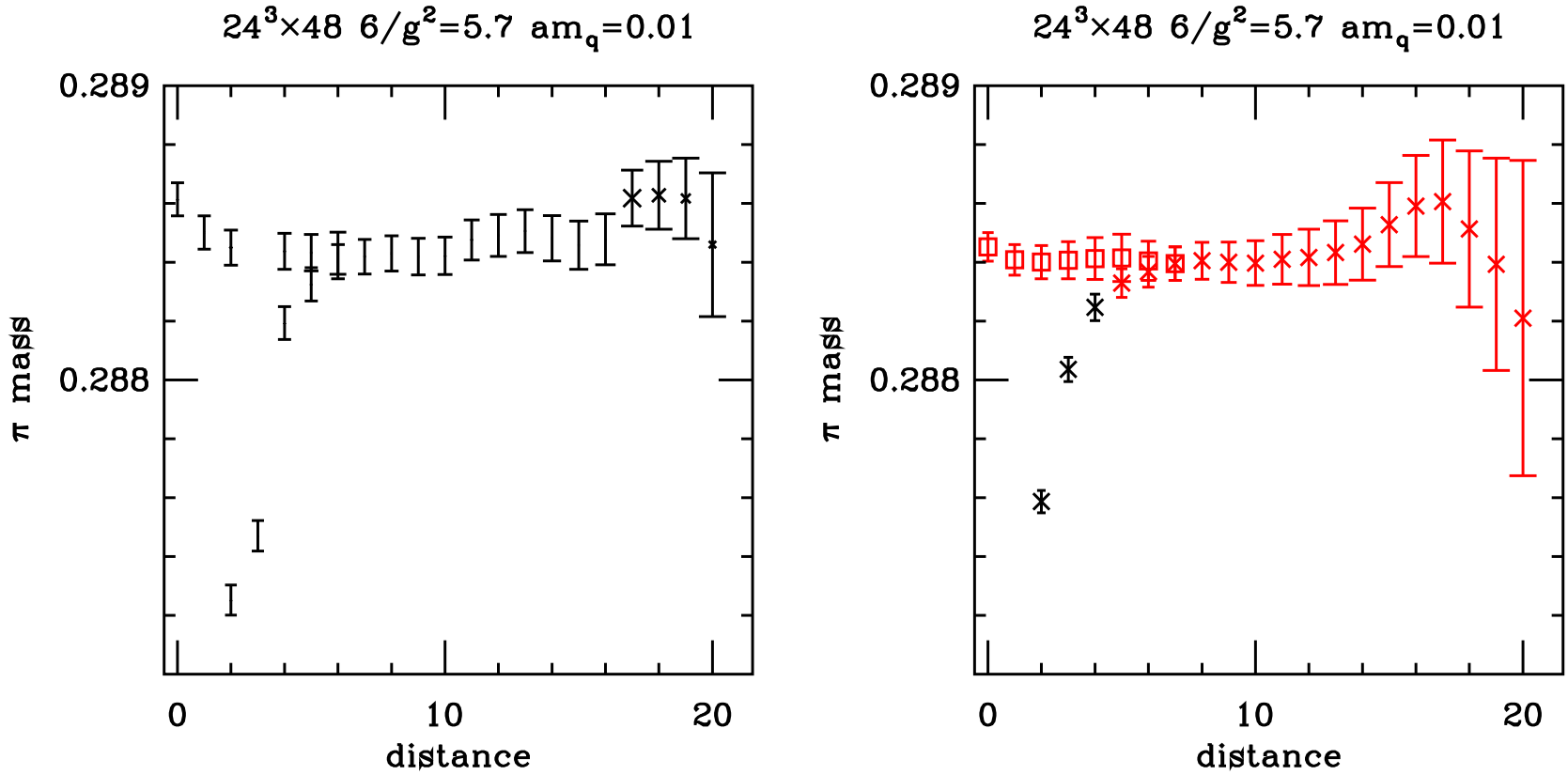
Fitting Correlated Data III

- First we fit including the covariance.
- In these fits we vary the minimum distance that is fit to try to exclude the region where the heavier particle may contribute.
- The squares come from fits with additional parameters for a heavier particle.



Fitting Correlated Data IV

- Which fit should we pick? Need confidence level.



- (L) The symbols are proportional to the confidence level of the fit. The best fit starts at distance 17.
- (R) We fit without the covariances. Red points have a confidence level $>$ 95%.

