Avoiding the sign-problem in lattice QCD

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Overview

- A method to avoid the sign-problem for physical one-dimensional systems was proposed.
- Avoiding the sign-problem with symmetric quadrature rules for one-dimensional integrals
- Reducing high-dimensional integrals to nested one-dimensional integrals
- Physical high-dimensional systems are still challenging

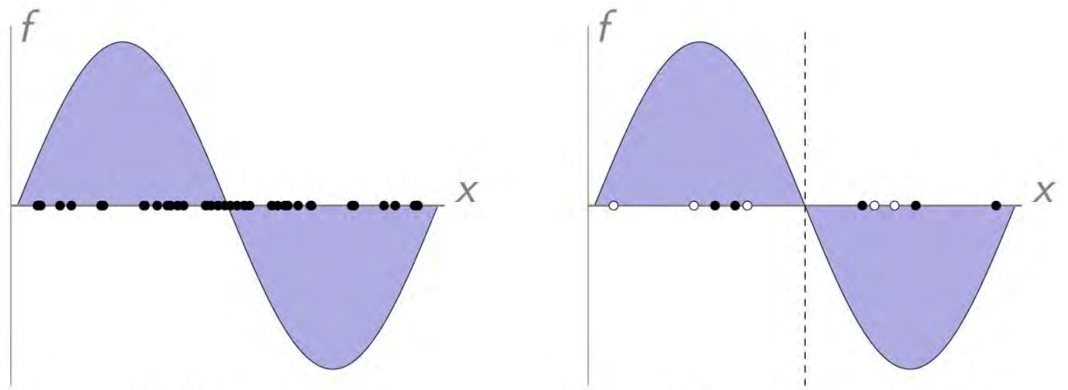
The sign-problem

- Computing high-dimensional integrals such as in lattice QCD
  → Markov Chain Monte Carlo (MCMC) methods are efficient in general

$$A = \frac{\int O[P]B[P]\,\mathrm{d}P}{\int B[P]\,\mathrm{d}P}$$

- Integral functions are sometimes oscillatory (e.g. finite density QCD)
  → non-perfect cancellation of positive and negative parts
  → **large quadrature errors in MCMC methods**
  → the sign problem

- Using some symmetry of the system



(a) MC sampling points (b) Symmetric sampling points

Symmetric quadrature rules

- A one-dimensional integration over the Haar measure of G

$$I(f) = \int_G f(U)\,\mathrm{d}U \qquad G \in \{\mathscr{U}(1), \mathscr{U}(2), \mathscr{U}(3), \mathscr{S}\mathscr{U}(2), \mathscr{S}\mathscr{U}(3)\}$$

- Rewriting the integral into an integral over spheres

$$\mathscr{S}\mathscr{U}(N) \simeq S^3 \times S^5 \times \ldots \times S^{2N-1}$$
$$\mathscr{U}(N) \simeq S^1 \times S^3 \times \ldots \times S^{2N-1}$$

$\Rightarrow$

$$\int_G \mathrm{d}U\, f(U) = \int_{S^{2N-1}} \left(\int_{S^{2N-3}} \left(\cdots \int_{S^{n+2}} \left(\int_{S^n} f\left(\Phi(\boldsymbol{x}_{S^{2N-1}}, \boldsymbol{x}_{S^{2N-3}}, \ldots, \boldsymbol{x}_{S^{n+2}}, \boldsymbol{x}_{S^n})\right) \mathrm{d}\boldsymbol{x}_{S^n} \right) \mathrm{d}\boldsymbol{x}_{S^{n+2}} \cdots \right) \mathrm{d}\boldsymbol{x}_{S^{2N-3}} \right) \mathrm{d}\boldsymbol{x}_{S^{2N-1}}$$

- Introducing quadrature rules with symmetric sampling points on spheres

$$Q_{S^k}(g) = \sum_{\gamma=1}^{N_{\mathrm{sym}}} w_\gamma\, g(\boldsymbol{t}_\gamma)$$

Symmetric quadrature rules (examples)

