NetKet Implementation Notes

1 Neural Density Matrix

We consider purified neural-network density matrices of the form

$$\rho(x,y) \quad = \quad \sum_{\mu}^{K} \Phi(x,\mu)\Phi(y,\mu)^{\star},$$

where μ is a suitable set of *mixing* variables [1].

For concreteness, let us consider the case of a complex-valued purified RBM density matrix, as used e.g in [2],. The corresponding pure state is RbmSpin with M hidden units. Define the standard pure case as

$$\begin{aligned} \Psi(x;W) \quad &= \quad \sum_{h} e^{\sum_j^M \sum_s^N x_s W_{sj} h_j + b_j h_j} \\ &\propto \quad \Pi_j^M \cosh(\theta_j(x;W,b)) \\ &= \quad \Psi(x;W,b) \end{aligned}$$

With

$$\theta_j(x;W,b) \quad = \quad \sum_s x_s W_{sj} + b_s.$$

We introduce mixing units with a coupling U_{sk} and bias c_k. Then

$$\rho(x,y) \quad = \quad \sum_{hh'\mu} \exp\left[\sum_{j,j',k} \theta_j(x;W,b)h_j + \theta^{\star}_{j'}(y;W,b)h'_{j'} + \theta_k(x;U,c)\mu_k + \theta^{\star}_k(y;U,c)\mu_k\right],$$

thus

$$\log\rho(x,y) \quad = \quad \sum_j G(\theta_j(x)) + \sum_{j'} G(\theta^{\star}_{j'}(y)) + \sum_k G(\theta_k(x) + \theta^{\star}_k(y)),$$

where $G(x) = \log\cosh(x)$ in the case of ± 1 hidden and mixing units.

References

[1] Torlai, G. & Melko, R. G. Latent Space Purification via Neural Density Operators. Phys. Rev. Lett. 120, 240503 (2018).

[2] Hartmann, M. J. & Carleo, G. Neural-Network Approach to Dissipative Quantum Many-Body Dynamics. Phys. Rev. Lett. 122, 250502 (2019).