methods for lattice QCD calculations of hadronic observables using stochastic locality

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in collaboration with
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based on
Exploiting stochastic locality in lattice QCD: hadronic observables and their uncertainties
arXiv:2307.15674

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motivations

stochastic locality in QCD: [Lüscher Lattice 2017]
fields in space-time regions that are far apart fluctuate largely independently

interest in generating large volume lattices

- more computational resources available • advances in communication-avoiding algorithms [plenary by Boyle]
- strong physics motivations to simulate larger volumes,
  e.g. reconstructing spectral functions from $\lim_{\sigma\to 0}\lim_{V\to\infty}\rho_{\sigma,V}$
- the master-field approach is also solution of the topological charge freezing problem,
  frozen topology bias: $O(1/V)$ $\ll$ statistical uncertainty: $O(1/\sqrt{V})$

⇒ e.g. master-field with • 192^4 lattice points • up to ≈ 18 fm length • $m_\pi L = 25$ [Fritzsch Lattice 2022]

in Bruno, MC, *et al.* arXiv:2307.15674 we investigate methods to exploit stochastic locality in lattice QCD calculations of (hadronic) observables:
in this talk, independent statistics from space-time decorrelation can be used to improve error estimates

notation

with one single gauge-field configuration with T and $L \gg 1/m_\pi$ [Lüscher Lattice 2017, Francis, Fritzsch, Lüscher, Rago 2020]

given a local observable $\mathcal{O}_\alpha(x)$, the best estimator for the true expectaion value $\langle \mathcal{O}_\alpha \rangle$

$$\langle\langle \mathcal{O}_\alpha \rangle\rangle = \frac{1}{N} \sum_x \mathcal{O}_\alpha(x)$$

is given by the translation average over a set of points $x \in \Lambda$, where $N = |\Lambda|$ is the number of sample points

the (co)variance of the estimator $\langle\langle \mathcal{O}_\alpha \rangle\rangle$ is [Lüscher Lattice 2017]

$$\Big\langle [\langle\langle \mathcal{O}_\alpha \rangle\rangle - \langle \mathcal{O}_\alpha \rangle][\langle\langle \mathcal{O}_\beta \rangle\rangle - \langle \mathcal{O}_\beta \rangle] \Big\rangle = \frac{1}{N^2} \sum_{x,y} \Gamma_{\alpha\beta}(x-y) = \frac{1}{N} \sum_y \Gamma_{\alpha\beta}(y)$$

where the correlation function Γ and its sum over y are

$$\Gamma_{\alpha\beta}(y) = \Big\langle [\mathcal{O}_\alpha(y) - \langle \mathcal{O}_\alpha \rangle][\mathcal{O}_\beta(0) - \langle \mathcal{O}_\beta \rangle] \Big\rangle, \qquad C_{\alpha\beta} = \sum_y \Gamma_{\alpha\beta}(y)$$

how to estimate $\Gamma_{\alpha\beta}$ from one single gauge-field configuration?

autocorrelation — Wolff's Γ method

in a traditional computation with (replicas of) a Monte Carlo chain, for a primary observable $\mathcal{O}_\alpha$ [Wolff 2003]

$$\Gamma_{\alpha\beta}(i-j) = \left\langle [\mathcal{O}^i_\alpha - \langle\mathcal{O}_\alpha\rangle][\,\mathcal{O}^j_\beta - \left\langle\mathcal{O}_\beta\right\rangle] \right\rangle$$

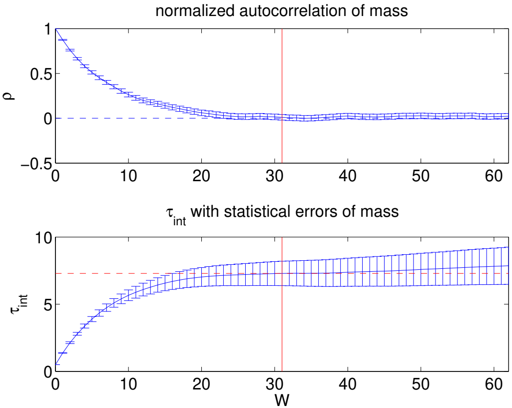
- define an integrated autocorrelation time τ_α

$$\tau_\alpha = \frac{1}{2\Gamma_{\alpha\alpha}(0)} \sum_{i=-\infty}^{+\infty} \Gamma_{\alpha\alpha}(i), \quad \mathrm{var}(\mathcal{O}_\alpha) = \frac{2\tau_\alpha}{N}\Gamma_{\alpha\alpha}(0)$$