- For $\mathscr{SU}(2)$

$$\Phi_{\mathscr{SU}(2)} : S^3 \to \mathscr{SU}(2),$$
$$x \mapsto \begin{pmatrix} x_1 + ix_2 & -(x_3 + ix_4)^* \\ x_3 + ix_4 & (x_1 + ix_2)^* \end{pmatrix}$$

- For $\mathscr{SU}(3)$

$$\Phi_{\mathscr{SU}(3)} : S_1^5 \times S^3 \to \mathscr{SU}(3),$$
$$(x, y) \mapsto A(\Psi^{-1}(x)) \cdot B(y)$$

$$\Psi : [0, 2\pi)^3 \times [0, \frac{\pi}{2}) \to S^5,$$
$$(\alpha_1, \alpha_2, \alpha_3, \phi_1, \phi_2) \mapsto \begin{pmatrix} \cos\alpha_1 \sin\phi_1 \\ \sin\alpha_1 \sin\phi_1 \\ \sin\alpha_2 \cos\phi_2 \sin\phi_2 \\ \cos\alpha_2 \cos\phi_2 \sin\phi_2 \\ \sin\alpha_3 \cos\phi_1 \cos\phi_2 \\ \cos\alpha_3 \cos\phi_1 \cos\phi_2 \end{pmatrix}$$

$$A(\Psi^{-1}(x)) = \begin{pmatrix} e^{i\alpha_1}\cos\phi_1 & 0 & e^{i\alpha_1}\sin\phi_1 \\ -e^{i\alpha_2}\sin\phi_1\sin\phi_2 & e^{-i(\alpha_1+\alpha_3)}\cos\phi_2 & e^{i\alpha_2}\cos\phi_1\sin\phi_2 \\ -e^{i\alpha_3}\sin\phi_1\cos\phi_2 & -e^{-i(\alpha_1+\alpha_2)}\sin\phi_2 & e^{i\alpha_3}\cos\phi_1\cos\phi_2 \end{pmatrix}$$

$$B(y) = \begin{pmatrix} x_1 + ix_2 & -(x_3 + ix_4)^* & 0 \\ x_3 + ix_4 & (x_1 + ix_2)^* & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Application to one-dimensional QCD

- Chiral condensate

$$\chi = \frac{\int_G \partial_m B[U]\, \mathrm{d}U}{\int_G B[U]\, \mathrm{d}U}$$

