Reweighting trajectories from the complex Langevin method

Jacques Bloch, Johannes Meisinger, Sebastian Schmalzbauer

University of Regensburg

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Introduction

- QCD at $\mu \neq 0$: $\det(D) \in \mathbb{C} \to$ sign problem.
- Most solutions: computational cost grows $\propto \exp(V)$
  $\to$ restricted to $\mu/T < 1$.
- Possible alternative: complex Langevin method.
- Recent investigations in heavy-dense QCD (Sexty et al., 2013) and full QCD (Fodor et al., 2015): method breaks down in transition region.
- Problems confirmed for low-dimensional strong-coupling QCD (Bloch et al., 2015): method converges to wrong values for small masses.
- New idea: combine CL method and reweighting of complex trajectory
  $\to$ reweighted complex Langevin (RCL) method.
- Reach regions of parameter space that are not simulated correctly by the CL method.

Complex Langevin Method

- Assume partition function

$$Z = \int dx\, e^{-S(x)}$$

  with real degrees of freedom x and complex action $S(x)$.
- Langevin equation with complex action: real variables driven into complex plane. So, $x \to z = x + iy$ satisfying the CL equation

$$\dot{z}(t) = -\frac{\partial S}{\partial z} + \eta(t)$$

- Stochastic Euler discretization:

$$z(t+1) = z(t) + \epsilon K + \sqrt{\epsilon}\,\eta,$$

  with drift $K = -\partial S/\partial z$, step size ϵ and independent Gaussian noise η (chosen real for better convergence) with mean 0 and variance 2.

Validity of CL method

- Do CL equations give correct expectation values?
- If action S and observable $\mathcal{O}$ holomorphic in complexified variables (up to singularities):

Equivalence identity

$$\langle \mathcal{O} \rangle \equiv \frac{1}{Z} \int dx\, w(x) \mathcal{O}(x) = \int dx dy\, P(x+iy) \mathcal{O}(x+iy)$$

  - $w(x) \equiv e^{-S(x)}$ with complex action $S(x)$ in the real variables x,
  - $P(z)$ is real probability of complexified variables z along CL trajectories.
- Validity conditions:
  - $P(z)$ suppressed close to singularities of drift and observable;
  - Sufficiently rapid decay of $P(z)$ in the imaginary direction;
- CL validity conditions satisfied for some parameter values but not for others $\rightarrow$ in latter case the CL method will fail.
- For QCD this depends on μ, m, β and lattice size.

Reweighted complex Langevin (RCL)

Aim

Extend applicability of CL method to parameter regions for which validity conditions are not satisfied.

Principle

- Generate CL trajectory for parameter values where CL is correct
- Reweight this complex trajectory to compute observables for other parameter values where CL could be wrong.

Advantage

Reweighting from $\mu \neq 0$: auxiliary ensemble closer to target ensemble than in traditional reweighting.

Reweighting the CL trajectories

- Consider target ensemble with parameters $\xi = (\mu, m, \beta)$ and auxiliary ensemble with parameters $\xi_0 = (\mu_0, m_0, \beta_0)$
- Reweight from auxiliary ensemble with parameters ξ_0 to target ensemble with parameters ξ:

$$\langle \mathcal{O} \rangle_\xi = \frac{\int dx\, w(x;\xi)\mathcal{O}(x;\xi)}{\int dx\, w(x;\xi)} = \frac{\int dx\, w(x;\xi_0)\left[\frac{w(x;\xi)}{w(x;\xi_0)}\mathcal{O}(x;\xi)\right]}{\int dx\, w(x;\xi_0)\left[\frac{w(x;\xi)}{w(x;\xi_0)}\right]}$$

$$= \frac{\left\langle \frac{w(x;\xi)}{w(x;\xi_0)}\mathcal{O}(x;\xi)\right\rangle_{\xi_0}}{\left\langle \frac{w(x;\xi)}{w(x;\xi_0)}\right\rangle_{\xi_0}}$$