Jackknife and Bootstrap I

- Jackknife and Bootstrap are known as resampling methods.
- In (single-elimination) jackknife, you remove one data point at a time from your sample and look at the variation of the resulting average.
- All the jackknife samples are highly correlated, so the resulting variance is too small and must be corrected by multiplying by N, number of points.
- If data is correlated, you can eliminate blocks of data to form each jackknife sample. If the calculated error grows as the blocksize increases, then you need to keep increasing the block size.

Jackknife and Bootstrap II

- Jackknife is also good for sample size bias reduction.
- In my class, I use a very simple example of a biased statistic.
- Say you can measure the velocity of particles, but you want the time for a particle with the average velocity to traverse 1 meter.

$$t = 1/\langle v \rangle$$

- An easy way to estimate the average velocity is to make n measurements and average.
- However, this will be a biased estimator for t, as can be worked out in great detail for a very simple velocity distribution. v is uniformly distributed between 0 and 1.

Jackknife and Bootstrap III

- For any statistic S, let the statitic measured on a sample of size n be denoted S_n. We assume the leading bias is order $1/n$, so:

$$S_n = S_\infty + \epsilon/n$$

$$S_\infty = nS_n - (n-1)S_{n-1}$$

- If we have n measurements, we have one evaluation of the statistic S_n, and by eliminating one measurement at a time, we can make n estimates of the statistic S_{n-1}
- It is easy to test this via a Monte Carlo.

Jackknife and Bootstrap III

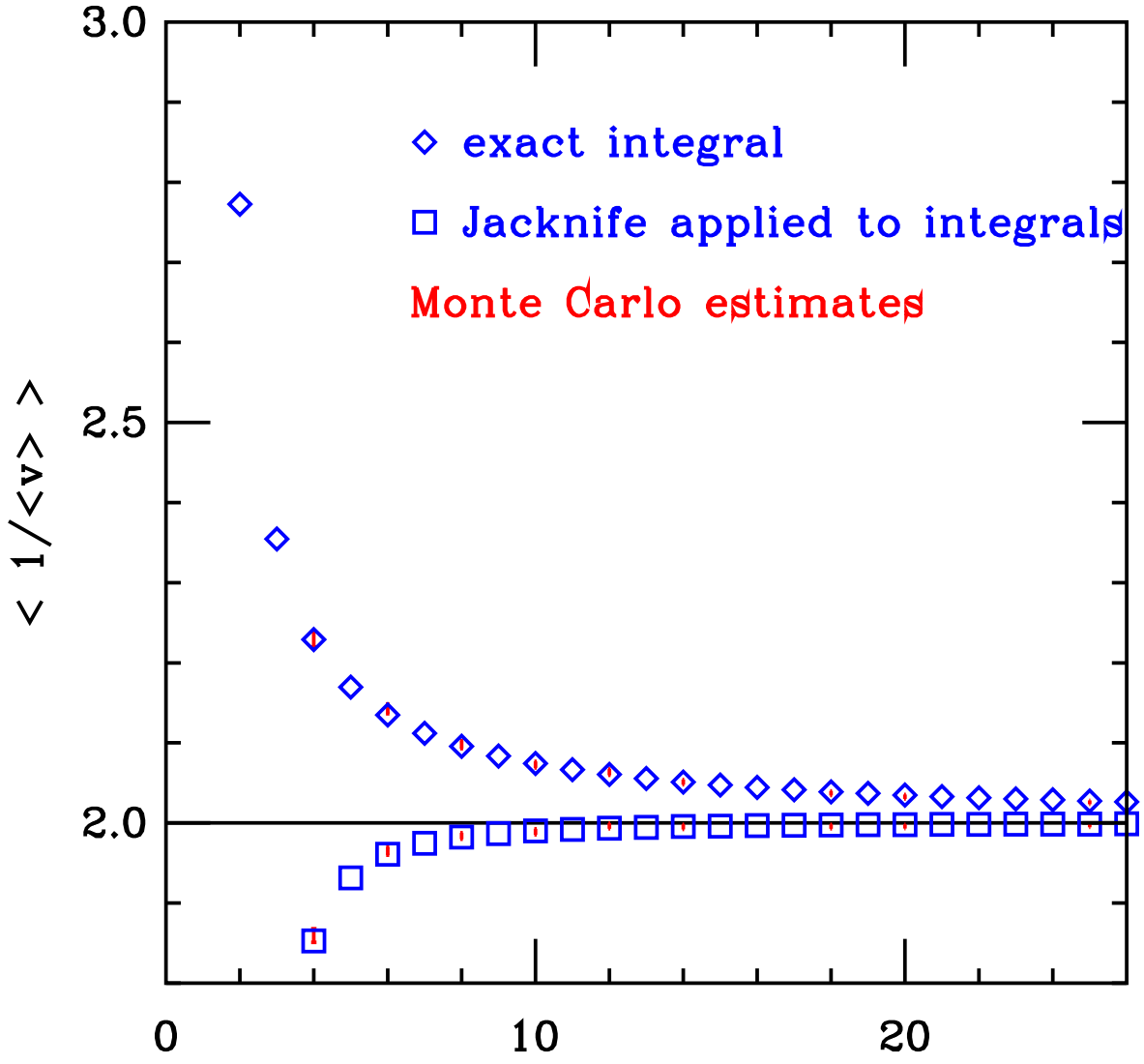
- It is also interesting to replace the Monte Carlo by an exact evaluation. If there are n measurements of v, then each possible measurement is a point uniformly distributed in $[0,1]^n$ and