$$B[U] = \det\left(c_1(m) + c_2(d,\mu)U^\dagger + c_3(d,\mu)U\right)$$

$$c_1(m) = \prod_{j=1}^{d.} \tilde{m}_j, \qquad \tilde{m}_1 = m,$$

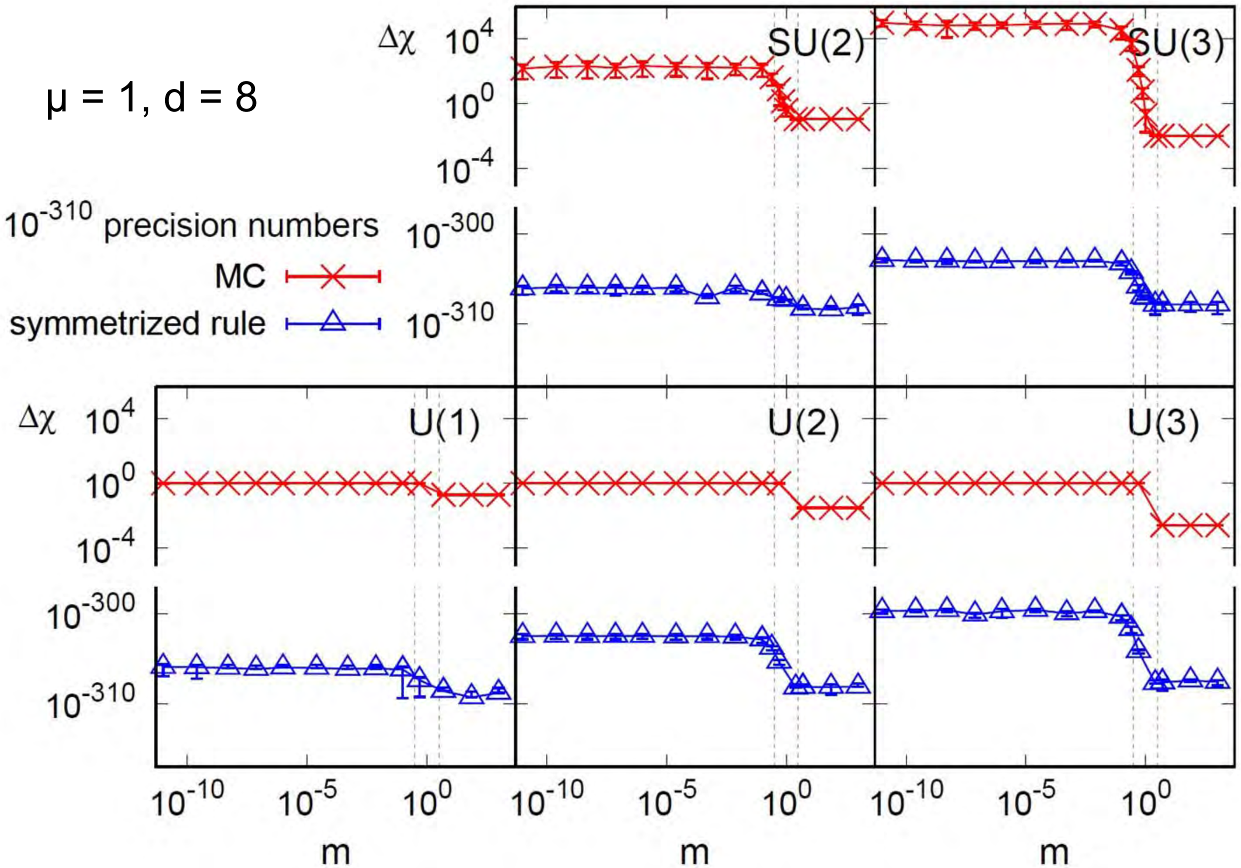
$$\tilde{m}_j = m + \frac{1}{4\tilde{m}_{j-1}} \quad \forall j \in \{2,3,\ldots,d-1\}$$

$$\tilde{m}_d = m + \frac{1}{4\tilde{m}_{d-1}} + \sum_{j=1}^{d-1} \frac{(-1)^{j+1} 2^{-2j}}{\tilde{m}_j \prod_{k=1}^{j-1} \tilde{m}_k^2},$$

$$c_2(d,\mu) = 2^{-d}\, \mathrm{e}^{-d\mu},$$

$$c_3(d,\mu) = (-1)^d 2^{-d}\, \mathrm{e}^{d\mu}.$$

Application to one-dimensional QCD (result)



$$\Delta\chi = \frac{|\chi_{\text{numerical}} - \chi_{\text{analytic}}|}{|\chi_{\text{analytic}}|}$$

$N \equiv N_{\text{sym}} = N_{\text{MC}} = 8$ for $\mathscr{SU}(2)$, $N = 96$ for $\mathscr{SU}(3)$, $N = 4$ for $\mathscr{U}(1)$, $N = 32$ for $\mathscr{U}(2)$ and $N = 384$ for $\mathscr{U}(3)$.

High-dimensional integrals to nested one-dimensional integrals

- A d-dimensional integral

$$I(f) = \int_{D^d} f[\varphi]\,\mathrm{d}\varphi \qquad \mathrm{d}\varphi = \prod_{i=1}^{d} \mathrm{d}\varphi_i \text{ and } D = [0, 2\pi)$$

