Topology and critical slowing down

Gergely Markó*

* University of Bielefeld, Department of Theoretical Physics

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- Importance sampling, Markov chains
- Autocorrelation
- Critical slowing down
- Topological charge

Importance sampling

- We want to calculate expectation values of random variables $\mathcal{O}(s)$ using a probability distribution $P(s)$ over a set of states $s \in E$.

$$\langle \mathcal{O} \rangle = \sum_{s \in E} \mathcal{O}(s) P(s) \, .$$

- Generating states with equal probability and then summing $\mathcal{O}(s)P(s)$ is the naive Monte Carlo integration, however very ineffective.

- Instead importance sampling: sample E, n-times according to $P(s)$: $\{s_1, s_2, ..., s_n\}$ is a representative ensamble.

- Then the expectation value is approximated by the sample average:

$$\langle \mathcal{O} \rangle = \frac{1}{n} \sum_{i=1}^{n} \mathcal{O}(s_i) + O\left(n^{-\frac{1}{2}}\right) \, .$$

Markov chains

- In our case $P(s) \sim \exp(-S_E[\Phi])$, we cannot draw our states (configurations) directly with this distribution.

- We can construct some stochastic method M which generates one state from an other with probability $M(s \to s')$.

- If M is such that

  1. $M(s \to s') \geq 0$ for all s, s' and $\sum_{s'} M(s \to s') = 1$ for all s, (M is a probability distribution wrt s')
  2. $\sum_s P(s) M(s \to s') = P(s')$ for all s', (preserves the wanted probability distribution)
  3. $M(s \to s) > 0$ for all s, (aperiodic)
  4. if E_1 is a non-empty proper subset of E there exists $s \in E_1$ and $s' \notin E_1$ such that $M(s \to s') > 0$. (ergodic)

  then M produces a Markov chain and generates a representative ensamble by acting multiple times on a starting state.

Markov chains

1. One can show that in the space of real valued functions over the set of states E, defining a suitable norm any $f(s)$ is such that

$$||\sum_s M(s \to s')f(s)|| \leq ||f(s)|| \,.$$

2. It can also be proved that if $\sum_s M(s \to s')f(s) = f(s')$ then $f(s) = cP(s)$, where c is a constant.

3. A further important property is that for functions $\sum_s f(s) = 0$ the inequality is stronger $||\sum_s M(s \to s')f(s)|| < ||f(s)||$.

These properties lead to both termalization and that expectation values can indeed be approximated the way we imagine.

Adding detailed balance

- A further property, which is not necessary but desirable, is detailed balance:

$$P(s)M(s \to s') = P(s')M(s' \to s)\,.$$

- We can define a symmetrized method T:

$$T(s, s') = [P(s')]^{-\frac{1}{2}} M(s \to s')[P(s)]^{\frac{1}{2}}$$

  which inherits all the properties of M.

- Since T is symmetric it's eigenvalues are real and can be ordered such that $\lambda_0 \geq \lambda_1 \geq \lambda_2 ...$

- Using the general statements about M one can show that $\lambda_0 = 1 > \lambda_n$ (for $n > 0$) and the corresponding eigenfunction is $\sqrt{P(s)}$.

Autocorrelation

- States generated from some starting state s_1 by the repeated application of M will not be statistically independent.

- We define the autocorrelation function of some observable $\mathcal{O}$ in a Markov chain by

$$\Gamma(t) = \lim_{k\to\infty} \frac{1}{k} \sum_{i=1}^{k} \mathcal{O}(s_i)\mathcal{O}(s_{i+t}) - \langle \mathcal{O} \rangle^2 .$$

- A better definition would be to imagine many Markov chains with the same starting point and take the average of

$$\mathcal{O}(s_k)\mathcal{O}(s_{k+t}) - \langle \mathcal{O} \rangle^2$$

  at some k large enough that the result does not depend on it. However, they coincide for large enough k and both can be shown to fall off exponentially with t over some time scale τ, the autocorrelation time.

Integrated autocorrelation time

- Using the same idea of many parallel chains, the variance of the sample mean ($\bar{\mathcal{O}} =$ average of $\mathcal{O}$ over one chain) can be shown to be

$$\mathrm{var}^2_{\bar{\mathcal{O}}} = \Gamma(0)\frac{2\tau_{\mathcal{O}}}{n} + O(n^{-2})\,,$$

  where n is the length of the chain and

$$\tau_{\mathcal{O}} = \frac{1}{2} + \sum_{t=0}^{\infty} \frac{\Gamma(t)}{\Gamma(0)}$$

  is the integrated autocorrelation time.

- This can also be approximated using a long enough chain, similarly to $\Gamma(t)$ itself.

- More importantly it show that the non-independence of the states causes an extra uncertainty in the determination of expectation values.

