Deep Learning Algorithms for Lattice Field Theory Calculations

Twenty-Second Lomonosov Conference on Elementary Particle Physics
Moscow/ August, 21-27, 2025

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25 August 2025

The work is supported by Basis Foundation.

Path Integral

$$\langle F(\phi)\rangle_\beta = \frac{1}{Z}\int D\left[\phi(x^\mu)\right] e^{-S_E[\phi]}\, F(\phi)\,, \qquad \phi(0,\mathbf{x}) = \phi(\beta,\mathbf{x})$$

$$\langle F\rangle_\beta = \frac{Tr\left(e^{-\beta H} F\right)}{Z} = \sum_n \langle n|F|n\rangle \frac{e^{-\beta E_n}}{Z}$$

$$\langle F\rangle_\beta = \langle 0|F|0\rangle + O\left(e^{-\beta(E_1-E_0)}\right)$$

Discretization

In the space $\mathbb{R}^{D+1}$ we introduce a rectangular lattice with a step size of a. The field corresponds to a finite-dimensional vector.

$$\phi(t, \mathbf{x}) \in C(\mathbb{R}^{D+1}) \quad \to \quad \phi_i^{\mathbf{x}} \in \mathbb{R}^N$$

$$S[\phi] \quad \to S_{latt}(\phi_i^{\mathbf{x}})$$

$$|e^{-S(\phi)} - e^{-S_{latt}(\phi_i^{\mathbf{x}})}| = O(a^n)$$

$$\int D\phi(x^\mu) e^{-S(\phi)} F(\phi) \approx \int d^N\phi_i^{\mathbf{x}} \; e^{-S_{latt}(\phi_i^{\mathbf{x}})} F_{latt}(\phi_i^{\mathbf{x}})$$

Monte-Carlo approach

$$x \in \mathbb{R}^N$$

$$P(x) = \frac{e^{-S(x)}}{Z}, \qquad \int d^N x \; P(x) = 1$$

$$\langle F \rangle = \int d^N x \; P(x) F(x) \approx \frac{1}{M} \sum_{k=1}^{M} F(x^{(k)})$$

$$\{x^{(k)}\} \sim P(x)$$

Computation of path integral = generating of sample $\{x^{(k)}\}$ from $P(x)$

Critical slowing down

Wolff "Critical Slowing Down"Nucl. Phys. B 17 (1990) 93-102

$$X^1 \to \dots \to X^n$$

$$\langle O \rangle \approx \frac{1}{n} \sum_{k=1}^{n} \bar{O}(X^k)$$

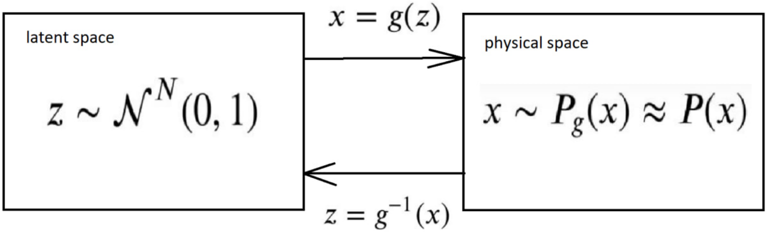
$$\sigma_O^2 = \left\langle \left(\frac{1}{n} \sum_{k=1}^{n} \bar{O}(X^k) - \langle O \rangle \right)^2 \right\rangle = \frac{1}{n^2} \sum_{i,k=1}^{n} \Gamma(i-k)$$

$$\Gamma(s) = \Gamma(0) e^{-s/\delta_{corr}}$$

$$\sigma_O^2 \approx \frac{2\delta_{corr}\Gamma(0)}{n}$$

$$\delta_{corr} \sim a^{-z} \qquad z \approx 2$$

Normalizing flow



$$r(z) = \frac{1}{(2\pi)^{N/2}} \exp\left(-\frac{1}{2}||z||^2\right) ,$$

$$P(x) = \frac{e^{-S(x)}}{Z}, \qquad P_g(x) = r(z)\left|\det \frac{\partial g}{\partial z}\right|^{-1}$$

Free field: $g(z) = wz$

w can be explicitly written.

Affine coupling layers

The map g is a composition of affine transformations

$$g = A_n \circ \ldots \circ A_1 \tag{1}$$

We devide z on two parts

$$z = u + v \tag{2}$$

For example, u contains coordinats of z with even numbers, and v – the odd one.

$$A(u) = u\,, \qquad [A(v)]_k = e^{\theta^w_{1k}(u)} v_k + \theta^w_{2k}(u)$$
$$\theta^w : \mathbb{R}^{N/2} \to \mathbb{R}^N$$

George Papamakarios, Eric Nalisnick, Danilo Jimenez Rezende, Shakir Mohamed, Balaji Lakshminarayanan "Normalizing Flows for Probabilistic Modeling and Inference" Journal of Machine Learning Research, 22(57):1-64, 2021

Optimization task

$$D_{KL}(p|q) = \int dx\, p(x) \ln \frac{p(x)}{q(x)}$$

$$D_{KL}(p|q) \geq 0\,, \qquad D_{KL}(p|q) = 0 \Longleftrightarrow p(x) = q(x)$$

$$L[w] = D_{KL}(P_g|P) - \ln Z$$

$$L[w] = D_{KL}(P_g|P) - \ln Z = \frac{1}{M} \sum_{k=1}^{M} \left[S(g(z_k|w)) - \ln \left| \det \frac{\partial g(z_k|w)}{\partial z} \right| \right]$$

M. S. Albergo, G. Kanwar, and P. E. Shanahan "Flow-based generative models for Markov chain Monte Carlo in lattice field theory" Phys. Rev. D 100, 034515

