frontiers

Supplementary Material

1 PARAMETER SHIFT RULE

The parameter shift rule (Romero et al., 2018; Mitarai et al., 2018; Schuld et al., 2019) is commonly used to update the parameters of VQA. We consider a single-parameterized unitary $U(\theta_i) = e^{-i\frac{\theta_i}{2}B}$, where B is an idempotent Hermitian operator satisfying $B^2 = I$. The derivative of the unitary $U(\theta_i)$ is given by $\frac{\partial U(\theta_i)}{\partial \theta_i} = -iU(\theta_i)B/2$, and its conjugate is $\frac{\partial U^\dagger(\theta_i)}{\partial \theta_i} = iBU^\dagger(\theta_i)/2$. For any operator ρ, we have

$$\begin{aligned}\frac{\partial U(\theta_i)\rho U^\dagger(\theta_i)}{\partial \theta_i} &= \frac{\partial U(\theta_i)}{\partial \theta_i}\rho U^\dagger(\theta_i) + U(\theta_i)\rho\frac{\partial U^\dagger(\theta_i)}{\partial \theta_i} \\ &= -iU(\theta_i)B\rho U^\dagger(\theta_i)/2 + iU(\theta_i)\rho B U^\dagger(\theta_i)/2 \\ &= U(\theta_i)(-iB\rho + i\rho B)U^\dagger(\theta_i)/2.\end{aligned} \tag{S1}$$

As $U(\theta_i) = \cos(\theta_i/2)I - i\sin(\theta_i/2)B$, we have

$$\begin{aligned}-iB\rho + i\rho B &= (I - iB)\rho(I + iB)/2 - (I + iB)\rho(I - iB)/2 \\ &= e^{-i\frac{\pi}{4}B}\rho e^{i\frac{\pi}{4}B} - e^{i\frac{\pi}{4}B}\rho e^{-i\frac{\pi}{4}B} \\ &= U(\frac{\pi}{2})\rho U^\dagger(\frac{\pi}{2}) - U(-\frac{\pi}{2})\rho U^\dagger(-\frac{\pi}{2}).\end{aligned} \tag{S2}$$

Thus,

$$\frac{\partial U(\theta_i)\rho U^\dagger(\theta_i)}{\partial \theta_i} = \frac{U(\theta_i + \frac{\pi}{2})\rho U^\dagger(\theta_i + \frac{\pi}{2}) - U(\theta_i - \frac{\pi}{2})\rho U^\dagger(\theta_i - \frac{\pi}{2})}{2}. \tag{S3}$$

For any observable O, the derivative of the expectation value $\mathrm{tr}\left[U(\theta_i)\rho U^\dagger(\theta_i)O\right]$ is given by

$$\frac{\partial \mathrm{tr}\left[U(\theta_i)\rho U^\dagger(\theta_i)O\right]}{\partial \theta_i} = \frac{\mathrm{tr}\left[U(\theta_i + \frac{\pi}{2})\rho U^\dagger(\theta_i + \frac{\pi}{2})O\right] - \mathrm{tr}\left[U(\theta_i - \frac{\pi}{2})\rho U^\dagger(\theta_i - \frac{\pi}{2})O\right]}{2}. \tag{S4}$$

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