- $w(x;\xi_0)$ is complex → no importance sampling → use CL

Reweighting the CL trajectories

- If CL method is valid for parameters ξ_0, the CL equivalence says

$$\langle \mathcal{O} \rangle_{\xi_0} \equiv \frac{\int dx\, w(x;\xi_0)\mathcal{O}(x;\xi_0)}{\int dx\, w(x;\xi_0)} = \int dx dy\, P(z;\xi_0)\mathcal{O}(z;\xi_0)$$

  where:
  - $w(x,\xi_0) \equiv e^{-S(x;\xi_0)}$ with complex action $S(x;\xi_0)$ in the real variables x.
  - $P(z;\xi_0)$ is real probability of complexified variable z along CL trajectory.
- Apply the CL equivalence to both $\langle \cdots \rangle_{\xi_0}$ in reweighting formula:

RCL equation

$$\langle \mathcal{O} \rangle_{\xi} = \frac{\int dx dy\, P(z;\xi_0) \left[\frac{w(z;\xi)}{w(z;\xi_0)} \mathcal{O}(z;\xi) \right]}{\int dx dy\, P(z;\xi_0) \left[\frac{w(z;\xi)}{w(z;\xi_0)} \right]}$$

$\rightarrow \langle \mathcal{O} \rangle_{\xi}$ in target ensemble is ratio of expressions evaluated along CL trajectory in the auxiliary ensemble.

- Does this reweighting along the complex trajectory work correctly?

Features of RCL

- Both $w(z_j;\xi)$ and $w(z_j;\xi_0)$ are complex.
- RCL based on fact that the effective observables are correctly evaluated in auxiliary ensemble when using a valid CL trajectory.
- Application to finite discretized CL trajectory:

$$\langle \mathcal{O} \rangle_\xi \approx \frac{\frac{1}{N}\sum_{j=1}^{N} \frac{w(z_j;\xi)}{w(z_j;\xi_0)} \mathcal{O}(z_j;\xi)}{\frac{1}{N}\sum_{j=1}^{N} \frac{w(z_j;\xi)}{w(z_j;\xi_0)}}.$$

  where z_j are complex configurations of CL trajectory at ξ_0.
- Note: reweighting factor cancels observable singularities in target ensemble explicitly.

Applied to:

- Random matrix model for QCD (Osborn, 2004)
- QCD in 1+1 dimensions (Bloch et al., 2015)

QCD – partition function

- Partition function of lattice QCD:

$$Z = \left[\prod_{x=1}^{V} \prod_{\nu=0}^{d-1} \int dU_{x,\nu} \right] \exp[-S_g] \det D(m;\mu)$$

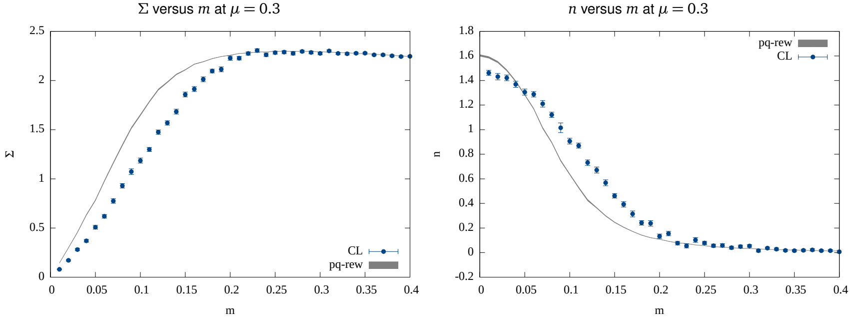
  with SU(3) matrices $U_{x,\nu}$.
- S_g: Wilson gauge action
- D: staggered Dirac operator for quark of mass m at chemical potential μ
- For $\mu \neq 0$: $\det(D) \in \mathbb{C} \to$ complex action and sign problem.