Critical slowing down

- The lattice continuum limit, $a \to 0$ is a second order phase transition.
- All physical scales in lattice units go to zero, therefore the lattice correlation length, ξ, diverges.
- Dynamical critical exponent: $\tau \sim \xi^z$. This universal scaling is something well known in non-equilibrium phase transitions.
- Extra problems arise because the physical volume becomes infinitly large in lattice units.
- Local updates become slow because they do not effect large enough parts of configurations.
- Global updates in principle can solve some of the problems (e.g. cluster algorithms or overrelaxation in spin models).

Critical slowing down

- The autocorrelation is defined for every observable.
- Not all observables are sensitive to critical slowing down.
- In the language of the eigenvalues of M: if

$$\lambda_1 \lessapprox 1$$

  then it is called a slow mode. If an observables couples strongly to the slow mode, its autocorrelation will be large.

- Global observables are particularly sensitive due to the updating problems.

Topological charge

- One example of a problematic global observable is the QCD topological charge

$$Q = \frac{1}{32\pi^2} \int d^4x \epsilon_{\mu\nu\rho\sigma} \mathrm{Tr}[F_{\mu\nu}(x) F_{\rho\sigma}(x)] \,.$$

- The value of Q is an integer, which is related to the number of zero modes of the Dirac operator through the Atiyah-Singer index theorem.

$$Q = n_+ - n_- \,,$$

  where $n_\pm$ is the number of zero modes with positive or negative chirality respectively.

- The topological charge is also a total derivative, hence adding θQ to the Lagrangian does not change the theory classically. The quantum theory is changed however, therefore the θ dependence of the free energy is a relevant question.

- Instead of the total θ dependence usually the susceptibility, χ, and higher moments are measured at $\theta = 0$.

Topological charge

- On the lattice the Atiyah-Singer theorem is no longer true.

- This leads to either a bosonic or fermionic definition of the topological charge.

  1. Volume sum of $\frac{1}{32\pi^2}\epsilon_{\mu\nu\rho\sigma}\mathrm{Tr}[F_{\mu\nu}(x)F_{\rho\sigma}(x)]$,
  2. Counting zero modes of the Dirac operator. Strictly speaking this can only be done using overlap fermions, but approximate definitions can be given for other formulations.

- Apart from the observable itself, the main challenge for lattic simulations is the fact that in the continuum, Q introduces homotopy classes in the configuration space, which are not continously connected.

- Lattice simulations use more or less continous paths in the configuration space. Luckily homotopy classes are broken on the lattice, but close to the continuum limit they are almost restored.

- Getting stuck in a homotopy class is called the topological freezing.

- All this leads to the $\tau \sim a^{-z}$ behaviour, the critical slowing down.

