

Suppose we have

$$\begin{aligned} O(W') &= \sqrt{\frac{|\langle \Psi_{W'} | \Phi \rangle|^2}{\langle \Psi_{W'} | \Psi_{W'} \rangle \langle \Phi | \Phi \rangle}} \\ &= \sqrt{\left\langle \frac{\Phi(B)}{\Psi_{W'}(B)} \right\rangle_{\Psi} \left\langle \frac{\Psi_{W'}(B)}{\Phi(B)} \right\rangle_{\Phi}^*} \end{aligned}$$

where $\langle f(B) \rangle_A \equiv \sum_B f(B) \frac{|A(B)|^2}{\sum_B |A(B)|^2}$ is the expectation value over variational state A .

Define Loss function as $L(W') = -\log O(W')$, we want to calculate the derivative.

$$\partial_{p_k} L(W') = -\frac{1}{2} \partial_{p_k} [\log(\left\langle \frac{\Phi(B)}{\Psi_{W'}(B)} \right\rangle_{\Psi}) + \log(\left\langle \frac{\Psi_{W'}(B)}{\Phi(B)} \right\rangle_{\Phi}^*)]$$

Lemma 1

Define $O_k(B) \equiv \partial_{p_k} \log(\Psi(B))$ and $O_k^*(B) \equiv \partial_{p_k} \log(\Psi^*(B))$, and

$$\partial_{p_k} \langle f \rangle_{\Psi} = \langle \partial_{p_k} f \rangle_{\Psi} + \langle f(B)(O_k(B) + O_k^*(B)) \rangle_{\Psi} - \langle f \rangle_{\Psi} \langle O_k(B) + O_k^*(B) \rangle_{\Psi}$$

Proof:

$$\langle f \rangle_{\Psi} = \frac{\sum_B f(B) |\Psi(B)|^2}{\sum_B |\Psi(B)|^2}$$

Then the derivative can be decomposed into 3 parts, where

$$\begin{aligned} \partial_{p_k} \langle f \rangle_{\Psi} &= \frac{\sum_B [\partial_{p_k} f(B)] |\Psi(B)|^2}{\sum_B |\Psi(B)|^2} \\ &+ \frac{\sum_B f(B) [\partial_{p_k} |\Psi(B)|^2]}{\sum_B |\Psi(B)|^2} \\ &+ \frac{\sum_B f(B) |\Psi(B)|^2}{\partial_{p_k} \sum_B |\Psi(B)|^2} \end{aligned}$$

The first part is $\langle \partial_{p_k} f \rangle_{\Psi}$

The second part:

$$\begin{aligned}
\frac{\sum_B f(B) [\partial_{p_k} |\Psi(B)|^2]}{\sum_B |\Psi(B)|^2} &= \frac{\sum_B f(B) [\Psi^*(B) \partial_{p_k} \Psi(B) + \Psi(B) \partial_{p_k} \Psi^*(B)]}{\sum_B |\Psi(B)|^2} \\
&= \frac{\sum_B f(B) |\Psi(B)|^2 \partial_{p_k} [\log(\Psi(B)) + \log(\Psi^*(B))]}{\sum_B |\Psi(B)|^2} \\
&= \langle f(B) (O_k(B) + O_k^*(B)) \rangle_\Psi
\end{aligned}$$

The third part:

$$\begin{aligned}
\frac{\sum_B f(B) |\Psi(B)|^2}{\partial_{p_k} \sum_B |\Psi(B)|^2} &= - \frac{\sum_B f(B) |\Psi(B)|^2}{(\sum_B |\Psi(B)|^2)^2} (\partial_{p_k} \sum_B |\Psi(B)|^2) \\
&= - \frac{\sum_B f(B) |\Psi(B)|^2}{\sum_B |\Psi(B)|^2} \frac{\partial_{p_k} \sum_B |\Psi(B)|^2}{\sum_B |\Psi(B)|^2} \\
&= - \langle f \rangle_\Psi \frac{\sum_B |\Psi(B)|^2 \partial_{p_k} (\log(\Psi(B)) + \log(\Psi^*(B)))}{\sum_B |\Psi(B)|^2} \\
&= - \langle f \rangle_\Psi \langle O_k(B) + O_k^*(B) \rangle_\Psi
\end{aligned}$$

Continue calculate

$$\partial_{p_k} L(W') = -\frac{1}{2} \partial_{p_k} [\log(\left\langle \frac{\Phi(B)}{\Psi_{W'}(B)} \right\rangle_\Psi) + \log(\left\langle \frac{\Psi_{W'}(B)}{\Phi(B)} \right\rangle_\Phi^*)]$$

Calculate the first part

Using Lemma 1 to the first part $\partial_{p_k} \log(\left\langle \frac{\Phi(B)}{\Psi_{W'}(B)} \right\rangle_\Psi)$, then