Complex Langevin and gauge cooling for QCD

- CL equations drive $U_{x,\nu}$ from SU(3) $\rightarrow$ $\mathrm{SL}(3,\mathbb{C})$.
- CL method invalid when complex trajectories wander off too far in the imaginary direction of the complexified variables.
- Gauge theories: problem resolved with gauge cooling (Seiler et al., 2012) $\rightarrow$ keep trajectories as close as possible to SU(3).
- Gauge cooling alters CL trajectories: validity conditions of CL *can* be restored, BUT no guarantee to achieve this for all parameter values.
- Validity of CL method in 1+1-dim strong-coupling QCD (Bloch et al., 2015):
  - Gauge cooling $\rightarrow$ valid results for some parameter range (m, μ).
  - At small masses: $P(z)$ not sufficiently suppressed for singularity of drift and observables at $\det(D) = 0$ $\rightarrow$ CL method gives wrong results.
- Investigate RCL in these cases.

2dQCD: Reweighting in m for 4×4 lattice

- 4×4 lattice at $\beta = 0, \mu = 0.3$: mild sign problem
- CL with gauge cooling: wrong for small masses ($m \lesssim 0.2$)



Chiral condensate and number density versus mass at $\mu = 0.3$ for a 4×4 lattice:
CL versus RCL.

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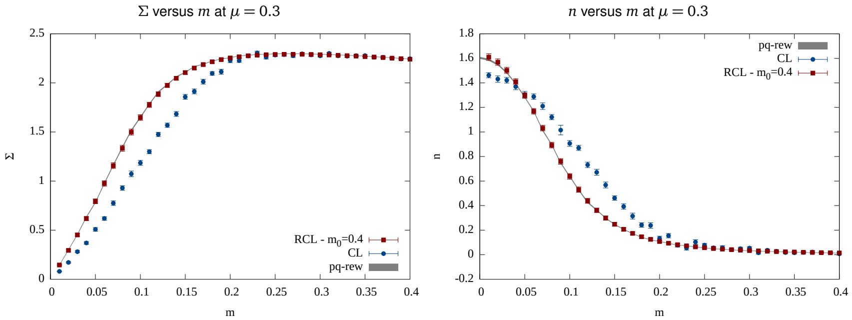
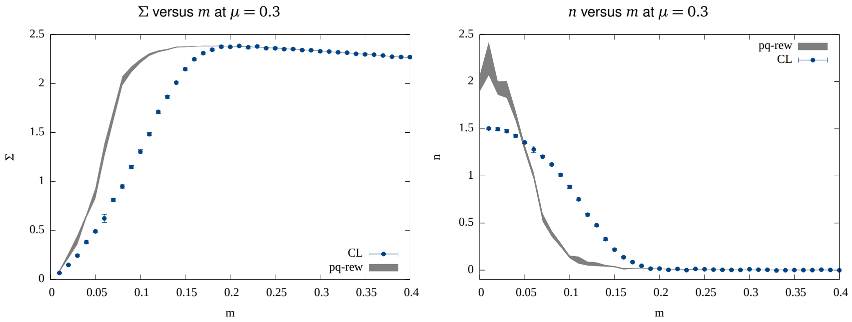
- CL with gauge cooling: wrong for small masses ($m \lesssim 0.2$)
- Apply RCL method: auxiliary ensemble at $m = 0.4, \mu = 0.3$.
- RCL in mass works over complete mass range.



Chiral condensate and number density versus mass at $\mu = 0.3$ for a 4×4 lattice: CL versus RCL.

