

Exercises for Lattice Field Theory – Hamiltonian and Lagrangian Methods (physics7520)

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For this exercise, please upload a single `.zip` file per group, containing both the notebooks with your solutions and a `.pdf` file with comments and answers to the questions.

1. $\mathbb{Z}_2$ Lattice Gauge Theory (10 pts)

In this exercise we will use Monte Carlo simulations to investigate a $\mathbb{Z}_2$ LGT in three spacetime dimension. The action of the theory is

$$S = -\beta \sum_x \sum_{\mu < \nu} P_{x,\mu\nu}, \quad P_{x,\mu\nu} = U_{x,\mu} U_{x+\hat{\mu},\nu} U_{x+\hat{\nu},\mu} U_{x,\nu}, \quad (1)$$

where the gauge field $U_{x,\mu} \in \{\pm 1\}$.

In this exercise you are given with a notebook, with some routines already provided, and you have to fill the incomplete ones and to numerically study the system. Notice that you are not asked to write the Monte Carlo routine yourself, nor the error analysis, and these are already implemented.

- (2 pts.) We are simulating a model in a L^3 lattice with periodic boundary conditions. Define a function `init_lattice` taking as input the linear size of the lattice L and returns a numpy array containing all the gauge fields initialized to +1, and two numpy arrays containing the coordinate of the positive and negative neighboring sites in each direction.
- (1 pts.) Write a function `delta_action` that computes the difference in the action once a single link is flipped.
- (2 pts.) Write two functions `avg_plaquette` and `avg_link` returning respectively the average value of the plaquette and the average value of the link. Are these quantities gauge invariant?
- (2 pts.) Study the average value of the plaquette in the β -range `np.linspace(0.1, 1.2, 15)`. For every value of β , discard the first 200 measurement and average over 500 samples. Plot the average value of the plaquette and the error computed with the jackknife routine (provided in the notebook) as a function of β .
- (2 pts.) In LGT there exist a theorem, the Elitzur's theorem, stating that the vacuum expectation value of non-gauge invariant observables vanishes. Repeat the same analysis as in the previous point for the link and explain what you observe.

- f) (1 pts.) Plot the Monte Carlo history of the plaquette (an example is provided in the notebook) for $\beta = 0.3, 0.7$ and 1.2 . Explain the differences you observe: which dataset looks more correlated?

See `z2_lgt_exercise.ipynb` for the exercises

2. Problems at finite chemical potential (10 pts)

In this exercise we will see the two biggest challenges faced by Monte Carlo simulations at finite chemical potential: the sign problem and the overlap problem. Since the overlap problem originates from re-weighting observables from a *different* distribution than the one we want to sample from, we will use the results developed in the previous exercise to investigate it.

Note: The role of chemical potential is played by the coupling β as the overlap problem is a general issue of Monte Carlo simulations and it is not specific to finite chemical potential. In fact, the overlap problem can be observed in any situation where one tries to re-weight observables from a different distribution, and it is not specific to finite chemical potential.

- a) (5 pts.) Consider the $\mathbb{Z}_2$ LGT studied in the previous exercise. Start by performing Monte-Carlo simulations as you did above, but now at $\beta \in \{0.2, 0.3, 0.6\}$. Write a function `reweight_plaquette` that takes as input the samples obtained at $\beta = 0.2$ and returns the re-weighted average value of the plaquette at $\beta = 0.3$ and $\beta = 0.6$. Plot the results for the average plaquette and compare them with the ones obtained by direct Monte Carlo simulation that you performed. Explain the differences you observe: do you get better or worse results as you try to predict the average plaquette at a coupling β that is further than the one you sampled from? What is the reason for this behaviour?
- b) (5 pts.) Consider the 1D oscillatory integral

$$I(\alpha) = \int_{-\infty}^{\infty} dx e^{-x^2} \cos(\alpha x), \quad \alpha \geq 0, \quad (2)$$

whose exact value is $I(\alpha) = \sqrt{\pi} e^{-\alpha^2/4}$. We use the sign decomposition $e^{-x^2} \cos(\alpha x) = W(x) \sigma(x)$, where $W(x) = e^{-x^2} |\cos(\alpha x)| \geq 0$ and $\sigma(x) = \text{sgn}(\cos(\alpha x)) = \pm 1$, so that $I(\alpha) = Z_+ \langle \sigma \rangle_W$ with $Z_+ = \int W dx$.

- i. Evaluate $I(\alpha)$ numerically using the trapezoidal rule on a uniform grid over $[-10, 10]$ for $\alpha \in [0, 10]$ and compare with the exact result. Show that the relative error stays near machine precision for a well-resolved grid ($n = 20001$ points), and degrades only when the grid is too coarse to resolve the period $2\pi/\alpha$. *Note: deterministic quadrature has no signal-to-noise problem.*
- ii. Use Metropolis–Hastings to draw $N = 10^5$ samples $x_i \sim p(x) \propto W(x)$ and estimate

$$\langle \sigma \rangle_W \approx \frac{1}{N} \sum_{i=1}^N \text{sgn}(\cos(\alpha x_i)), \quad \hat{I}_N = Z_+ \langle \sigma \rangle_W. \quad (3)$$

For $\alpha \in \{0.5, 2, 5, 8\}$ report the MC estimate, its standard error, the exact sign average $I(\alpha)/Z_+$, and the ratio *error/signal*. What do you observe for large α ?

iii. Show that the per-sample signal-to-noise ratio is

$$\text{SNR}_1(\alpha) = \frac{|\langle \sigma \rangle_W|}{\sqrt{1 - \langle \sigma \rangle_W^2}} \xrightarrow{\alpha \rightarrow \infty} \frac{\pi}{2} e^{-\alpha^2/4}, \quad (4)$$

and that fixed relative precision requires $N \sim e^{\alpha^2/2}$ samples. Verify numerically by plotting the measured SNR and the cost N for 10% relative error against α .