- $\Gamma_{\alpha\alpha}(0)$ is the "naive" variance of $\mathcal{O}_\alpha$
- in practice, extract from $i = 1, \ldots, N$ configurations

$$\bar{\Gamma}_{\alpha\beta}(t) = \frac{1}{N-t} \sum_{i=1}^{N-t} [\mathcal{O}^i_\alpha - \bar{\mathcal{O}}_\alpha][\mathcal{O}^{i+t}_\beta - \bar{\mathcal{O}}_\beta]$$

- $\sum \bar{\Gamma}(t)$ truncation ⇒ systematic error
- the statistical error of the error is given by Madras-Sokal formula [Madras, Sokal 1988]



⇒ automatic windowing procedure to balance statistical and systematic uncertainties

Γ method for space-time correlations

straightforward generalization

$$\Gamma_{\alpha\beta}(y) = \left\langle [\mathcal{O}_\alpha(y) - \langle \mathcal{O}_\alpha \rangle][\mathcal{O}_\beta(0) - \langle \mathcal{O}_\beta \rangle] \right\rangle \sim \exp\{-m|y|\}$$

is expected to fall off exponentially with the distance $|y|$ and a mass m

- $\langle \mathcal{O}_\alpha \rangle \neq 0 \Rightarrow$ typically $m = 2m_\pi$ (the energy of the 0^{++} state)

in practice, we replace $\langle \mathcal{O}_\alpha \rangle \to \langle\!\langle \mathcal{O}_\alpha \rangle\!\rangle$

$$\left\langle\!\!\left\langle \Gamma_{\alpha\beta}(y) \right\rangle\!\!\right\rangle = \frac{1}{N} \sum_x \delta\mathcal{O}_\alpha(x+y)\delta\mathcal{O}_\beta(x), \qquad \delta\mathcal{O}_\alpha(x) = \mathcal{O}_\alpha(x) - \langle\!\langle \mathcal{O}_\alpha \rangle\!\rangle$$

- a biased estimator: $\left\langle \left\langle\!\!\left\langle \Gamma_{\alpha\beta}(y) \right\rangle\!\!\right\rangle \right\rangle - \Gamma_{\alpha\beta}(y) = -C_{\alpha\beta}/N$

and truncate the sum at a finite summation radius R

$$\left\langle\!\!\left\langle C_{\alpha\beta}(R) \right\rangle\!\!\right\rangle = \sum_{|y|<R} \left\langle\!\!\left\langle \Gamma_{\alpha\beta}(y) \right\rangle\!\!\right\rangle$$

such that

$$\left\langle \left\langle\!\!\left\langle C_{\alpha\beta}(R) \right\rangle\!\!\right\rangle \right\rangle = C_{\alpha\beta}\left[1 + O\left(\mathrm{e}^{-mR}\right) + O(1/N)\right]$$

a higher-dimensional generalization

Λ can be any D-dimensional subspace of space-time, e.g.

$$\Lambda_T = \{x_0 \mid x_0 \in [0, T-a]\}$$
$$\Lambda_{TL} = \{(x_0, x_1) \mid x_0 \in [0, T-a], x_1 \in [0, L-a]\}$$
$$\Lambda_{L^3} = \{\vec{x} \mid x_1, x_2, x_3 \in [0, L-a]\}$$

or even an irregular subset of randomly sampled points

with more than one configuration
e.g. in the case of traditional ensembles of gauge field configurations U_i, $i = \{1, \ldots, N_{MC}\}$

