Reweighting trajectories from the complex Langevin method

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QCD at $\mu \neq 0$: $\text{det}(D) \in \mathbb{C} \rightarrow \text{sign problem}$.

Most solutions: computational cost grows $\propto \exp(V)$ $\rightarrow$ 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 $\rightarrow$ 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, \( x \rightarrow z = x + iy \) 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 \( K = -\frac{\partial S}{\partial z} \), step size \( \epsilon \) and independent Gaussian noise \( \eta \) (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):

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

- $w(x) \equiv e^{-S(x)}$ 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 → in latter case the CL method will fail.
- For QCD this depends on $\mu, m, \beta$ and lattice size.
# Reweighted complex Langevin (RCL)

<table>
<thead>
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<th><strong>Aim</strong></th>
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<td>Extend applicability of CL method to parameter regions for which validity conditions are not satisfied.</td>
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<th><strong>Principle</strong></th>
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| - 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. |

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<th><strong>Advantage</strong></th>
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<td>Reweighting from $\mu \neq 0$: auxiliary ensemble closer to target ensemble than in traditional reweighting.</td>
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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 $\xi_0$ to target ensemble with parameters $\xi$:

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

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

- $w(x; \xi_0)$ is complex $\rightarrow$ no importance sampling $\rightarrow$ use CL
Reweighting the CL trajectories

- If CL method is valid for parameters $\xi_0$, 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:

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

→ $\langle \mathcal{O} \rangle_{\xi}$ 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:

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

where \( z_j \) are complex configurations of CL trajectory at \( \xi_0 \).
- 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 \( \mu \)
- For \( \mu \neq 0 \): \( \det(D) \in \mathbb{C} \rightarrow \) complex action and sign problem.
CL equations drive $U_{x,y}$ from $\text{SU}(3) \rightarrow \text{SL}(3, \mathbb{C})$.

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) → 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 → valid results for some parameter range $(m, \mu)$.
- At small masses: $P(z)$ not sufficiently suppressed for singularity of drift and observables at $\det(D) = 0$ → CL method gives wrong results.

Investigate RCL in these cases.
2dQCD: Reweighting in $m$ for $4 \times 4$ lattice

- $4 \times 4$ 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 $4 \times 4$ lattice:

- CL versus RCL.
2dQCD: Reweighting in $m$ for $4 \times 4$ lattice

- $4 \times 4$ lattice at $\beta = 0, \mu = 0.3$: mild sign problem
- 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 $4 \times 4$ lattice: CL versus RCL.
2dQCD: Reweighting in $m$ for $6 \times 6$ lattice

- $6 \times 6$ lattice at $\beta = 0, \mu = 0.3$: stronger sign problem
- Again, 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 $6 \times 6$ lattice: CL versus RCL.
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- $6 \times 6$ 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 $m \approx 0.05$.

Chiral condensate and number density versus mass at $\mu = 0.3$ for a $6 \times 6$ lattice:

CL versus RCL.
2dQCD – Reweighting in $\mu$ at $\beta = 0$

$\Sigma$ versus $\mu$ at $m = 0.1$

$n$ versus $\mu$ at $m = 0$

Jacques Bloch
Reweighting trajectories from the complex Langevin method
Leaving the strong-coupling limit: $\Sigma$ versus $\beta$

- At $m = 0.3$: CL agrees with benchmark (phase-quenched reweighting)
- At $m = 0.1$: CL only agrees at large $\beta$ (> 8)

Chiral condensate $\beta$ at $\mu = 0.3$, $m = 0.3$ (left) and $m = 0.1$ (right) for a $4 \times 4$ lattice: CL versus RCL.
Leaving the strong-coupling limit: $\Sigma$ versus $\beta$

At $m = 0.3$: CL agrees with benchmark (phase-quenched reweighting)
At $m = 0.1$: CL only agrees at large $\beta$ ($>8$)

However, RCL only brings little improvement

Chiral condensate $\beta$ at $\mu = 0.3$, $m = 0.3$ (left) and $m = 0.1$ (right) for a $4 \times 4$ 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: $w_0 = |\text{det}(D)|$. Auxiliary and target are in different phases for $\mu > m_\pi/2$: 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 \((\mu, m, \beta)\), 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 \(m, \mu\) and \(\beta\) at \(\mu \neq 0\) and verified that the RCL procedure works correctly.
- **Efficiency:**
  - RCL in \(m\) works best,
  - RCL in \(\mu\) works in limited window,
  - RCL in \(\beta\) hardly works as gauge probability is narrow and sensitive to \(\beta\).
- Method could be optimized by making a multiparameter RCL in \(\mu, m, \beta\) (Fodor et al., 2002).
- **Usual overlap/sign problem \(\rightarrow\)** 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 \((\mu, \beta)\) and reweight in \( m \).
- Alternatively: follow a line in \((m, \mu)\)-plane keeping \( \beta \) fixed.
- Learn how to reweight most efficiently.
- Make validity map of 2dQCD in \((m, \mu, \beta)\) plane and devise best reweighting path to cover all parameter values.
- New possibility: extend reweighting to interpolate rather then extrapolate: use auxiliary ensembles at \( \mu_0 \) above and below critical region → improve reliability of results.