Update on the improved lattice calculation of direct CP-violation in K decays

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Lattice 2019

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Motivation

- Significant goal of RBC & UKQCD is physical lattice calculation of ε’, the measure of direct CP-violation in $K \to \pi\pi$ decays.
- Direct CPV heavily suppressed in Standard Model hence ε’ is very sensitive to BSM sources of CPV.
- When compared to experiment, any deviations may help shed light on origin of matter/antimatter asymmetry.
- Understanding I=0 $\pi\pi$ system is crucial:
  - Energy is needed for time dependence of correlation function from which extract finite-volume $K \to \pi\pi$ matrix element.
  - Phase shift enters Lellouch-Luscher finite-volume correction to matrix element.

Calculation details

- 741 configurations of domain wall fermions with Iwasaki+DSDR gauge action (a^{-1}=1.73 GeV) and physical pion masses.
- 32^3x64 volume ~ $(4.7\ \mathrm{fm})^3$ - large volume helps control finite-volume effects.
- G-parity BCs in 3-directions, lowest energy pion momentum (1,1,1)π/L. $E_{\pi\pi}$~m_K ensuring physical decay.
- 3 ππ operators: ππ(111), ππ(311), σ (scalar)
- Significant improvement in determination of ground-state energy (cf Tianle Wang's talk)
- $E_{\pi\pi}$= 0.3614(74) [2015, 216cfgs, 1 op] [Phys.Rev.Lett. 115 (2015) no.21, 212001]

  → ~0.3488(9)* [2019, 741 cfgs, 3 op]
- Result now agrees well with dispersive prediction.
- Good evidence that excited state contamination formerly underestimated.
- Effect on K→ππ as yet undetermined, awaiting final ππ numbers

Multi-operator ππ fits

- Obtain parameters by simultaneous fitting to matrix of correlation functions

$$C_{ij}(t) = \langle 0|O_i^\dagger(t) O_j(0)|0\rangle \;= C + \sum_\alpha A_{i,\alpha} A_{j,\alpha} e^{-E_\alpha t}$$

round-the-world single pion propagation small compared to errors - drop

- Correlated fits to obtain most precise result and **goodness-of-fit metric**
- Jackknife procedure to determine statistical errors.
- Full variation in covariance matrix over jackknife samples taken into account with double-jackknife technique.

Outstanding issues

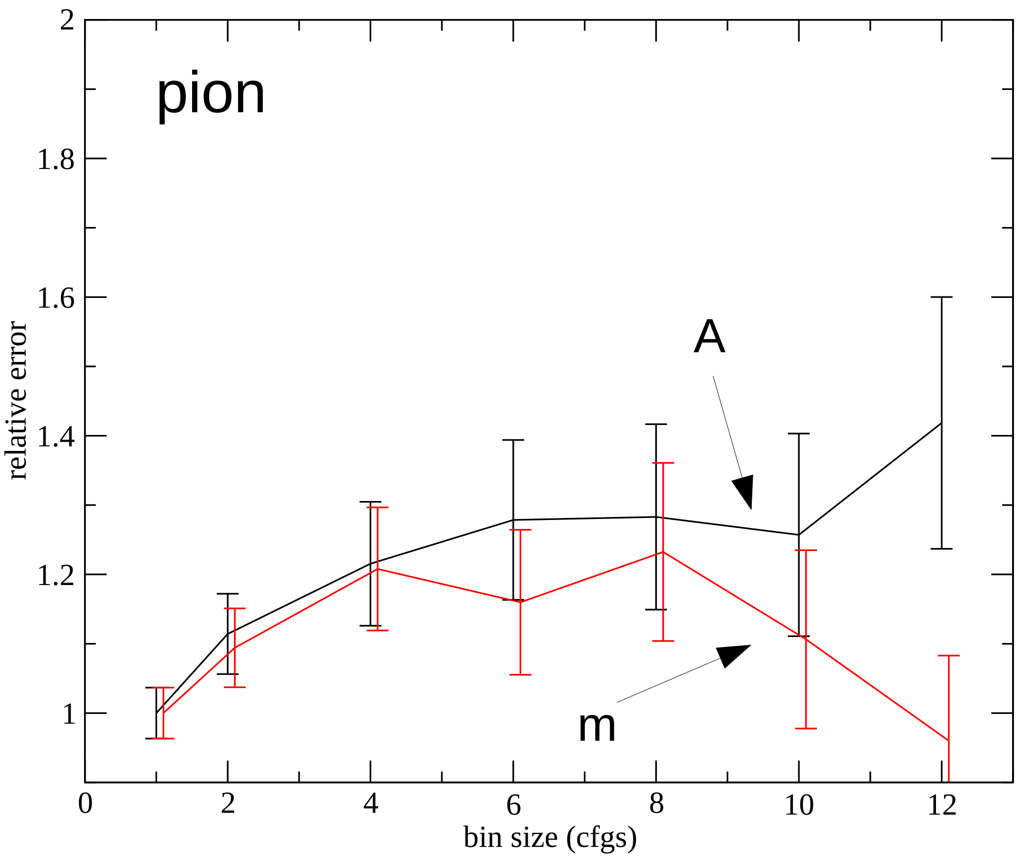
- I=0 $\pi\pi$ calculation looks very solid and excited state contamination appears negligible.
- Why the delay in publication then?
    - With vastly more statistics, now some evidence of autocorrelation effects which may lead to underestimation of errors.
    - Despite high degree of stability under changing fit ranges, goodness of fit typically quite poor and display unexpected dependence on bin size and fit ranges.
- Importance of reliable $\pi\pi$ fits strongly motivates resolving these issues.

