Tensor networks based quantum optimization algorithm

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In this work, we propose a quantum realization for power iterations–a well known classical optimization algorithm. Considering low-rank tensor network representations, such as Matrix Product Operators (MPO) for arbitrary matrices, we provide a systematic approach by which one can perform power iterations on a quantum computer. Specifically, our methodology involves variaitonally tuning an MPO ansatz; wherein the indexed matrices (or tensor cores) are constrained to be unitary, to approximate a given target MPO. Such unitary MPOs can easily be implemented as a quantum circuit with the addition of ancillary qubits. Thereafter, with appropriate initialization and post-selection on the ancillary space, we realize a single iteration (and any subsequent iterations) of the classical algorithm on a quantum computer. Our approach therefore features a run-time advantage when compared to tensor network variants of power iterations. Moreover, by exploiting Riemannian optimization and cross-approximation techniques, our methodology becomes instance agnostic and thus allows for addressing black-box optimization within the framework of quantum computing.

Background: Consider the following setting, let $f(x)$ represent some real-valued function we wish to maximize over an input domain, $x \in [a,b]$. Given access to n qubits, one can exploit 2^n discretization points to amplitude encode $f(x)$ into a quantum state, $|f\rangle = \sum_{k=0}^{2^n-1} f(x_k)\,|k\rangle$. Here x_k represents discetized inputs and $\{|k\rangle\}_{k=0}^{2^n-1}$ is the computational basis. The optimization problem now becomes, $\max_k f(x_k) \equiv \max_k p_k$, where $p_k = |\langle k|f\rangle|^2$ are the measurement probabilities of state $|f\rangle$ with respect to projections onto the computational basis. Therefore, if one could prepare such a state, measuring it would allow for recovering a candidate optima. Power iterations simply improve on this idea by considering powers of $f(x)$ via:

$$\left|f^{(j+1)}\right\rangle = \frac{\mathrm{H}^j\,|f\rangle}{\|\mathrm{H}^j\,|f\rangle\|}, \tag{1}$$

where, $\mathrm{H} = \sum_{k=0}^{2^n-1} f(x_k)\,|k\rangle\langle k|$ and $\|\cdot\|$ is the 2-norm. Ideally, as $j \to \infty$, the resultant state becomes $|k^*\rangle$, where $k^* = \arg\max_k p_k$, is the optimum.

Quantum Power Iterations: In order to prepare $|f\rangle$ and subsequently the powers: $\left|f^{(j)}\right\rangle$, on a quantum computer, we start by considering a r-rank MPO representation for the diagonal matrix H as in Eq. (1):

$$\mathrm{H}_{\mathrm{mpo}} = \sum_{\boldsymbol{K}} \left[{A^{(1)}}_{k_1} {A^{(2)}}_{k_2} \cdots {A^{(n)}}_{k_n} \right] |\boldsymbol{K}\rangle\langle\boldsymbol{K}|\,. \tag{2}$$

Here, $\max_j \ \mathrm{rank}\left({A^{(j)}}_{k_j}\right) \leq r$. Such representations can be obtained efficiently by employing matrix cross-approximation techniques. Next, we approximate this target MPO via a unitary MPO of ranks $R \geq r$. To do this, we consider the following variational minimization:

$$(c^*, \mathrm{U}_{\mathrm{mpo}}) \in \arg\min_{\substack{c\in\mathbb{R}\\ \mathrm{U}\in\boldsymbol{\Omega}}} \left\| c\cdot\tilde{\mathrm{U}} - \mathrm{H}_{\mathrm{mpo}} \right\|_F^2, \tag{3}$$

where $\boldsymbol{\Omega}$ is the space of MPOs for which the indexed matrices (as in Eq. (2)), satisfy unitarity. This optimal $\mathrm{U}_{\mathrm{mpo}}$ can straightforwardly be implemented as a quantum circuit with $\log(R)$ ancillary qubits. With the input state, $\left(|0\rangle^{\otimes \log(R)} \otimes |+\rangle^{\otimes n}\right)$, and performing post-selection, one can prepare $|f\rangle$. Subsequent powers can then be addressed by simply concatenating multiple circuit blocks. In Fig. 1, we perform a noiseless simulation of our approach to recover the function landscape for the two-dimensional Rosenbrock function.

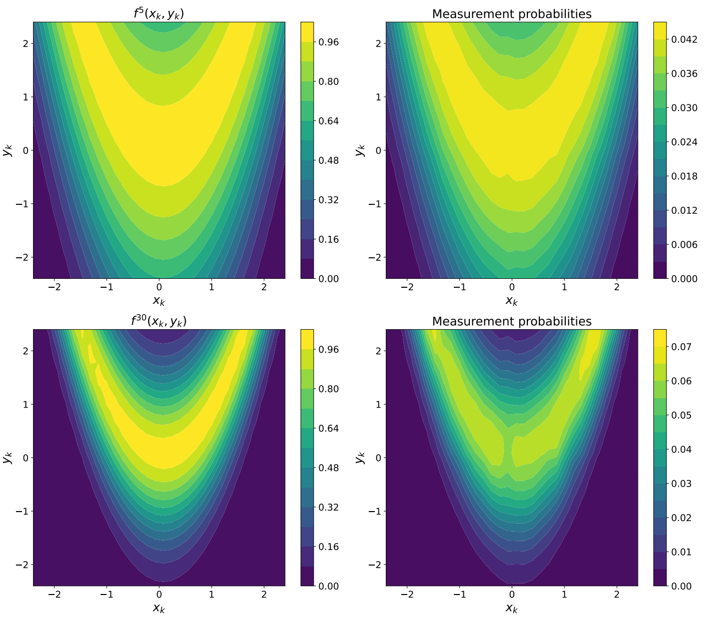

Figure 1: Quantum power iterations for the two-dimensional Rosenbrock function. The left panels indicate the powers of the exact function, $f^j(x_k, y_k)$, $j \in \{5, 30\}$, and the right panels indicate the measurement probabilities obtained via simulations. With increasing powers, we observe that the banana valley is faithfully reproduced.