MCMC+Normalizing flow = Decorrelation of trajectories

- At a certain iteration of the Markov chain, apply the inverse transformation and compute the probability

$$z = g^{-1}(x), \qquad P_g(x) = (2\pi)^{-N/2} e^{-|z|^2/2} \left| \det \frac{\partial g^{-1}(x)}{\partial x} \right|$$

- Generate a new trajectory

$$x' = g(z'), \qquad P_g(x') = (2\pi)^{-N/2} e^{-|z|^2/2} \left| \det \frac{\partial g(z')}{\partial z'} \right|^{-1}$$

- Accept the trajectory with probability

$$\pi(x', x) = \min\left(\frac{q(x')}{q(x)}, 1\right), \qquad q(x) = \frac{P(x)}{P_g(x)}$$

Non-relativistic quantum mechanics

$$H = \frac{p^2}{2} + V(x)$$

$$S(x) = \sum_i \frac{1}{2a}(x_{i+1} - x_i)^2 + aV(x_i)$$

A. Vasiliev, A. Ivanov, D. Salnikov, V. Chistiakov, "Application of neural networks for calculating functional integrals in quantum field theory" Phys. Part. Nucl., 2025, Vol. 56, No. 3, pp. 704–708.

Relativistic quantum mechanics

$$H = \sqrt{p^2 + m^2} - m + V(x)$$

$$S(x) = \sum_i \left[-\ln \left(\frac{m^2 a}{\pi} \frac{K_1(\eta_i)}{\eta_i} \right) + aV(x_i) \right],$$

$$\eta_i = ma\sqrt{1 + \left(\frac{x_{i+1} - x_i}{a} \right)^2}$$

D. V. Salnikov, V. V. Chistiakov, A. S. Ivanov and A. V. Vasiliev, "Application of Neural Networks for Path Integrals Computation in Relativistic Quantum Mechanics"Moscow University Physics Bulletin, 2024, Vol. 79, Suppl. 2, pp. S639–S646

https://github.com/Vsevolod2001/NF_QFT

Scalar field on the lattice

$$S = v\left[\frac{1}{2}(K\phi,\phi) + (J(x),\phi) + \frac{m^2}{2}(\phi,\phi) + \sum_i V_{int}(\phi_i)\right]$$

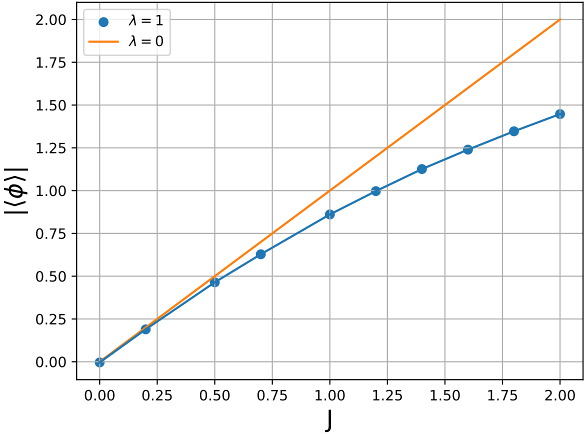
$$K = \sum_\mu I \otimes \ldots\mathcal{D}^2\ldots \otimes I \sim -\partial_\mu\partial_\mu$$

$$\mathcal{D}^2 = 2I - T - T^{-1}$$

$$T_{ij} = \delta_{i+1,j}$$

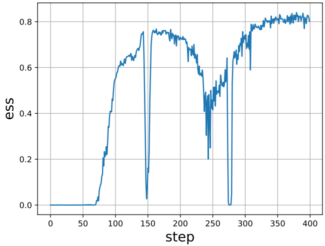
$J = const$

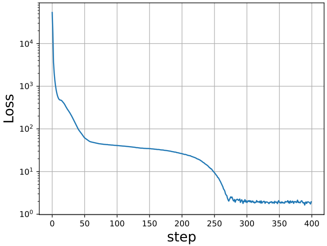
$$V_{int}(\phi) = \frac{\lambda}{24}\phi^4$$



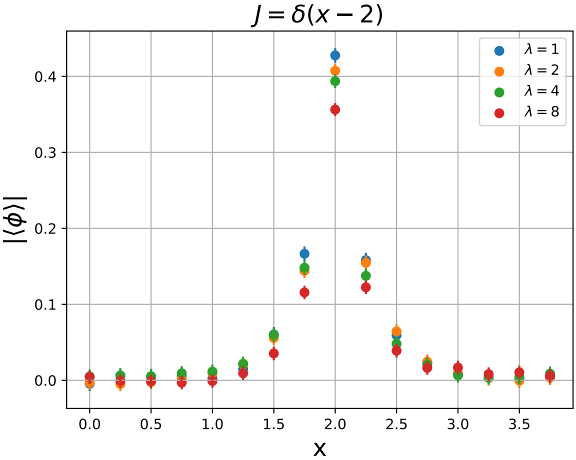
Metric

$$Q(\phi) = \frac{e^{-S(\phi)}}{P_g(\phi)}, \quad ess = \frac{\left(\frac{1}{M}\sum_{k=1}^{M} Q(\phi^{(k)})\right)^2}{\frac{1}{M}\sum_{k=1}^{M} Q^2(\phi^{(k)})}$$





$J(x)$


$J = \delta(x-2)$
$\lambda = 1$
$\lambda = 2$
$\lambda = 4$
$\lambda = 8$
0.4
0.3
0.2
0.1
0.0
$|\langle\phi\rangle|$
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
x