See `z2_lgt_exercise.ipynb` for 2a and `sign_problem_exercise.ipynb` for 2b.

3. Lefschetz Thimble Regularization (10 pts)

In this exercise we study the zero-dimensional ϕ^4 “field theory”, i.e. a single integral over the real line with a complex action:

$$Z = \int_{\mathbb{R}} d\phi e^{-S(\phi)}, \quad S(\phi) = \frac{1}{2} \sigma \phi^2 + \frac{1}{4} \lambda \phi^4, \quad \lambda \in \mathbb{R}^+, \quad \sigma \in \mathbb{C}. \quad (5)$$

When $\text{Im } \sigma \neq 0$ the Boltzmann weight $e^{-S(\phi)}$ is complex, causing sign oscillations that make naive Monte Carlo impractical. The Lefschetz thimble approach deforms the integration contour into $\mathbb{C}$ so that $\text{Im } S$ is constant on each contour, removing the oscillations. You are given the companion notebook `lefschetz_thimble_phi4_exercise.ipynb` with helper routines already provided.

a) (1 pts.) Show that the critical points of $S(\phi)$ (solutions of $S'(\phi) = 0$) are

$$\phi_0 = 0, \quad \phi_{\pm} = \pm \sqrt{-\sigma/\lambda}. \quad (6)$$

For $\sigma = 0.5 + 0.75i$ and $\lambda = 2$, compute the numerical values of ϕ_0, ϕ_+, ϕ_- and verify that they are in general off the real axis. Implement the function `critical_points( $\sigma, \lambda$ )` in the notebook.

b) (2 pts.) To trace a thimble we integrate the steepest-ascent ODE

$$\frac{d\phi}{dt} = \overline{S'(\phi)}, \quad (7)$$

starting from a small perturbation of a critical point in the direction tangent to the thimble. The Hessian of $S^R \equiv \text{Re } S$ at a critical point ϕ_σ has eigenvalues $\pm |S''(\phi_\sigma)|$; if $S''(\phi_\sigma) = |S''| e^{i\alpha}$, the positive-eigenvalue eigenvector points along angle $\theta = -\alpha/2$.

Implement `hessian_direction` and use it together with the provided `trace_thimble` routine to draw stable (steepest-ascent) and unstable (steepest-descent) thimbles through all three critical points for $\sigma = 0.5 + 0.75i$, $\sigma = 0.75i$, and $\sigma = -0.5 + 0.75i$. Display the three portraits side by side. Describe qualitatively what changes between the three cases.

c) (2 pts.) A key property of stable thimbles is that $\text{Im } S$ is *constant* along each one. Verify this numerically: for $\sigma = -0.5 + 0.75i$ and $\lambda = 2$, trace the stable thimbles through all three critical points and plot $\text{Im } S(\phi(t))$ as a function of the ascent time t for each branch. What is the constant value of $\text{Im } S$ on each thimble?

- d) (1 pts.) The Picard–Lefschetz decomposition states that the original integral can be written as

$$\int_{\mathbb{R}} d\phi \phi^n e^{-S(\phi)} = \sum_{\sigma} m_{\sigma} \int_{\mathcal{J}_{\sigma}} d\phi \phi^n e^{-S(\phi)}, \quad (8)$$

where $m_{\sigma} \in \mathbb{Z}$ are integer weights and each contour integral is computed numerically along the traced thimble using

$$\int_{\mathcal{J}_{\sigma}} d\phi \phi^n e^{-S(\phi)} = \int dt \overline{S'(\phi(t))} \phi(t)^n e^{-S(\phi(t))}. \quad (9)$$

For $\sigma_R > 0$ only $\mathcal{J}_0$ contributes ($m_0 = +1$). For $\sigma_R < 0$ all three thimbles contribute; determine the correct integer weights m_{σ} numerically by comparing with the reference integral computed by direct quadrature on $\mathbb{R}$.

- e) (4 pts.) Compute $\langle \phi^8 \rangle = Z^{-1} \int_{\mathbb{R}} d\phi \phi^8 e^{-S(\phi)}$ via the thimble decomposition for $\sigma_R \in [-0.6, 0.6]$ at fixed $\sigma_I = 0.75$ and $\lambda = 2$, (in steps of 0.1 and excluding the point $\sigma_R = 0$), using the appropriate decomposition on each side of the Stokes line $\sigma_R = 0$. Compare your result with the exact answer obtained by direct numerical integration on $\mathbb{R}$ and comment on the agreement.

See `lefschetz_thimble_phi4_exercise.ipynb`