- Using the structure of the integrand in one physical dimensional

$$f[\varphi] = \prod_{i=1}^{d} f_i(\varphi_{i+1}, \varphi_i)$$

$\varphi_{d+1} = \varphi_1$: Periodic boundary condition

Only next-neighbor coupling

⇨

$$I(f) = \int_D \cdots \int_D \prod_{i=1}^{d} f_i(\varphi_i, \varphi_{i+1})\,\mathrm{d}\varphi_d \cdots \mathrm{d}\varphi_1$$

$$= \underbrace{\int_D \Bigg(\cdots \underbrace{\Bigg(\int_D f_{d-2}(\varphi_{d-2}, \varphi_{d-1}) \cdot \underbrace{\Bigg(\int_D f_{d-1}(\varphi_{d-1}, \varphi_d) \cdot f_d(\varphi_d, \varphi_{d+1})\,\mathrm{d}\varphi_d \Bigg)}_{I_d} \mathrm{d}\varphi_{d-1} \Bigg)}_{I_{d-1}} \cdots \Bigg) \mathrm{d}\varphi_1}_{I_1}$$

High-dimensional integrals to nested one-dimensional integrals

- Quadrature rules

$$Q_d(\varphi_{d-1}, \varphi_{d+1}) = \sum_{\gamma=1}^{N_{\text{quad}}} w_\gamma \, f_{d-1}(\varphi_{d-1}, t_\gamma) \, f_d(t_\gamma, \varphi_{d+1})$$

$$Q_{d-1}(\varphi_{d-2}, \varphi_{d+1}) = \sum_{\gamma=1}^{N_{\text{quad}}} w_\gamma \, f_{d-2}(\varphi_{d-2}, t_\gamma) \, Q_d(t_\gamma, \varphi_{d+1})$$

$$\vdots$$

$$Q = Q_1 = \sum_{\gamma=1}^{N_{\text{quad}}} w_\gamma Q_2(t_\gamma, t_\gamma) = \text{tr}\left[\prod_{i=1}^{d} \left(M_i \cdot \text{diag}(w_1, \ldots, w_{N_{\text{quad}}})\right)\right] \qquad (M_i)_{\alpha\beta} = f_i(t_\alpha, t_\beta)$$

- Choosing an efficient quadrature rule

  → Gaussian-Legendre

$$\sigma \sim \mathcal{O}\left(\exp(-2N_{\text{quad}} \ln N_{\text{quad}}) \frac{1}{\sqrt{N_{\text{quad}}}}\right)$$

For MC, $\sigma \sim O(1/\sqrt{N_{\text{MC}}})$

Application to topological oscillator

- Topological charge susceptibility

$$\chi_{\text{top}} = \frac{\int O[\varphi] B[\varphi]\, \mathrm{d}\varphi}{\int B[\varphi]\, \mathrm{d}\varphi}$$

$$B[\varphi] = \exp\left(-c \sum_{i=1}^{d} (1 - \cos(\varphi_{i+1} - \varphi_i))\right)$$

φ : [0, 2π)

$$O[\varphi] = \frac{1}{T}\left(\frac{1}{2\pi} \sum_{i=1}^{d} (\varphi_{i+1} - \varphi_i) \mod 2\pi\right)^2$$

Application to topological oscillator (result)