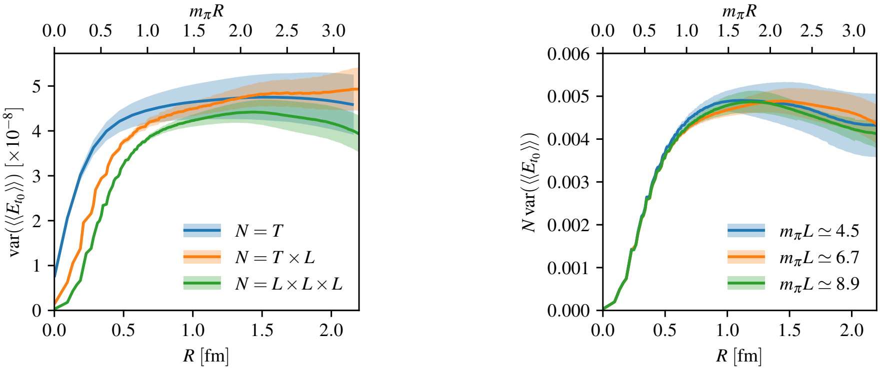
$$\left\langle\!\left\langle \Gamma^i_{\alpha\beta}(y) \right\rangle\!\right\rangle = \frac{1}{N} \sum_x \delta\mathcal{O}_\alpha(x+y)\delta\mathcal{O}_\beta(x), \qquad \delta\mathcal{O}^i_\alpha(x) = \mathcal{O}_\alpha(x) - \left\langle\!\left\langle \bar{O}_\alpha \right\rangle\!\right\rangle$$

correlations also in MC time ⇒ "five-dimensional" gamma method

- improve the error estimate if not enough configurations are available
- first explorations along these lines Blum *et al.* (RBC/UKQCD) 2023

numerical tests — energy density

of the gauge action with gradient flow at flow-time $t \approx t_0 = (t \mid t^2 E_t = 0.3)$ [Lüscher 2010]



the variance of $\langle\langle E_{t_0}\rangle\rangle$ plateaus for $R \gtrsim 1.0$ fm

left with different sets of $\Lambda \Rightarrow$ compatible plateau values, different approach

right and scaling the volume, $L/a \in \{32, 48, 64\} \Rightarrow m_\pi L \in \{4.5, 6.7, 8.9\}$
$\Rightarrow$ perfect scaling of the variance with $N \propto L^3$

the error of the error

extending Madras–Sokal formula derived in Wolff 2003, see also Madras, Sokal 1988

$$\mathrm{var}\big(\langle\!\langle C_{\alpha\beta}(R)\rangle\!\rangle\big) \approx \frac{N(R)}{N}\Big[C_{\alpha\alpha}C_{\beta\beta} + C_{\alpha\beta}^2\Big]$$

where $N(R)$ is the number of points $|y| < R$, $\approx \pi^{D/2}(R/b)^D/\Gamma(D/2+1)$

- grows with R
- has to be balanced with the systematic bias

$$\Big\langle \langle\!\langle C_{\alpha\beta}(R)\rangle\!\rangle \Big\rangle = C_{\alpha\beta}\Big[1 + O\big(\mathrm{e}^{-mR}\big) + O(1/N)\Big]$$

as in the Γ method case, we can define an integrated autocorrelation volume

$$\tau_\alpha = \frac{C_{\alpha\alpha}}{\Gamma_{\alpha\alpha}(0)} \qquad \Rightarrow \qquad \mathrm{var}(\langle\!\langle O_\alpha\rangle\!\rangle) = \tau_\alpha \Gamma_{\alpha\alpha}(0)/N$$

- dimension D dependent definition!
- estimator as a function of R

$$\tau_\alpha(R) = \frac{1}{\Gamma_{\alpha\alpha}(0)}\langle\!\langle C_{\alpha\beta}(R)\rangle\!\rangle = \frac{1}{\Gamma_{\alpha\alpha}(0)}\sum_{|y|<R}\langle\!\langle \Gamma_{\alpha\alpha}(y)\rangle\!\rangle$$

hadronic observables

the mesonic two-point function projected to zero momentum, $\Gamma, \Gamma' \in \{\gamma_5, \gamma_\mu, \gamma_5\gamma_\mu, \dots\}$

$$\tilde{C}(x_0 - y_0, \vec{x}) = -a^3 \sum_{\vec{y}} \mathrm{Re}\,\mathrm{Tr}\big[\Gamma D^{-1}(y,x)\Gamma' D^{-1}(x,y)\big]$$