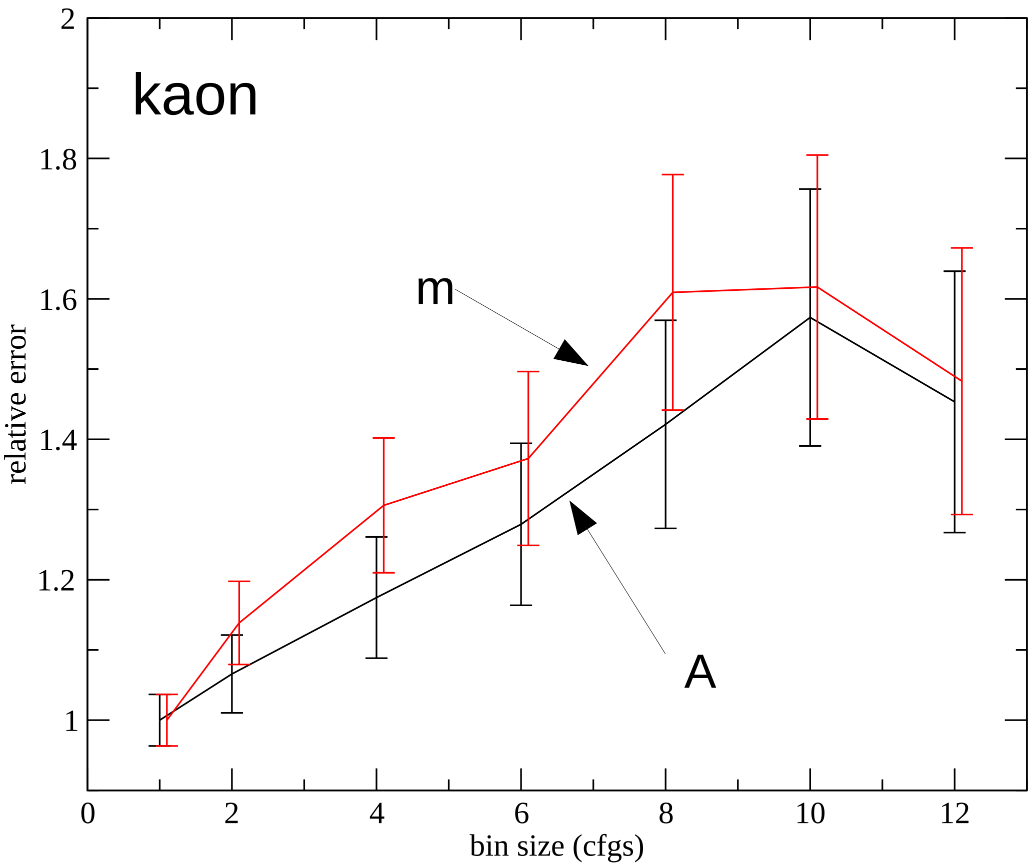
Autocorrelations

Dealing with autocorrelations

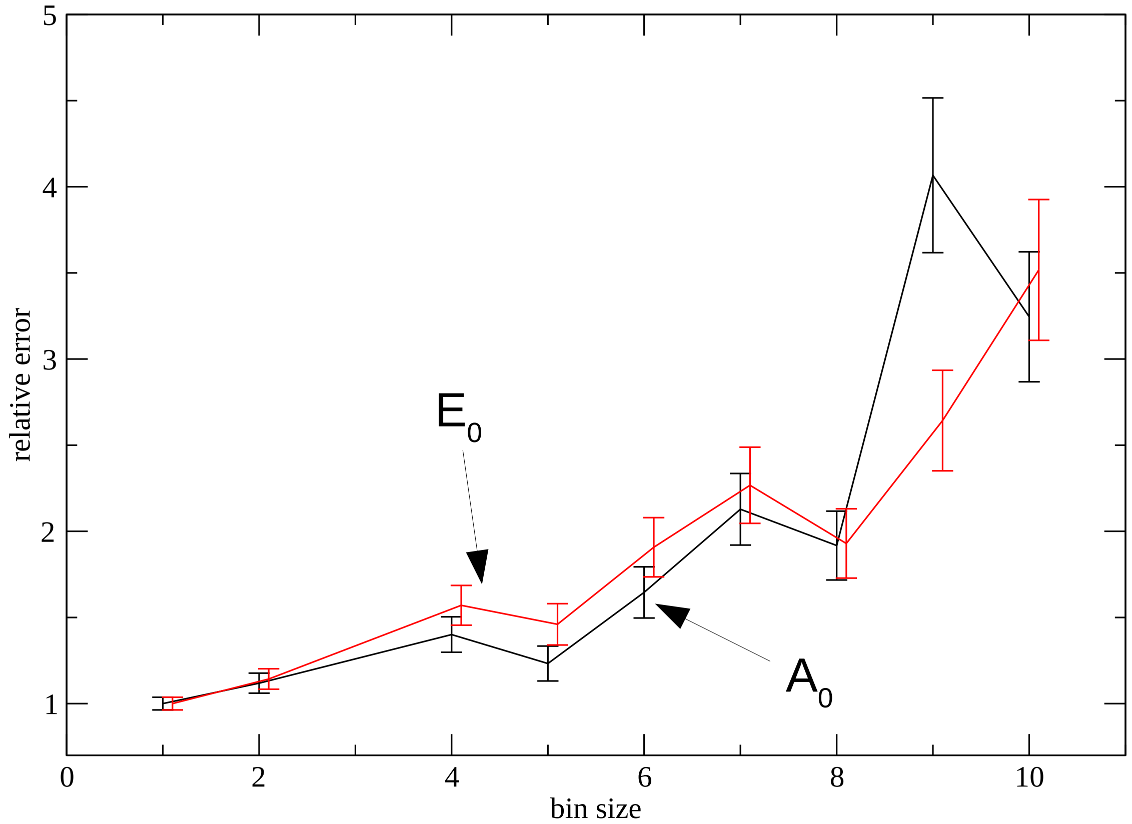
- Evidence suggests τ_{int} ~ 4 MDTU (1 cfg)
- Naively $\sigma \propto \sqrt{\frac{2\tau_{\mathrm{int}}}{n}}$ expect ~1.4x larger errors.
- Standard (crude) strategy is to bin (average) the data over blocks sufficiently large to make the blocks independent.
- Typically see errors grow then stabilize when bin size large enough.

