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On the Complexity of Eigenvalue Approximation

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We deal with the complexity of approximating the smallest eigenvalue of a Sturm-Liouville eigenvalue problem, i.e., the ground state eigenvalue of the time-independent Schrödinger equation for a many-particle system. In particular, we consider the eigenvalue problem $-\Delta u + qu = \lambda u$ on the d-dimensional unit cube with a Dirichlet boundary condition, and we assume that q and its partial derivatives are continuous and uniformly bounded. We are interested in the potential power of quantum over classical computation, and we study the complexity of classical and quantum algorithms approximating the smallest eigenvalue with respect to their accuracy ε.

In the classical worst case we obtain the optimal algorithm by discretizing the differential operator on a grid of size ε^{-1} and then solving the corresponding matrix eigenvalue problem. The worst case complexity is $\Theta(\varepsilon^{-d})$. We remark that we obtain the complexity lower bound by reducing the eigenvalue problem to high-dimensional integration. For this, we use a perturbation formula.

The complexity lower bounds for classical randomized algorithms are also obtained from high-dimensional integration. Namely, the randomized complexity is $\Omega(\varepsilon^{-2d/(d+2)})$. We show an algorithm that uses $O(\varepsilon^{-\max(2/3,d/2)})$ evaluations of q plus $O(\varepsilon^{-d}\log\varepsilon^{-1})$ arithmetic operations. This algorithm is optimal only when $d \leq 2$. Determining the randomized complexity for $d > 2$ and determining whether the randomized complexity is an exponential function of d are important open questions.

Similarly, we show that the quantum complexity is $\Omega(\varepsilon^{-d/(d+1)})$. For $d = 1$, using the perturbation formula mentioned above and the amplitude amplification algorithm, we derive an algorithm for the eigenvalue problem that uses $O(\varepsilon^{-1/2})$ quantum queries, which is optimal.

For general d, the complexity is not known exactly. We only have the upper bound $O(\varepsilon^{-p})$ with $p \leq 6$ (modulo polylog factors). The best quantum algorithm known is based on phase estimation. In particular, we apply phase estimation to the matrix $e^{i\gamma M_\varepsilon}$, where M_ε is the matrix obtained from the problem discretization as in the classical worst case. The parameter γ is chosen appropriately so that the resulting phase belongs to $[0, 2\pi)$. We use a splitting formula to approximate the necessary powers of the matrix exponential. The largest eigenvalue of the matrix is $O(\varepsilon^{-2})$, which implies that the resulting number of queries does not grow exponentially with d. Finally, we address the efficient preparation of the initial state of the algorithm.

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