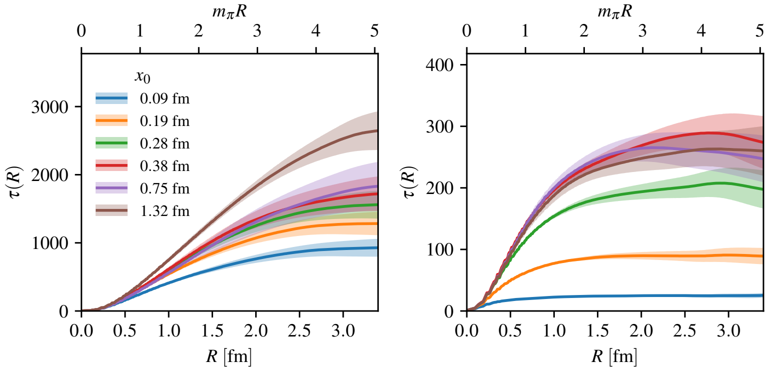
estimated using random $3d$-volume source $\Rightarrow \vec{x} \in \Lambda_{L^3}$
has an error given by

$$\Big\langle \big[\langle\!\langle \tilde{C}(t) \rangle\!\rangle - \langle \tilde{C}(t) \rangle\big]^2(R) \Big\rangle = \frac{1}{L^3}\Bigg[\sum_{|y|\leq R} \langle\!\langle \tilde{C}(t;\vec{x})\tilde{C}(t;0) \rangle\!\rangle_c + O\big(\mathrm{e}^{-mR}\big) + O\big(L^{-3}\big)\Bigg]$$

where each source-sink separation t defines a different observable

scaling with source-sink separation

left: pseudoscalar $\tilde{C}_{PP}$, right: vector $\tilde{C}_{VV}$, each source-sink separation defines a different observable

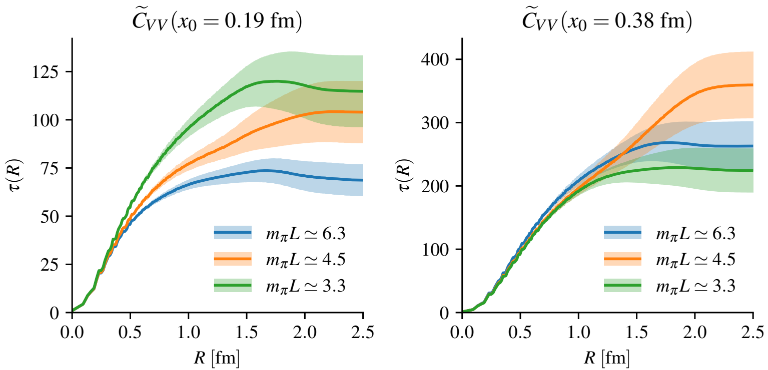


important: saturation is a function of the statistical precision!

- at large source-sink separations, the noise hides space-time correlations
- just as in the case of autocorrelations in Monte Carlo time

scaling with pion mass

as a function of $m_\pi \in \{215, 293, 410\}$MeV with $L = 32a$, for $\tau(R)$ of the vector correlator $\tilde{C}_{VV}$



left: at very short distance $x_0 \approx 0.19$ fm: lighter pions $\Rightarrow$ larger $\tau(R)$, plateau at larger R

right: at $x_0 \approx 0.38$ fm or larger: noisier data $\Rightarrow$ $\tau(R)$ approchaes are comparable

extrapolation to large volumes

our investigation on moderately-large volumes up to 96×64^3 / $m_\pi L \approx 8.9$
$\Rightarrow$ fit of the variance of the pion correlator at source-sink separation $x_0 = 4a$
$\Rightarrow$ estimate the error of the same observable on a different volume
e.g. we project a $0.5\,\%$ error on the pseudoscalar correlator from a single configuration with $T = L = 192a$

preliminary exploration: numerical tests a single 192^4 / $m_\pi L \approx 25$ master-field configuration [Fritzsch Lattice 2022]
(same lattice spacing $a \approx 0.095$ fm but slightly different $m_\pi \approx 270$ MeV!)
stochastic $3d$-volume sources at two source times: $x_0 = 0$ and $96a$

$$\tilde{C}_{PP}(x_0 = 4a) = 0.061\,01(23) \quad \text{and} \quad am_\pi = 0.126\,32(27)$$