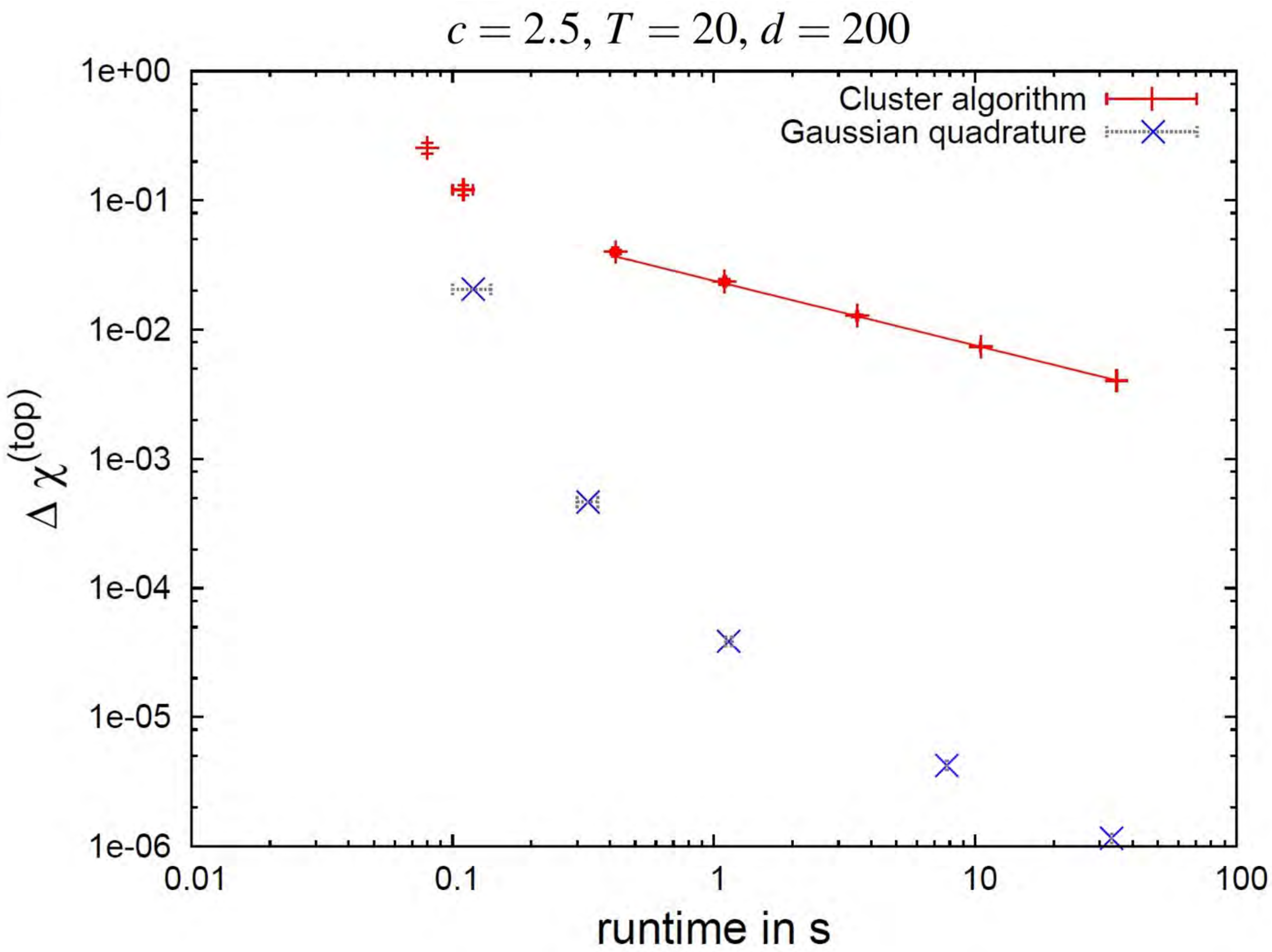
For the quadrature rule

$$\Delta\chi_{\text{top}}(N_{\text{quad}}) = |\chi_{\text{top}}(N_{\text{quad}}) - \chi_{\text{top}}(N^g_{\text{quad}})|$$

N^g_{quad} : Large number corresponding to the actual value of χ_{top}

For MC, Δχtop is usual standard error

$N_{MC} = 10^2 - 10^6$ for MC
$N_{quad} = 10 - 300$ with $N^g_{quad} = 400$



Application to topological oscillator with the sign-problem

$$B[U] = \exp\left(-c\sum_{i=1}^{d}\Re(1 - U_{i+1}U_i^*)\right)\cdot\prod_{j=1}^{d}U_j^{-\theta}$$

$$U_j = \mathrm{e}^{i\varphi_j} \in \mathscr{U}(1)$$

$$plaquette = \frac{\int O[U]B[U]\,\mathrm{d}U}{\int B[U]\,\mathrm{d}U}$$

$$O[U] = \frac{1}{d}\Re\left(\sum_{i=1}^{d}U_{i+1}U_i^*\right)$$

Θ = π