Analysis of the extended hitting time and its properties

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1 Introduction

Quantum walks are quantum mechanical analogues of classical random walks or Markov chains [Amb03]. Many quantum algorithms based on the quantum walk concept have been discovered [Amb07, MSS07, BS06, MN07, AA05, CCD⁺03, Sze04]. In many cases the quantum walks are used as a tool for search.

Krovi, Magniez, Ozols and Roland in [KMOR10] studies the spatial search problem by means of quantum walks. The spatial search problem is modelled by an undirected graph G = (X, E); the set of marked vertices is denoted by M. Classically a simple way to find a marked vertex is to repeatedly apply a random walk P on G until a marked vertex is reached. The *classical hitting time* – the expected number of steps it takes for this algorithm to find a marked vertex, starting from a stationary distribution of P – is denoted by HT(P, M).

The concept of the hitting time has been generalized to the quantum case [AKR05, Kem05, Sze04, KB06, MNRS11, MNRS12], usually yielding a quadratic improvement over the classical algorithms. However, as it is pointed out in [KMOR10], these results impose serious restrictions: for being able to find a marked vertex the Markov chain *P* has to be reversible, state-transitive, and with a unique marked vertex [MNRS12, Tul08].

The authors of [KMOR10] provide a quantum algorithm for finding a marked element for any reversible and ergodic Markov chain P. The algorithm is based on modifying the original walk P to an interpolated walk P(s) and constructing a quantum analogue of the modified walk. Their technique allows to achieve quadratic improvement over the classical algorithm for all reversible, ergodic Markov chains in case of a single marked element.

In 2014 the authors of [KMOR10] published an update [KMOR14] of their preliminary paper, clarifying that the complexity of their quantum algorithm is characterized by the quantity $HT^+(P, M)$ (called the *extended hitting time*), i.e., the algorithm finds a marked vertex with large probability in $O\left(\sqrt{HT^+(P, M)}\right)$ steps.

It follows from the definition of the extended hitting time that in case of a single marked vertex equality $HT^+(P, M) = HT(P, M)$ holds, but in general $HT^+(P, M) \ge HT(P, M)$. There is a simple example of P and M in [KMOR14] such that $HT^+(P, M) = 5$, whereas HT(P, M) = 4. Hence the case of multiple marked elements remains open.

Due to the possible gap between the extended hitting time and the classical hitting time, a question arises whether the algorithm by Krovi et al can achieve quadratic speed-up over the classical algorithm. We try to approach this problem by studying the extended hitting time and comparing it to its classical counterpart. We establish that even in case of three vertices, two of them being marked, the ratio $\frac{HT^+(P,M)}{HT(P,M)}$ can be arbitrarily large.

However, we note that a large gap between the hitting times implies that P is 'close to non-ergodic', in the sense its spectral gap, a common measure of ergodicity, is 'small',

thus leading to our main result: the ratio $\frac{HT^+(P,M)}{HT(P,M)}$ is upper bounded by the reciprocal of the spectral gap of P.

2 Summary of results

We show that the ratio $\frac{HT^+(P,M)}{HT(P,M)}$ can be arbitrarily large, namely, there exists a sequence of Markov chains $\{P_n\}_{n\in\mathbb{N}}$ and appropriated marked sets $\{M_n\}_{n\in\mathbb{N}}$ such that

$$\lim_{n \to +\infty} \frac{HT^+(P_n, M_n)}{HT(P_n, M_n)} = +\infty.$$

Our main result is that the extended hitting time is upper-bounded in terms of the classical hitting time and the spectral gap of the transition matrix of the original Markov chain. Recall that P is ergodic and reversible Markov chain. The transition matrix of such chain has real eigenvalues, the largest eigenvalue is 1 and the remaining eigenvalues are strictly smaller than 1 in absolute value; without loss of generality it can be assumed that the eigenvalues are positive. Under these assumptions the following inequality holds:

$$HT^{+}(P,M) \le \frac{HT(P,M)}{1-\lambda_{n-1}},$$
 (1)

where λ_{n-1} is the second largest eigenvalue of P. In particular, this implies that in case of the spectral gap of P being lower-bounded by a constant, the algorithm by Krovi et al does achieve quadratic improvement over the classical algorithm.

Unlike its classical counterpart, the extended hitting time has an interesting property which relates the extended hitting time for the set M being marked with the extended hitting time for its complement, $U = X \setminus M$ being marked:

$$HT^{+}(P, M) \cdot p_{M} = HT^{+}(P, U) \cdot (1 - p_{M}),$$
(2)

where p_M is the probability of drawing a marked vertex from the stationary distribution. This equation shows how the extended hitting time changes when the marked and unmarked vertices swap their roles: all the vertices in M are unmarked and all the vertices in U are marked.

Next we consider an important special case when the graph G is the 2D-grid of size $\sqrt{n} \times \sqrt{n}$ with periodic boundary conditions and self-loops; then G is a 5-regular graph. The Markov chain P_n is chosen so that at any vertex the probability to move to any of its four neighbours is 0.2 and the probability of staying at the same vertex is also 0.2.

For the 2D-grid we show the existence of sets M_n such that $HT^+(P_n, M_n) = \Theta(n)$, whereas $HT(P_n, M_n) = \Theta(1)$. We also provide an example of sets M'_n satisfying

$$HT^+(P_n, M'_n) = \Omega(n), \quad HT(P_n, M'_n) = \Theta(\sqrt{n}\log n), \quad p_{M'_n} = \frac{|M'_n|}{n} = o(1).$$

These results imply that the gap between the hitting times can be large also in the case when G is the 2D-grid.

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