Part IV

quantum optimization problems

quantum optimization problem

Never, never, never, never, never give up.

Strings 2003, Tokyo
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quantum objective function

gradient-based algorithms

quantum objective function

$$f(\theta; A) = \mathrm{tr}\left(\rho(\theta)A\right)$$

conventionally

$$\rho(\theta) = U(\theta)\rho_0 U(\theta)^\dagger = \mathtt{exp}(\mathrm{ad}(X(\theta)))\rho_0$$

where

$$\mathrm{ad}(X(\theta))\rho_0 = \left[X(\theta), \rho_0\right].$$

quantum optimization problem

$$\min_{\theta} f(\theta; A).$$

quantum objective function

gradient-based algorithms

gradient of quantum objective functions

Let

$$\begin{aligned} U(\theta) &= U(\theta_1)U(\theta_2)\ldots U(\theta_n) \\ &= \mathtt{exp}(\theta_1 X_1)\,\mathtt{exp}(\theta_2 X_2)\ldots \mathtt{exp}\left(\theta_n X_n\right). \end{aligned}$$

then

$$\mathtt{exp}(\mathrm{ad}X(\theta)) = \mathtt{exp}(\theta_1 \mathrm{ad}X_1)\,\mathtt{exp}(\theta_2 \mathrm{ad}X_2)\ldots \mathtt{exp}(\theta_n \mathrm{ad}X_n).$$

gradient of quantum objective function

$$\frac{\partial f(\theta; A)}{\partial \theta_i} = \mathrm{tr}\left(A \,\mathtt{exp}(\theta_1 \mathrm{ad} X_1)\, \mathtt{exp}(\theta_2 \mathrm{ad} X_2) \ldots \mathtt{exp}(\theta_i \mathrm{ad} X_i)\, [X_i, \rho_i]\right)$$

where

$$\rho_i = \mathtt{exp}(\theta_{i+1} \mathrm{ad} X_{i+1})\, \mathtt{exp}(\theta_{i+2} \mathrm{ad} X_{i+2}) \ldots \mathtt{exp}(\theta_n \mathrm{ad} X_n) \rho_0.$$

parameter-shift rule

Quaternions $(\mathbf{1}, \mathbf{i}, \mathbf{j}, \mathbf{k})$:

$$\begin{array}{c|cccc} & \mathbf{1} & \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \hline \mathbf{1} & \mathbf{1} & \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \mathbf{i} & \mathbf{i} & -\mathbf{1} & \mathbf{k} & -\mathbf{j} \\ \mathbf{j} & \mathbf{j} & -\mathbf{k} & -\mathbf{1} & \mathbf{i} \\ \mathbf{k} & \mathbf{k} & \mathbf{j} & -\mathbf{i} & -\mathbf{1} \end{array} . \tag{1}$$

Sigma algebra $\sigma_a = \left(-\frac{i}{2}\mathbf{1}, \frac{1}{2}\mathbf{i}, \frac{1}{2}\mathbf{j}, \frac{1}{2}\mathbf{k}\right)$

$$\left[\sigma_i, \sigma_j\right] = \sum_{k=1}^{3} \epsilon_{ijk}\sigma_k, \quad i, j = 1, 2, 3.$$

sigma strings

$$\sigma_{a_1 a_2 \ldots a_n} = 2i\sigma_{a_1} \otimes \sigma_{a_2 a_3 \ldots \sigma_{a_n}}$$

we have

$$\exp(\theta \operatorname{ad} \sigma_A) = \cos\theta \mathbf{1} + \sin\theta \operatorname{ad} \sigma_A$$
$$\rightarrow \operatorname{ad} \sigma_A = \exp\left(\frac{\pi}{2} \operatorname{ad} \sigma_A\right)$$

parameter-shift rule

$$\frac{\partial f(\theta; A)}{\partial \theta_i} = \mathrm{tr}\left(A \,\mathtt{exp}(\theta_1 \mathrm{ad} X_1)\,\mathtt{exp}(\theta_2 \mathrm{ad} X_2) \ldots \mathtt{exp}(\theta_i \mathrm{ad} X_i)\,[X_i, \rho_i]\right)$$

$$= \mathrm{tr}\left(A \,\mathtt{exp}(\theta_1 \mathrm{ad} X_1)\,\mathtt{exp}(\theta_2 \mathrm{ad} X_2) \ldots \mathtt{exp}\left(\left(\theta_i + \frac{\pi}{2}\right) \mathrm{ad} X_i\right) \rho_i\right).$$

quantum optimization problem: discussion

- What are we doing? Optimization or quantum computing?
- Is the gradient-based algorithm suitable for our purpose?
- How do we initialize parameters?
- Do we have any barrier-method for a quantum ansatz?