a $0.38\,\%$ and $0.22\,\%$ error respectively, obtained using `pyobs`

conclusions

- very general method, Wolff's Γ method is the $1d$ version of this
- already used in recent studies to improve error estimates with few configurations [Blum *et al.* (RBC/UKQCD) 2023]
- large-separation correlators have a larger footprint in space
  ⇒ estimation of the integrated correlation volume depends on the statistics
- the whole procedure can be automated, see e.g. M. Bruno's `pyobs` Python package
  https://mbruno46.github.io/pyobs/
- results for $\Gamma_{\alpha\beta}$ on a intermediate-volume lattices
  ⇒ can inform (at fixed lattice spacing) and help plan large-volume / master-field simulation

details in the recent paper: Bruno, MC, *et al.* arXiv:2307.15674

position-space correlators

- studied on the same intermediate volumes [MC *et al.* Lattice 2021; Bruno, MC, *et al.* arXiv:2307.15674]
- and preliminary results on 96^4, 192^4 master fields [MC *et al.* Lattice 2022]
- using blocking; or Γ method with a sufficiently high density of points

long-T approach as a solution of topological charge freezing [Francis *et al.* Lattice 2022; Bruno, MC, *et al.* arXiv:2307.15674] thanks

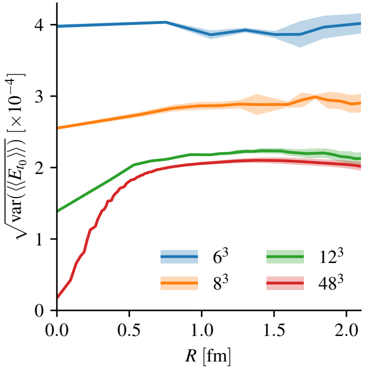
for your attention!

questions?

backup slides

saturation of the error

scaling the density of the points on which the observable E_{t_0} is computed



- red line at 48^3 is each point on the time slice, i.e. Λ_{L^3}
- green, orange, blue: artificial subsampling
- the error increases for a very sparse grid
- the error saturates as a the grid get denser:
  orange: $N = 12^3$ point samples on a grid with spacing $4a$
  $\Rightarrow$ same error as the whole time slice (red)

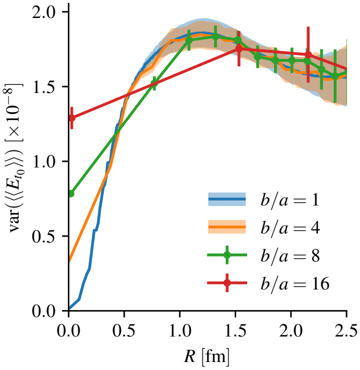
$\Rightarrow$ possible strategy for hadronic observables:
evaluate (a) stochastic volume sources vs. (b) a (more or less dense) grid of source points

- source points can also be randomly distributed

blocking

of the observable $\mathcal{O}_\alpha$ over small blocks of size b^4

$$\mathcal{O}_{B\alpha}(u) = \frac{N_B}{N} \sum_{x \in \text{block}} \mathcal{O}_\alpha(x)$$



- this can significantly reduce the cpu and memory footprint of the Γ method, in case of very large volumens
  e.g. 192^4 lattice points $\Rightarrow$ 48^4 blocks of length $4a$
- moderate blocking does not compromise the error of the error
- the scaling of $\Gamma_{\alpha\beta}$ is non-trivial, $\mathrm{var}(\mathcal{O}_\alpha) = \tau_\alpha \Gamma_{\alpha\alpha}/N$
  $\Rightarrow$ $\tau_\alpha(R)$ depends on the blocking
  possible solution: define τ_α with the non-blocked $\Gamma_{\alpha\alpha}(0)$

truncated $3d$ sums

$$\tilde{C}^{\text{cut}}(t, r_{\text{max}}) = \int \mathrm{d}^3\vec{x}\,\theta(r_{\text{max}} - |\vec{x}|)C(\vec{x}, t)$$

- explored in e.g. Liu, Liang, Yang 2018
- larger t require larger r_{max} to reach the same $\tilde{C}^{\text{cut}}/\tilde{C}$
- the pion correlator (top) is especially slow, does not saturate!
- the nucleon one (bottom) saturates at $r_{\text{max}} \approx 20a$, but also the error saturates

$\Rightarrow$ no statistical benefit