Pion and kaon 2pt functions





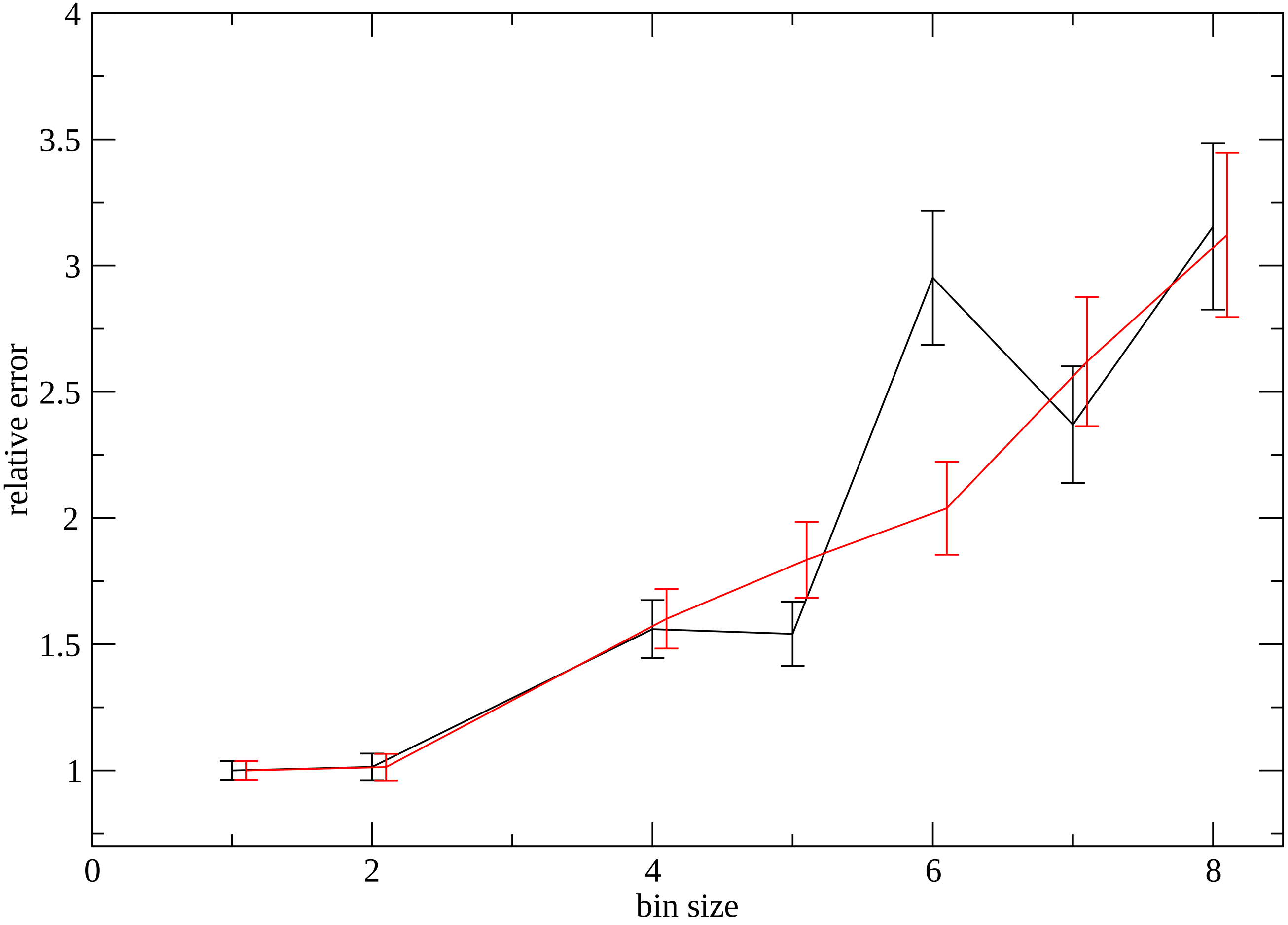
I=0 ππ 2pt function



- ππ errors continue growing with bin size and do not stabilize. Why?
- Covariance matrix is 66x66 here!
- As bin size increased, fewer data points enter determination of covariance matrix ⇒ matrix becomes less and less well resolved.
- Fluctuations of low eigenvalues increase, causing error growth unrelated to autocorrelation

Scrambled data

- Isolate effect of loss of resolution of covariance matrix by randomly scrambling data to destroy autocorrelations

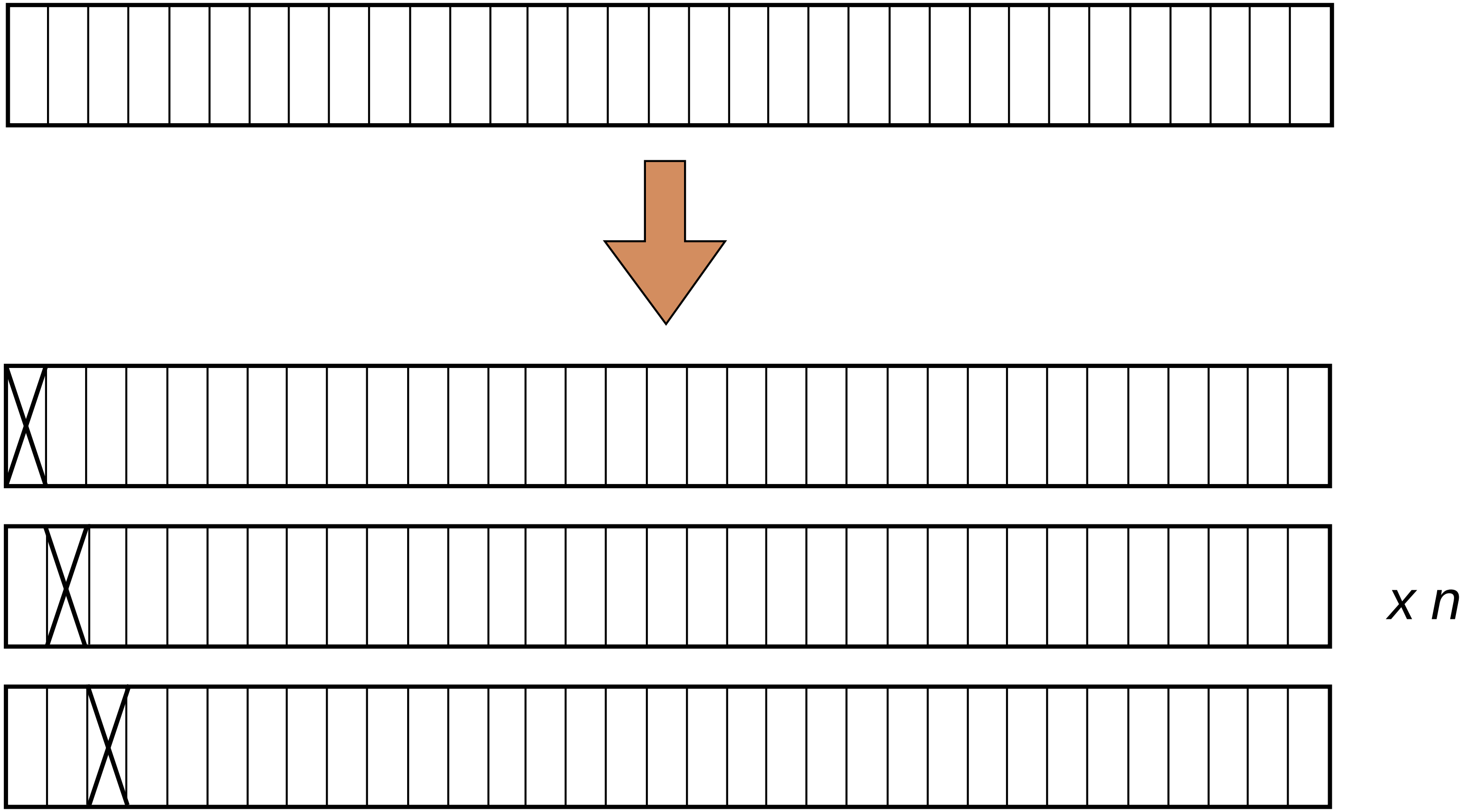


- Error growth essentially the same!

