Quantum State Tomography Proposal

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1 Restrict Boltzmann Machine

In generative modeling, we want to train a density $p_\lambda(x,h) = \frac{1}{Z}e^{-E(x,h)}$ to approach a ground truth $P(x)$. Like supervised learning, we need some cost function to minimize. But unlike supervised learning, the cost function here is defined via Kullback-Leibler divergence

$D(P|p_\lambda) \equiv \sum_x P(x) log \frac{P(x)}{p_\lambda(x)} = \sum_x P(x) log P(x) - \sum_x P(x) log p_\lambda(x)$

To define a tractable cost function, we need to get rid of the unknown $P(x)$. Make the approximation $P_X(x) \equiv \frac{1}{|X|}\sum_{x_k} \delta_{x,x_k}$, where $|X|$ is the number of data point in our dataset, then we have

$D(P|p_\lambda) \approx -H_X - \frac{1}{|X|}\sum_{x_k} log p_\lambda(x_k)$

Only second term depends on the parameters of model, thus we define the cost function

$C_\lambda = -\frac{1}{|X|}\sum_{x_k} log p_\lambda(x_k)$

with gradient descent process

$\lambda \Longrightarrow \lambda - \eta \nabla_\lambda C_\lambda$

So far it is generative modeling in general, since we haven't assigned any specific form of p_λ. We now assign the following form

$p_\lambda(x,h) = \frac{1}{Z}e^{-E(x,h)}$

where

$E(x,h) = -\sum_{i,j}^{n_x,n_h} W_{ij} x_i h_j - \sum_i^{n_x} b_i x_i - \sum_i^{n_h} c_i h_i$

this model is called the **Restricted Boltzmann Machine(RBM)**.

RBM makes the training very tractable as

$\nabla_\lambda C_\lambda = < \frac{\partial E}{\partial \lambda} >_{p_\lambda(x|h)} - < \frac{\partial E}{\partial \lambda} >_{p_\lambda(x,h)}$

where $\frac{\partial E}{\partial \lambda}$ can be very easily derived in RBM. The remaining task is to compute expectation value by samples, and only the second term needs some additional technique to tackle. Gibbs sampling is the most common one to do it.[1]

2 Quantum State Tomography

With RBM, we can always reveal the probability distribution from which the states are sampled. If the samples are from quantum measurements, the probability distribution we want to find is just from density matrix[3] or quantum states[2] with respect to the some basis of measurement. For simplicity, we illustrate the case of pure state in Ising spin basis. We simplify the case further by considering real value wave function.

We model the probability distribution by RBM

$p_\lambda(\sigma) = \sum_h p_\lambda(\sigma, h) = |\psi_\lambda(\sigma)|^2$

Since the wave function we consider is real, we can just reconstruct the wave function by

$\psi_\lambda(\sigma) = \sqrt{p_\lambda(\sigma)}$.

To check the result, we can examine the expectation value of physical observable.

$< \hat{O} > \approx < \hat{O} >_\lambda = < \psi_\lambda|\hat{O}|\psi_\lambda > = \sum_{\sigma\sigma'} \psi_\lambda(\sigma') < \sigma'|\hat{O}|\sigma > \psi_\lambda(\sigma)$

$= \sum_{\sigma\sigma'} \sqrt{p_\lambda(\sigma')}\sqrt{p_\lambda(\sigma)} O_{\sigma'\sigma}$

Then we can compare the result to that of other methods.[2]

Note that for complex-valued wave function, there are two ways to represent by RBM. One is directly set parameter λ of RBM complex. The other way is to add another RBM to parametrize the phase part of wave function[2].

References

[1] Hinton, G. E., 2002, Neural Comput. 14, 1771.

[2] Torlai, G., G. Mazzola, J. Carrasquilla, M. Troyer, R. Melko, and G. Carleo, 2018, Nat. Phys. 14, 447.

[3] Torlai, G., and R. G. Melko, 2018, Phys. Rev. Lett. 120, 240503.