$$t_n = \prod_{i=1,n} \int_0^1 dv_i \; n/(\sum_{j=1,n} v_j)$$

- I have my students use Mathematica to evaluate these integrals. We need some tricks beyond say $n = 7$, but jackknife bias reduction can be applied either to the computed integral or the Monte Carlo samples.

Jackknife and Bootstrap IV

We can apply the jackknife bias reduction either to Monte Carlo samples or the exact values of the integrals defined above.



Jackknife and Bootstrap V

- Finally, with bootstrap and jackknife you don't have to do complicated error propagation calculations. You just carry out your entire analysis on the samples and estimate the final errors from variation seen in the samples.
- For bootstrap, results are usually histogrammed and errors determined by usual probability distribution of a gaussian distribution. Not very sensitive to outliers.
- For jackknife, need to multiply variance by N to account for correlations.

Sparse Matrix Methods

- Sparse Matrix Methods are very important for lattice QCD problems that include quarks. One frequently needs to invert the quark matrix (Dirac Operator).
- In the early days, Gauss-Seidel was used, but a number of more modern and faster methods quickly replaced it.
  - Conjugate Gradient (CG)
  - Minimum Residual (MRES)
  - Biconjugate Gradient Stabilized (BiCGStab)
- Newer methods, which are still being researched include
  - Multigrid algorithms (acutally been trying to make this work for years)
  - Alternating Schwartz method

Higher Order Integration Schemes

- Sometimes students don't want to go beyond the Euler algorithm. Current computers are so fast, it is hard to convince them to think instead of decreasing step size.
- Leap-frog or half step algorithm has long been popular in lattice QCD.
- Recently, Omelyan type methods have come into vogue. [Comp. Phys. Comm. **151** 272 (2003)]

Concluding Remarks

- Students can learn methods needed to work on research level problems without needing research level supercomputers:
  - by working on models more simple than lattice QCD,
  - by working on problems that were research level 10–20 years ago.
- Statistical techniques and analysis have become very important in ways a classically trained physicist of my generation might not have imagined.
- Hopefully, students can gain insight and expertise by doing ‘experiments’ on model systems for which they can generate voluminous results.
- I also hope my students have as much fun as I do exploring different systems and the resulting physics.

References

These reference slides were added after the conference.

- Another useful book on Monte Carlo Methods is “A Guide to Monte Carlo Simulations in Statistical Physics” by D. P. Landau and K. Binder, Cambridge University Press (2nd edition). It includes a chapter on lattice gauge theory.
- There are several books on lattice gauge theory available. I will plug one by current and former collaborators: “Lattice Methods for Quantum Chromodynamics” by T. DeGrand and C. DeTar, World Scientific, 2006.
- Reweighting methods are covered in Sec. 15.11 of Gould, Tobochnik and Christian and Chapter 7 of Landau and Binder. For original work see A.M. Ferrenberg and R.H. Swendsen, Phys Rev Lett. 61, 2536 (1988); 63, 1195 (1989).
- Autocorrelation is discussed in Gould, Tobochnik and Christian on page 239.
- One of the responses to my email to LatticeNews came from U. Wolff who mentioned his paper “Monte Carlo Errors with less errors”, Comp. Phys. Comm. 156, 143 (2004) [arXiv:hep-lat/0306017].
- One of the classic references for resampling methods is the monograph “The Jackknife, the Bootstrap and Other Resampling Plans,” by B. Efron, (SIAM) 1982.

- “Matrix Computations” by G.H. Golub and C.F van Loan, Johns Hopkins, 1989 covers many of the important algorithms.
- A recent talk by W. Wilcox at Lattice 2007 reviews some of the most recent methods: `http://www.physik.uni-regensburg.de/lat07/hevea/wilcox.pdf` and includes numerous references to original papers.