Block jackknife

- To prevent loss of resolution of covariance matrix while still take into account autocorrelations, we perform **block jackknife**

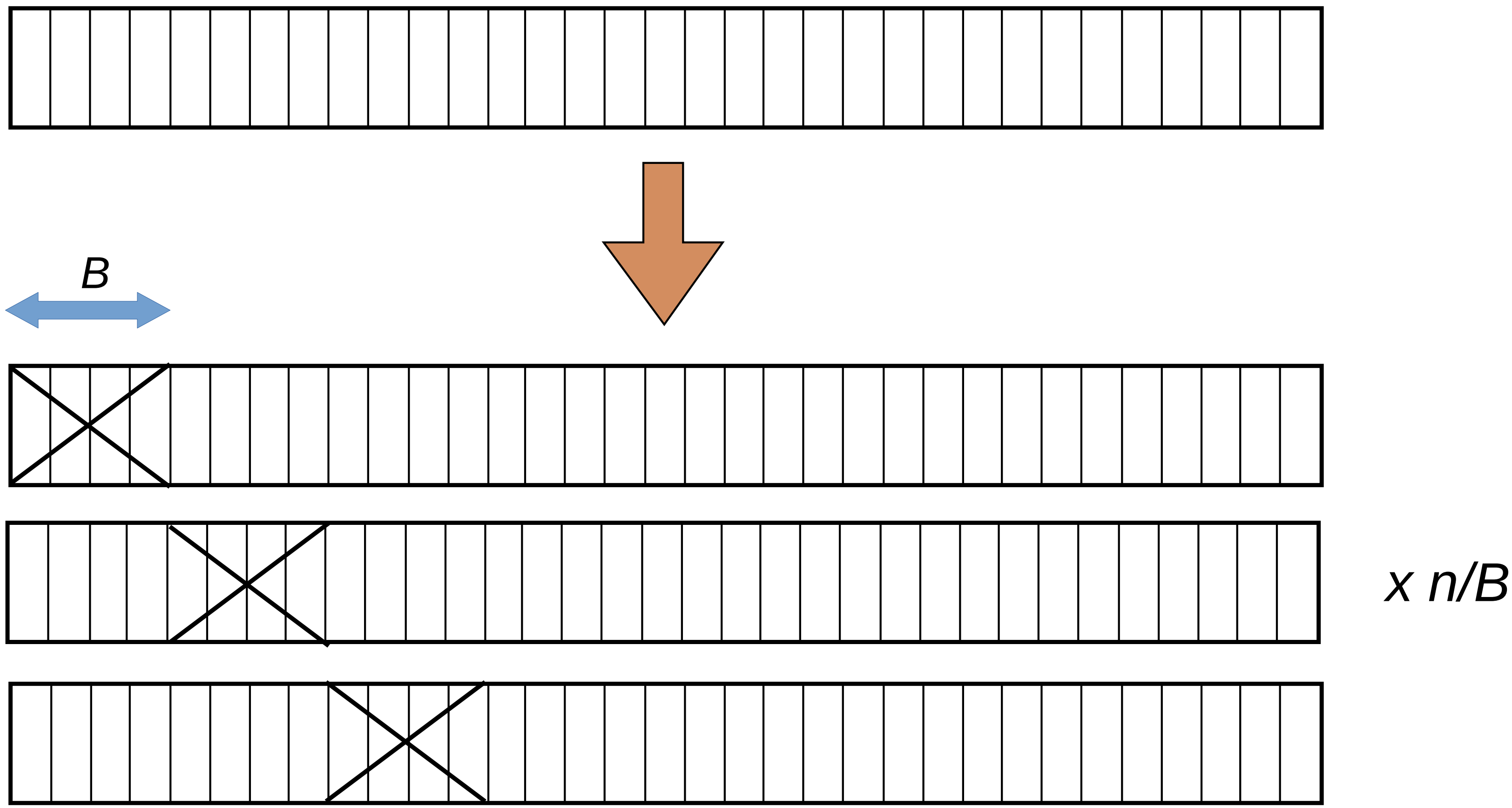
Regular jackknife: generate *n* “reduced ensembles” of size *n-1* by dropping successive samples



- With binning, covariance matrix obtained from just *n/B-1* samples

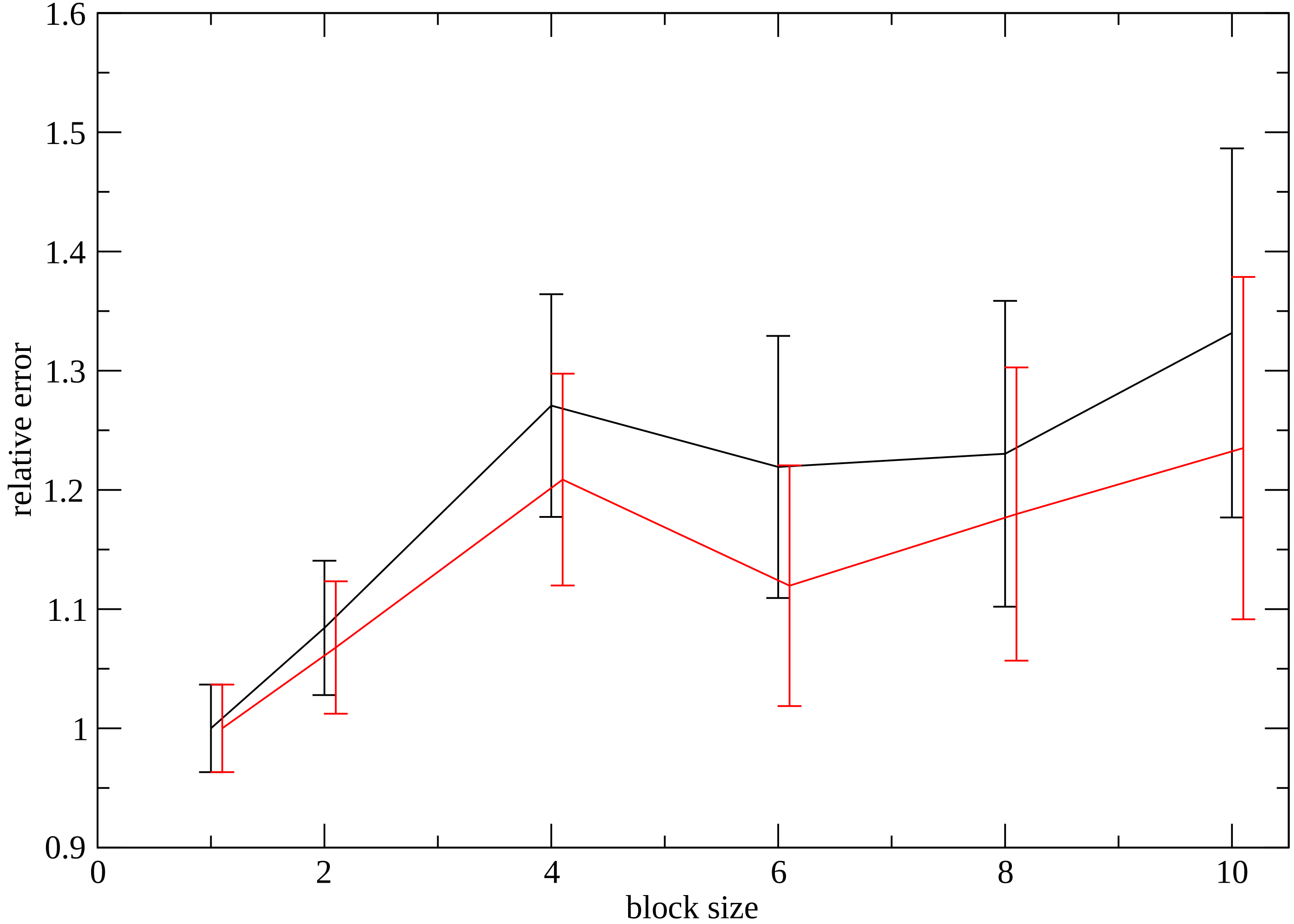
Block jackknife II

block jackknife: generate *n/B* reduced ensembles of size *n-B* by throwing away successive **blocks** of size *B*