Topological charge

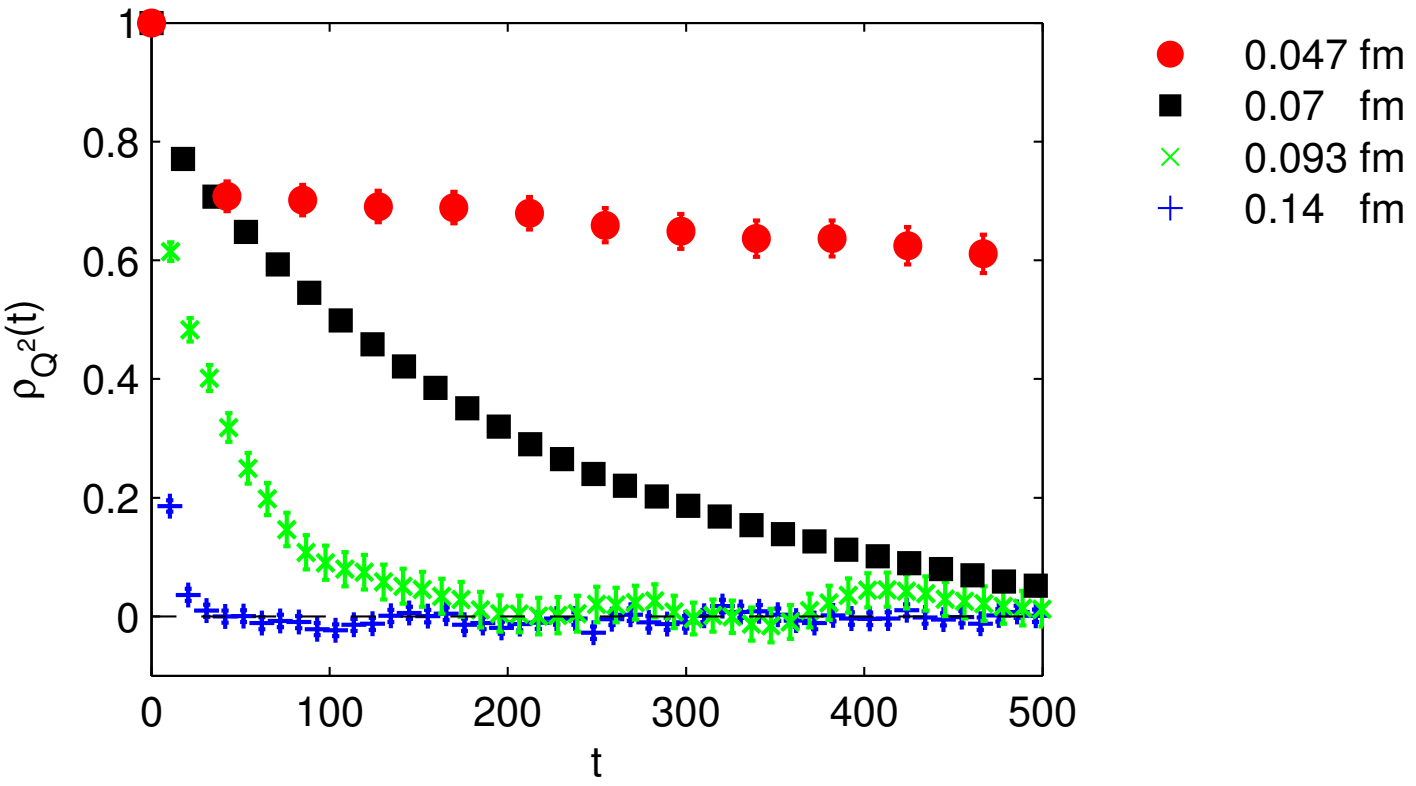

Figure 2: Normalized auto-correlation function of Q_1^2 at various lattice spacings. The Monte Carlo time is given in molecular dynamics units multiplied by R.

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Topological charge

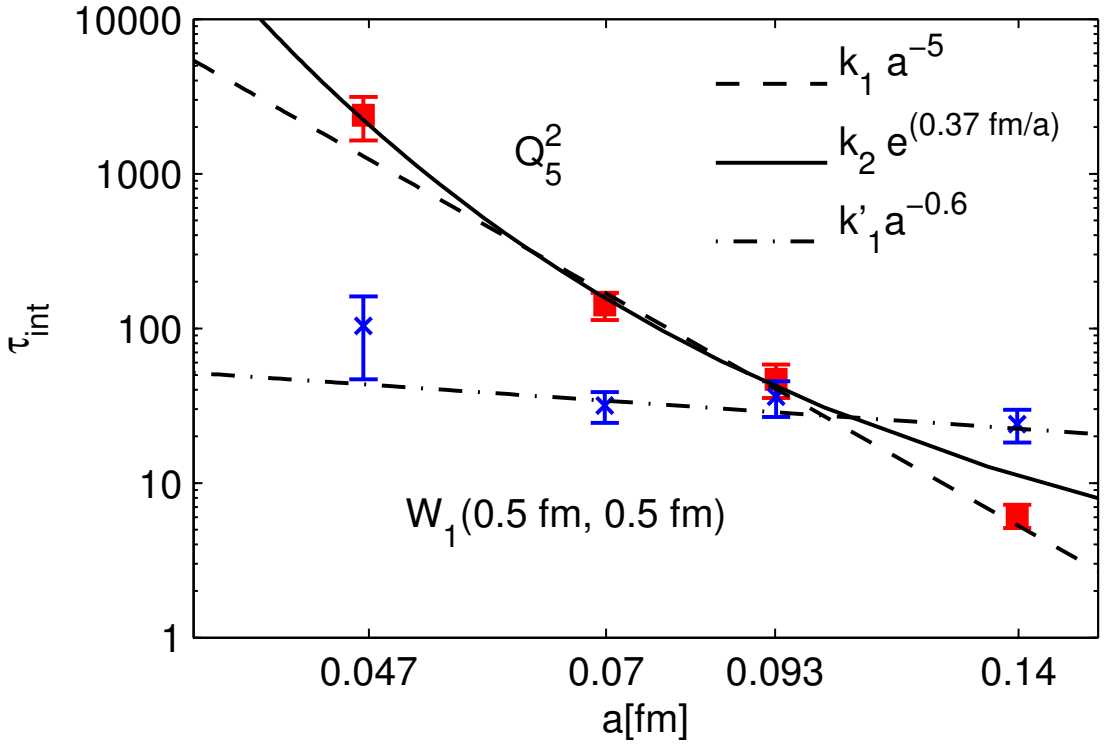

Figure 4: Auto-correlation time of Q_5^2 and the (0.5 fm) $\times$ (0.5 fm) square Wilson loop as a function of the lattice spacing using the DD-HMC algorithm. For Q_5^2 the two curves are fits through the last three points of the two ansätze of Eq. (4.1). For the Wilson loop only the fit to the power law has been performed, through all points.

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