$$\begin{aligned}
\partial_{p_k} \log\left(\left\langle \frac{\Phi(B)}{\Psi_{W'}(B)} \right\rangle_{\Psi}\right) &= \frac{1}{\left\langle \frac{\Phi}{\Psi} \right\rangle_{\Psi}} \partial_{p_k} \left\langle \frac{\Phi(B)}{\Psi_{W'}(B)} \right\rangle_{\Psi} \\
&= \frac{1}{\left\langle \frac{\Phi}{\Psi} \right\rangle_{\Psi}} \left\langle \partial_{p_k} \frac{\Phi(B)}{\Psi_{W'}(B)} \right\rangle_{\Psi} \\
&+ \frac{1}{\left\langle \frac{\Phi}{\Psi} \right\rangle_{\Psi}} \left\langle \frac{\Phi(B)}{\Psi_{W'}(B)} \partial_{p_k} (\log(\Psi(B)) + \log(\Psi^*(B))) \right\rangle_{\Psi} \\
&- \frac{1}{\left\langle \frac{\Phi}{\Psi} \right\rangle_{\Psi}} \left\langle \frac{\Phi(B)}{\Psi_{W'}(B)} \right\rangle_{\Psi} \langle \partial_{p_k} (\log(\Psi(B)) + \log(\Psi^*(B))) \rangle_{\Psi} \\
&= -\frac{1}{\left\langle \frac{\Phi}{\Psi} \right\rangle_{\Psi}} \left\langle \frac{\Phi(B)}{\Psi_{W'}(B)} \partial_{p_k} \log(\Psi(B)) \right\rangle_{\Psi} \\
&+ \frac{1}{\left\langle \frac{\Phi}{\Psi} \right\rangle_{\Psi}} \left\langle \frac{\Phi(B)}{\Psi_{W'}(B)} \partial_{p_k} (\log(\Psi(B)) + \log(\Psi^*(B))) \right\rangle_{\Psi} \\
&- \langle \partial_{p_k} (\log(\Psi(B)) + \log(\Psi^*(B))) \rangle_{\Psi} \\
&= \frac{\left\langle \frac{\Phi(B)}{\Psi_{W'}(B)} \partial_{p_k} \log(\Psi^*(B)) \right\rangle_{\Psi}}{\left\langle \frac{\Phi}{\Psi} \right\rangle_{\Psi}} - \langle \partial_{p_k} (\log(\Psi(B)) + \log(\Psi^*(B))) \rangle_{\Psi}
\end{aligned}$$

Write it in the observable form, we get

$$\partial_{p_k} \log\left(\left\langle \frac{\Phi(B)}{\Psi_{W'}(B)} \right\rangle_{\Psi}\right) = \frac{\left\langle \frac{\Phi(B)}{\Psi_{W'}(B)} O_k^*(B) \right\rangle_{\Psi}}{\left\langle \frac{\Phi}{\Psi} \right\rangle_{\Psi}} - \langle O_k(B) + O_k^*(B) \rangle_{\Psi}$$

Calculate the second part

The second part $\partial_{p_k} \log\left(\left\langle \frac{\Psi_{W'}(B)}{\Phi(B)} \right\rangle_{\Phi}^*\right)$ can be easily calculated by

$$\partial_{p_k} \log\left(\left\langle \frac{\Psi_{W'}(B)}{\Phi(B)} \right\rangle_{\Phi}^*\right) = \frac{\left\langle \frac{\partial_{p_k} \Psi_{W'}(B)}{\Phi(B)} \right\rangle_{\Phi}^*}{\left\langle \frac{\Psi_{W'}(B)}{\Phi(B)} \right\rangle_{\Phi}^*}$$

Combining together

Combine the first and second parts together, we get

$$\partial_{p_k} L(W') = \frac{1}{2} \langle O_k(B) + O_k^*(B) \rangle_\Psi - \frac{1}{2} \frac{\left\langle \frac{\Phi(B)}{\Psi(B)} O_k^*(B) \right\rangle_\Psi}{\left\langle \frac{\Phi}{\Psi} \right\rangle_\Psi} - \frac{1}{2} \frac{\left\langle \frac{\partial_{p_k} \Psi_{W'}(B)}{\Phi(B)} \right\rangle_\Phi^*}{\left\langle \frac{\Psi_{W'}(B)}{\Phi(B)} \right\rangle_\Phi^*}$$

Which is not consistent with the result in the original paper, that is

$$\partial_{p_k} L(\Psi_{\mathcal{W}'}) = \langle \mathcal{O}_k^*(\mathcal{B}) \rangle_\Psi - \frac{\left\langle \frac{\Phi(\mathcal{B})}{\Psi(\mathcal{B})} \mathcal{O}_k^*(\mathcal{B}) \right\rangle_\Psi}{\left\langle \frac{\Phi(\mathcal{B})}{\Psi(\mathcal{B})} \right\rangle_\Psi}, \quad (\text{B3})$$

Possible solution

Maybe we should turn into loss function as

$$L(W') = \frac{\langle \Psi_{W'} | \Phi \rangle}{\langle \Psi_{W'} | \Psi_{W'} \rangle} \sqrt{\langle \Psi_{W'} | \Psi_{W'} \rangle}$$

and this time the derivative should give us expectation only depends on distribution $\Psi_{W'}$

Appendix: Result in original paper

$$\begin{aligned} \text{O}(\mathcal{W}') &= \sqrt{\frac{|\langle \Psi_{\mathcal{W}'} | \Phi \rangle|^2}{\langle \Psi_{\mathcal{W}'} | \Psi_{\mathcal{W}'} \rangle \langle \Phi | \Phi \rangle}} \\ &= \sqrt{\left\langle \frac{\Phi(\mathcal{B})}{\Psi_{\mathcal{W}'}(\mathcal{B})} \right\rangle_\Psi \left\langle \frac{\Psi_{\mathcal{W}'}(\mathcal{B})}{\Phi(\mathcal{B})} \right\rangle_\Phi^*}, \end{aligned} \quad (\text{B1})$$

$$L(\mathcal{W}') = -\log \text{O}(\mathcal{W}'), \quad (\text{B2})$$

$$\partial_{p_k} L(\Psi_{\mathcal{W}'}) = \langle \mathcal{O}_k^\star(\mathcal{B}) \rangle_\Psi - \frac{\left\langle \frac{\Phi(\mathcal{B})}{\Psi(\mathcal{B})} \mathcal{O}_k^\star(\mathcal{B}) \right\rangle_\Psi}{\left\langle \frac{\Phi(\mathcal{B})}{\Psi(\mathcal{B})} \right\rangle_\Psi}, \quad (\text{B3})$$

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