- Covariance matrix obtained from *n-B* samples !
- Jackknife procedure ensures correct statistical error

I=0 ππ 2pt function with block jackknife



- Bravissimo! Problem solved

Goodness of fit

Techniques

- Test statistic is q^2 (often called χ^2).

$$q^2 = \sum_{t,t'=t_{\min}}^{t_{\max}} \left[\bar{v}_t - f(t,\vec{p})\right] C^{-1}_{tt'} \left[\bar{v}_{t'} - f(t',\vec{p})\right]$$

With covariance matrix obtained from sample covariance:

$$C_{tt'} = \frac{1}{n(n-1)} \sum_{i=1}^{n} \left[v_{i,t} - \bar{v}_t\right] \left[v_{i,t'} - \bar{v}_{t'}\right]$$

- **Stone age:** compare q^2/dof to 1.
  Doesn't take into account fact that deviations from 1 less likely for large dof *k* as std.dev of distribution

$$\text{std. dev}(q^2/\text{dof}) \sim \sqrt{2/k}$$

- **Bronze age:** compare q^2 to χ^2(k = dof) distribution, compute **p-value:**

$$p(q^2,k) = \int_{q^2}^{\infty} dx \; \text{PDF}_{\chi^2}(x,k)$$

Doesn't take into account fluctuations in covariance matrix between experiments when cov. mat obtained from data

Techniques II

- **Iron age:** For *normally-distributed, independent data*, effects of fluctuations of covariance matrix incorporated in the Hotelling T^2 distribution:

$$q^2 \sim T^2(k, n-1)$$

Doesn't take into account effects of non-normality or autocorrelations.

Correction to χ^2 significant for large k (dof) :

$$\langle T^2(k,n)\rangle - \langle \chi^2(k)\rangle \approx k^2/n$$

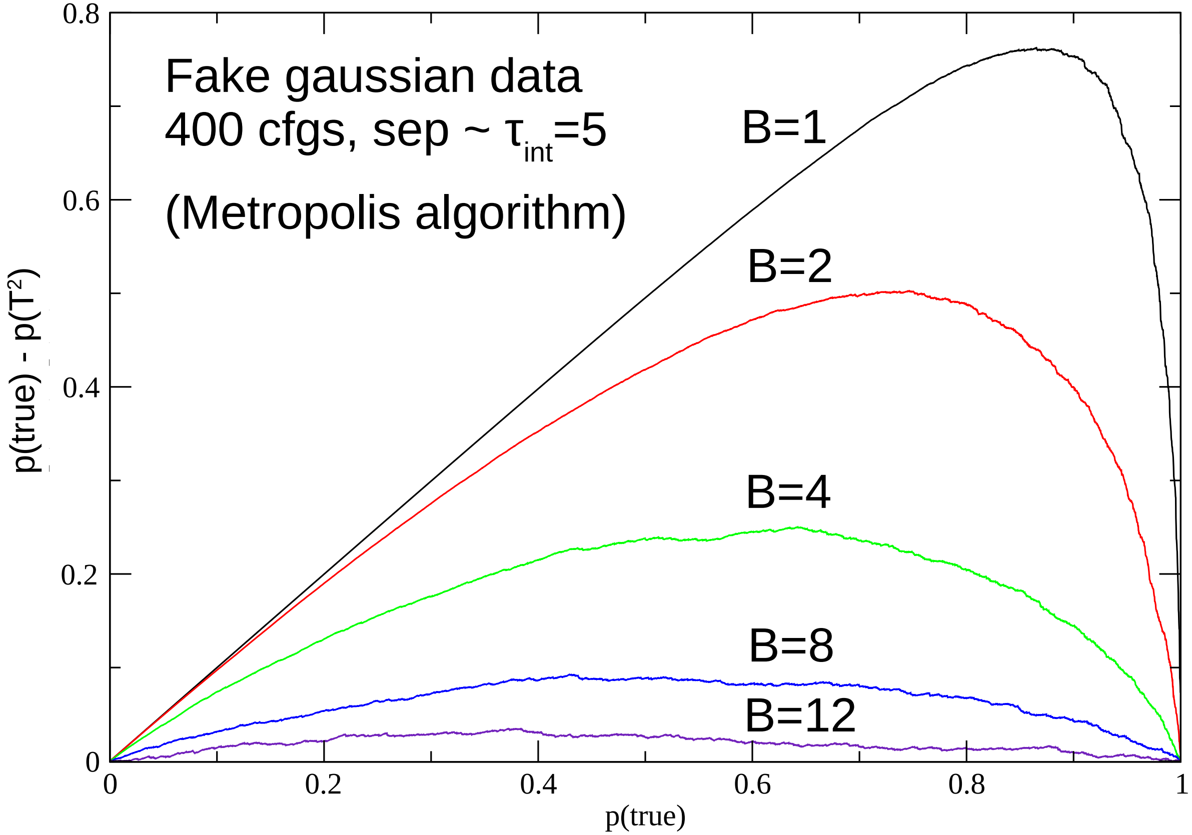
Example:

I=0 ππ fit, range 5-15 (no binning): k=54, q^2=74

$$q^2/\mathrm{dof} = 1.37 \qquad p(\chi^2) = 0.04 \qquad p(T^2) = 0.1$$

Is the Hotelling distribution sufficient?

- Numerical experiments with fake data show Hotelling T^2 relatively tolerant of non-normality.
- **However** T^2 relies on independent configurations: *extremely* sensitive to autocorrelations.
- Even with binning, slow convergence to true distribution:

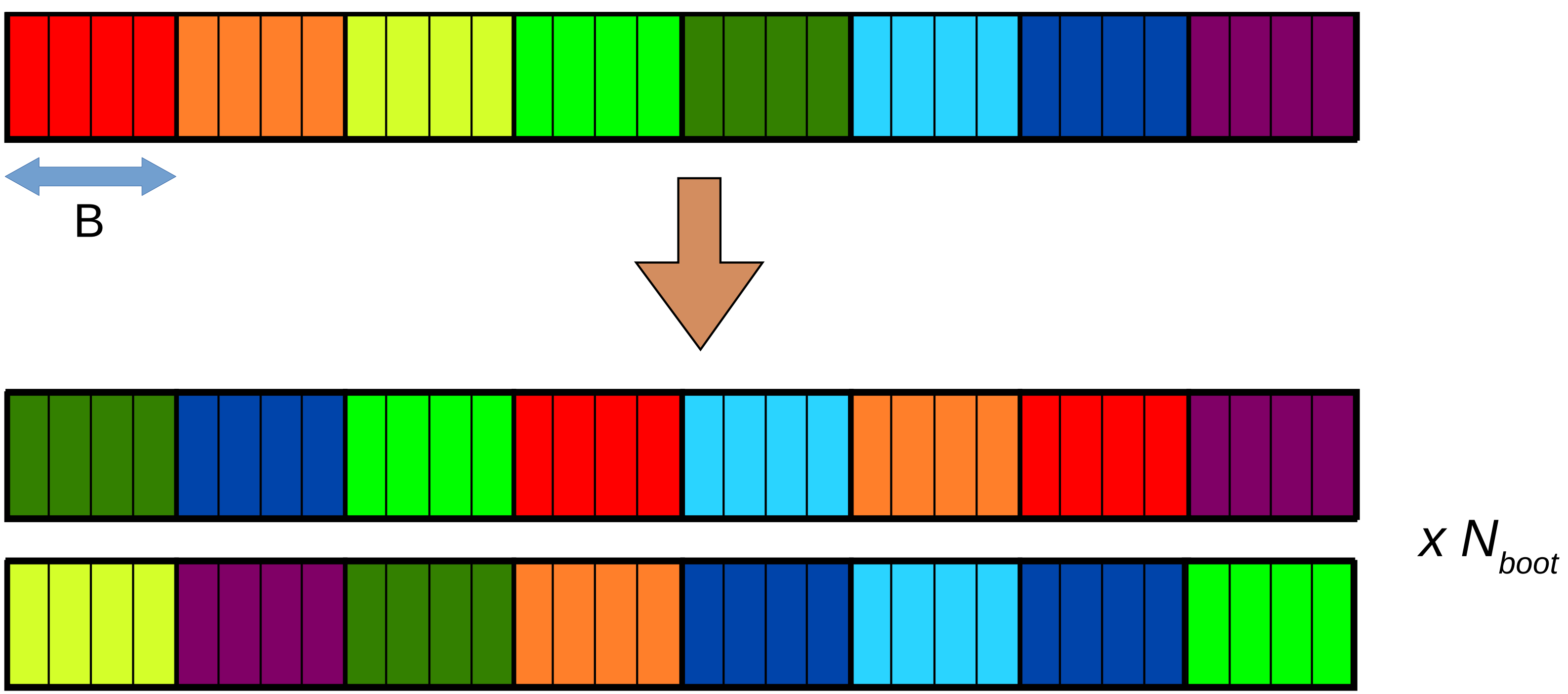


dramatically underestimates p

- Wish to avoid binning due to explosion in statistical error from reduced resolution of covariance matrix

Space age: Non-overlapping block bootstrap (NBB)

- The **bootstrap** technique allows us to estimate properties of the population from just one ensemble, by randomly resampling (with replacement).
- The (non-overlapping) block variant resamples blocks rather than single configurations, much like block jackknife, in order to account for autocorrelations:



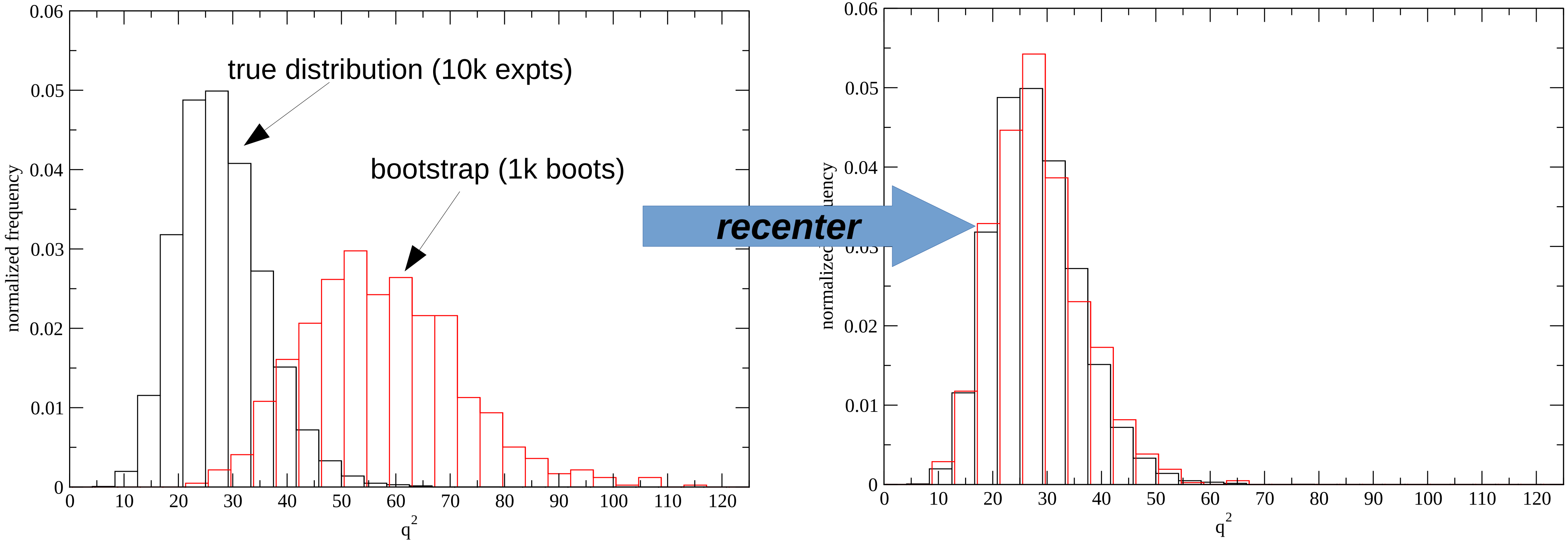
Space age II

- Use NBB to directly compute the distribution of q^2!
  - ✓ No normality assumption
  - ✓ Blocking accounts for autocorrelations without binning
- Minor subtlety: bootstrap ensemble means $\bar{b}^\alpha$ distributed about ensemble mean $\bar{v}$ ***not population mean***
- Results in broader distribution of q^2 with higher mean
- Correct by "recentering": $\bar{b}^\alpha(t) \to \bar{b}^\alpha(t) + [f(t, \vec{p}) - \bar{e}(t)]$

