

Machine Learning Approach for Lattice Quantum Field Theory Calculations

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Path Integral

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

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

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

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.

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

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

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

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

Monte-Carlo approach

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

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

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

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

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

$$X^1 \rightarrow \dots \rightarrow X^n$$

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

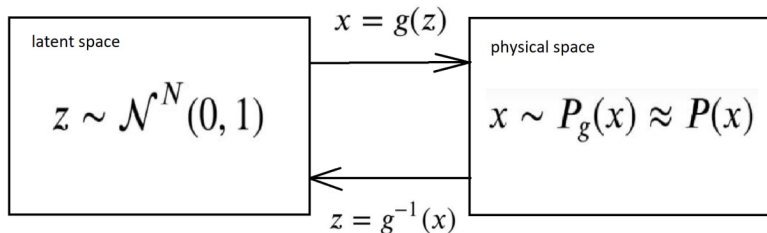
$$\sigma_O^2 = \left\langle \left(\frac{1}{n} \sum_{k=1}^n \bar{O}(X^k) - \langle O \rangle \right)^2 \right\rangle = \frac{1}{n^2} \sum_{i,k=1}^n \Gamma(i-k)$$

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

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

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

Normalizing flow



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

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

Free field: $g(z) = wz$
 w can be explicitly written.

Affine coupling layers

The map g is a composition of affine transformations

$$g = A_n \circ \dots \circ A_1 \quad (1)$$

We divide z on two parts

$$z = u + v \quad (2)$$

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

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

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

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

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

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

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

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

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

- Generate a new trajectory

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

- Accept the trajectory with probability

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

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

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

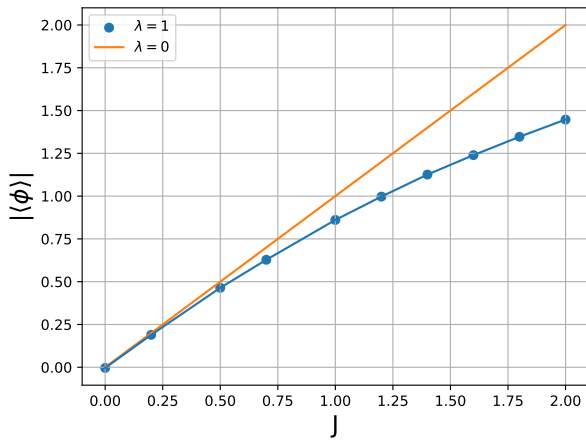
$$K = \sum_{\mu} I \otimes \dots \mathcal{D}^2 \dots \otimes I \sim \partial_{\mu} \partial_{\mu}$$

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

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

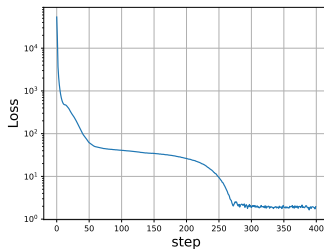
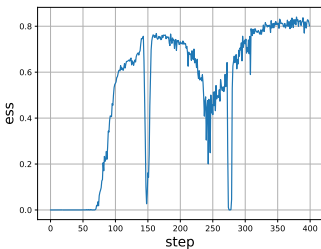
$J = \text{const}$

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



Metric

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



$$J(x)$$