2dQCD: Reweighting in m for 6×6 lattice

- 6×6 lattice at $\beta = 0, \mu = 0.3$: stronger sign problem
- Again, CL with gauge cooling: wrong for small masses ($m \lesssim 0.2$)



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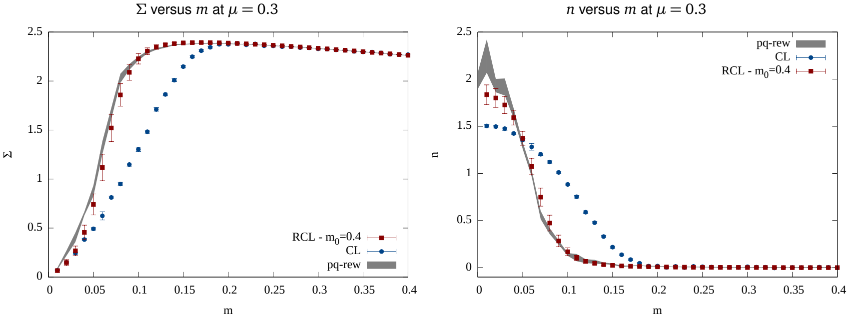
2dQCD: Reweighting in m for 6×6 lattice

- 6×6 lattice at $\beta = 0, \mu = 0.3$: stronger sign problem
- Again, CL with gauge cooling: wrong for small masses ($m \lesssim 0.2$)
- Apply RCL method: auxiliary ensemble at $m = 0.4$, $\mu = 0.3$.
- RCL works down to $m \approx 0.05$.



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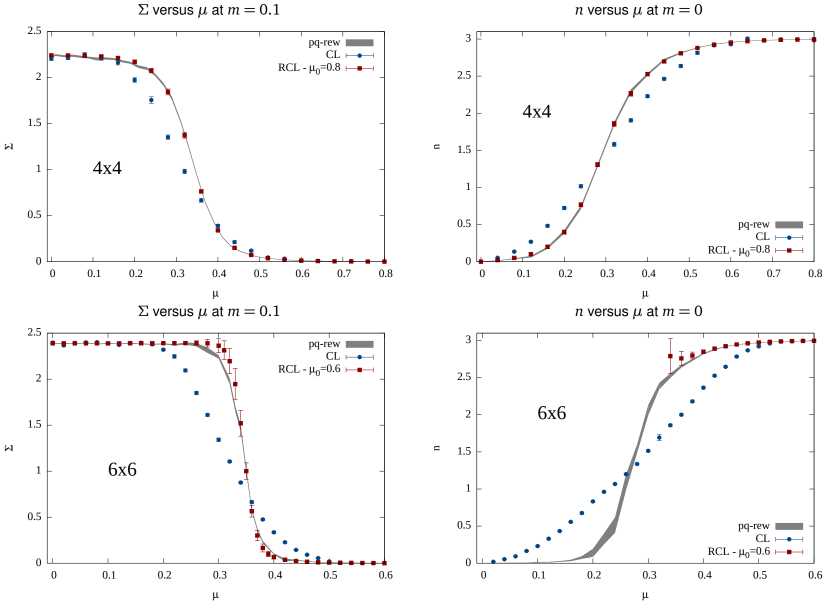
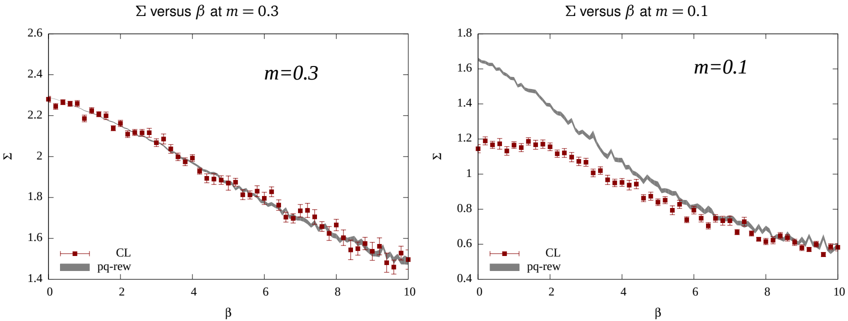
2dQCD – Reweighting in μ at $\beta = 0$