fit to original ensemble

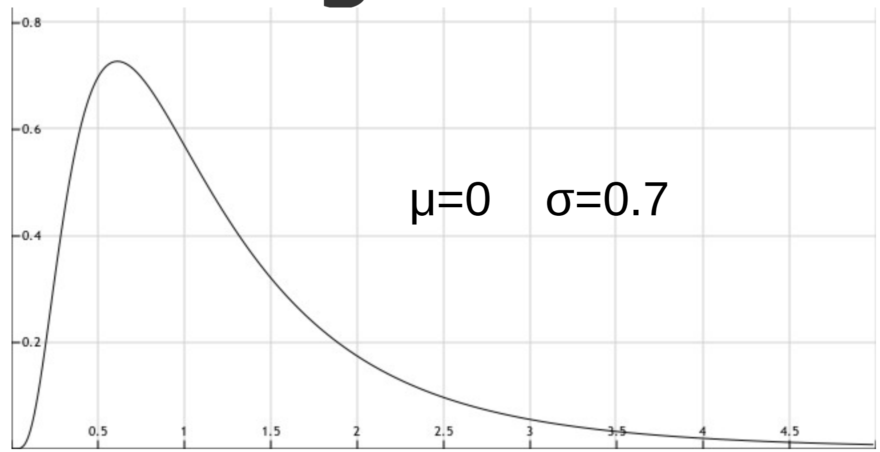
Demonstration

gaussian data, no autocorrelations, 400 samples

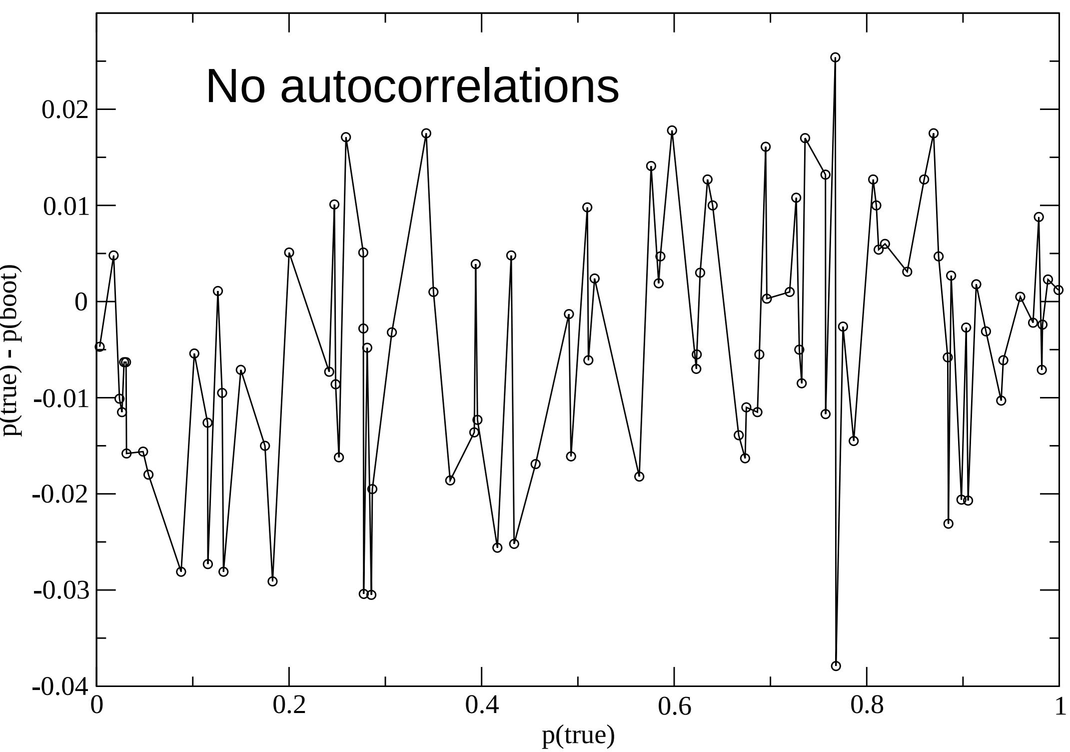


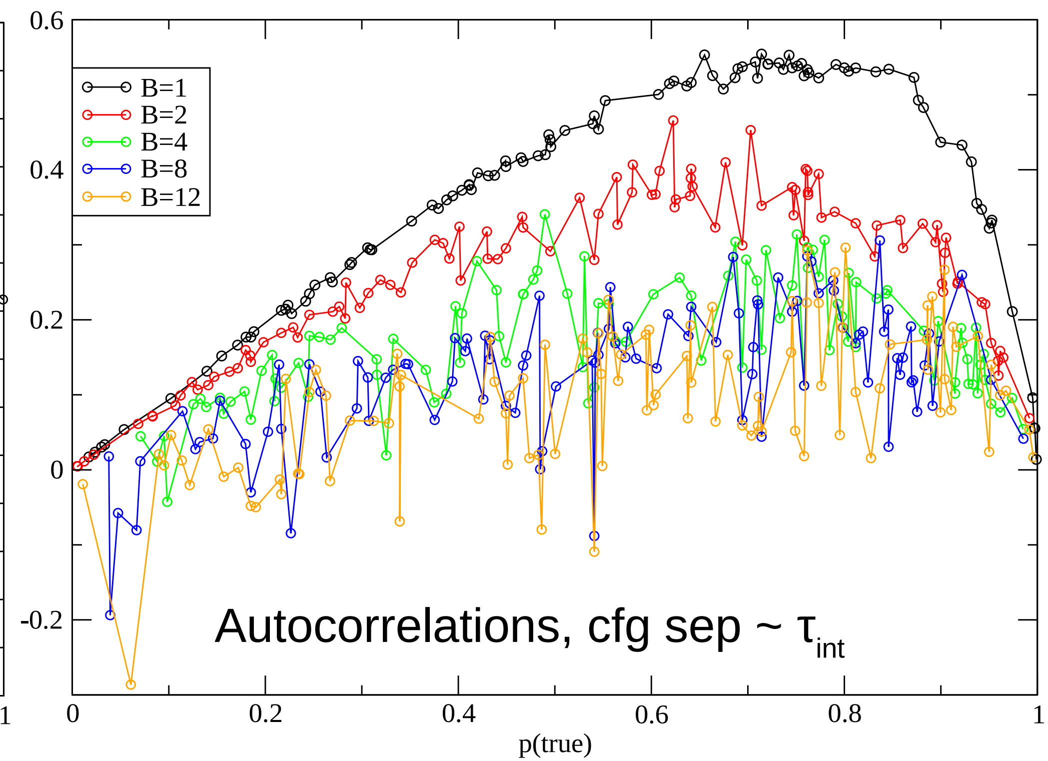
Demonstration II - log-normal

400 cfgs, log-normal

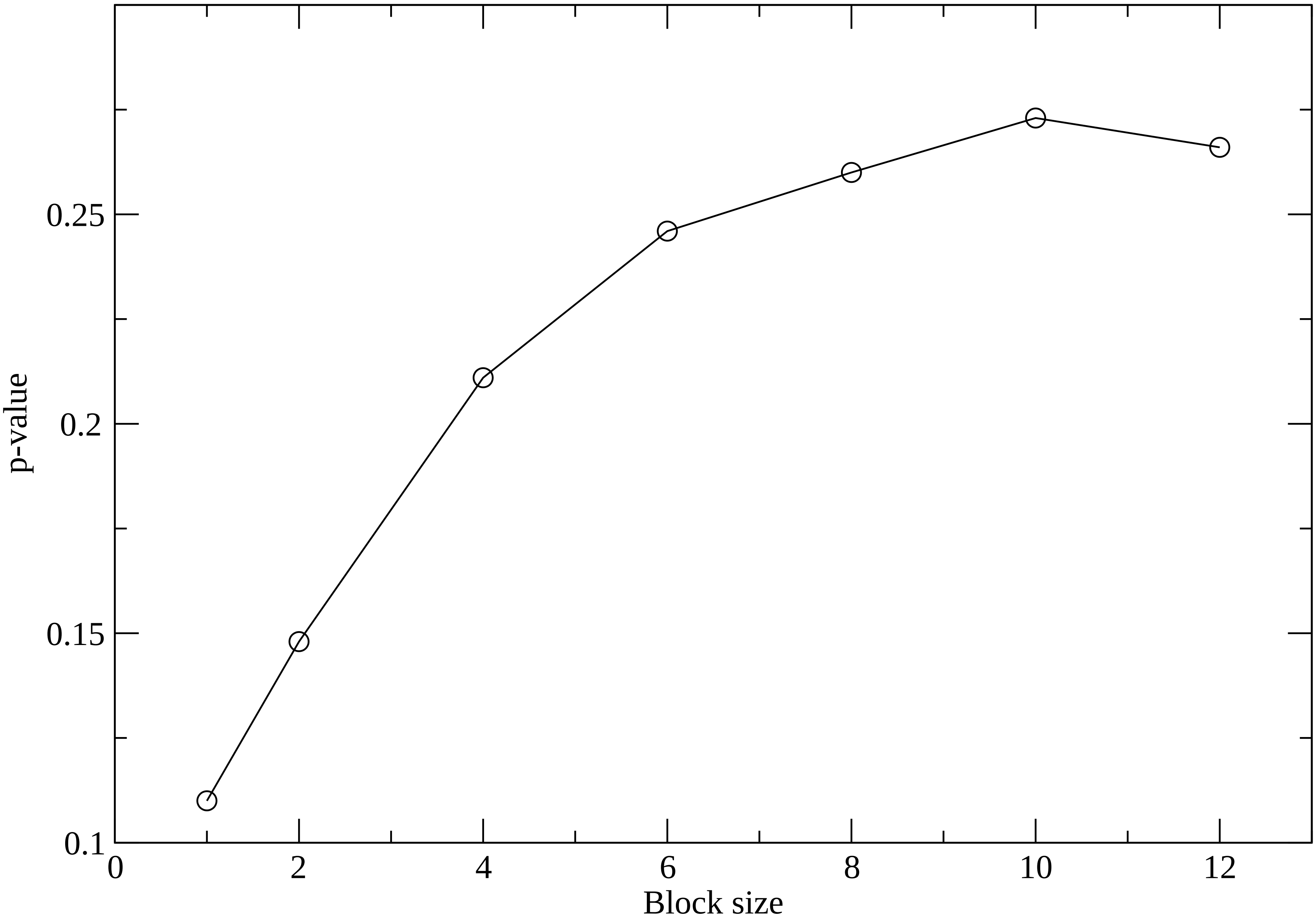


Stat error and bias fall as $n, B \to \infty \quad (B \ll n)$



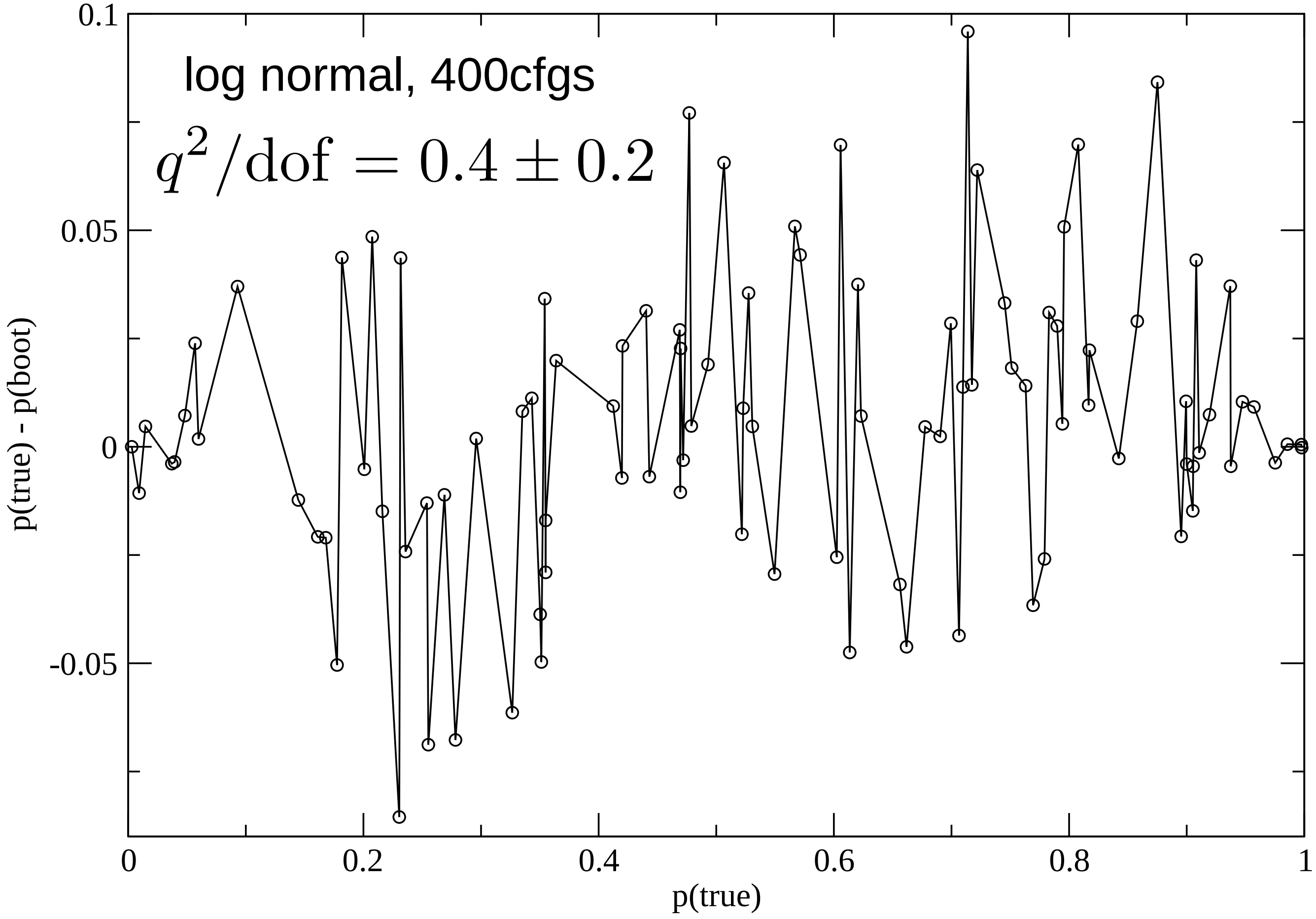


I=0 ππ fit bootstrap p-value



Incidentally....

- Conventional wisdom is that one cannot obtain the goodness-of-fit for uncorrelated fits. Space-age man can!



Conclusions

Conclusions

- Publication delayed by desire to account for autocorrelations and obtain reliable goodness-of-fit metrics for fits.
- Binning causes uncontrolled error growth due to loss of resolution of covariance matrix.
- Solve by performing block jackknife and computing covariance matrix from unbinned data.
- Even most advanced of old-fashioned approaches to computing goodness-of-fit fail to account for effects of autocorrelations or non-normality.
- Use non-overlapping block bootstrap to directly predict the distribution of q^2 from which a p-value can be obtained without any assumptions.
- Expect no further hurdles to completion of project and we aim to publish within the next few months.

Thank you!