2dQCD – Reweighting in $\beta - 4 \times 4 - \mu = 0.3$

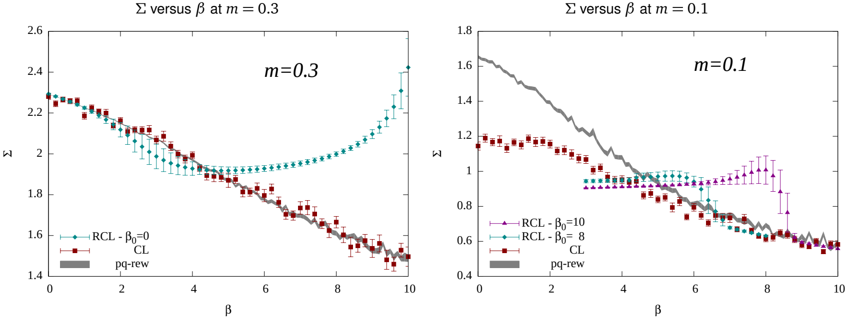
- Leaving the strong-coupling limit: Σ versus β
- At $m = 0.3$: CL agrees with benchmark (phase-quenched reweighting)
  At $m = 0.1$: CL only agrees at large β (> 8)



Chiral condensate β at $\mu = 0.3$, $m = 0.3$ (left) and $m = 0.1$ (right)
for a 4×4 lattice: CL versus RCL.

2dQCD – Reweighting in β – 4×4 – $\mu = 0.3$

- Leaving the strong-coupling limit: Σ versus β
- At $m = 0.3$: CL agrees with benchmark (phase-quenched reweighting)
  At $m = 0.1$: CL only agrees at large β (> 8)
- However, RCL only brings little improvement



Chiral condensate β at $\mu = 0.3$, $m = 0.3$ (left) and $m = 0.1$ (right)
for a 4×4 lattice: CL versus RCL.

Remarks on RCL

- RCL has usual overlap/sign problem, but could be less severe than with phase-quenched or Glasgow reweighting, because auxiliary ensemble is *closer* to target ensemble.
  1. Glasgow reweighting: $\mu_0 = 0$. RCL from $\mu_0 \neq 0$: auxiliary closer to target.
  2. Phase-quenched reweighting: $w_0 = |\det(D)|$. Auxiliary and target are in different phases for $\mu > m_\pi/2$: $\rightarrow$ little overlap between relevant configurations. RCL from $\mu \neq 0$: auxiliary and target both taken in full QCD.
- RCL can use one CL trajectory to reweight to range of parameter values (contrast to phase-quenched reweighting).

Summary

- For some theories with complex action the CL method works correctly for some range of parameters (μ, m, β), but fails for other parameter values.
- Propose new method: *reweighted complex Langevin* (RCL) method, which combines CL with reweighting of the complex trajectories.
- Proof of principle: applied RCL on RMT model and on 2dQCD using reweighting in m, μ and β at $\mu \neq 0$ and verified that the RCL procedure works correctly.
- Efficiency:
  - RCL in m works best,
  - RCL in μ works in limited window,
  - RCL in β hardly works as gauge probability is narrow and sensitive to β.
- Method could be optimized by making a multiparameter RCL in μ, m, β (Fodor et al., 2002).
- Usual overlap/sign problem → efficiency should be investigated further.

Outlook

- Try out on full 4dQCD where CL breaks down in phase transition region.
- As mass RCL works best: choose high enough m to get valid CL trajectory for particular (μ, β) and reweight in m.
- Alternatively: follow a line in (m, μ)-plane keeping β fixed.
- Learn how to reweight most efficiently.
- Make validity map of 2dQCD in (m, μ, β) plane and devise best reweighting path to cover all parameter values.
- New possibility: extend reweighting to interpolate rather then extrapolate: use auxiliary ensembles at μ_0 above and below critical region $\rightarrow$ improve reliability of results.