Quantum sampling in Markov chains

Dante Bencivenga, Xining Chen and Peter Høyer

Department of Computer Science
University of Calgary
AB, Canada

We consider the problem of sampling from a target distribution $\vec{\tau}$ in a Markov chain P. The random walk starts in a state drawn from the stationary distribution $\vec{\pi}$ of P, walks according to P, and eventually stops once some predefined conditions are satisfied. We want the walk to stop in a state drawn from the target distribution $\vec{\tau}$. If the predefined conditions ensure that the final state is drawn from $\vec{\tau}$, the conditions are called a *stopping rule* from $\vec{\pi}$ to $\vec{\tau}$ [Pit77, LW95]. The minimum expected number of steps required by any stopping rule from $\vec{\pi}$ to $\vec{\tau}$ is called the *access time* from $\vec{\pi}$ to $\vec{\tau}$ in P.

The access time is related to, but distinct from, the hitting time. The access time is a measure of the cost of sampling from a target distribution $\vec{\tau}$, whereas the hitting time is a measure of the cost of sampling from a marked subset $\mathcal{M}$.

The access time is computed with respect to a given Markov chain P. Related, but distinct, sampling problems are where the Markov chain is constructed as part of the algorithm, as in e.g. the Metropolis algorithm [MRR+53, TOV+11, YA12]. Related, but also distinct, sampling problems are where the input is an oracle providing samples from one distribution, and the aim is to generate a sample from another distribution. Such re-sampling problems can be solved quantumly by rejection sampling [ORR13].

The goal of this work is to give a quantum algorithm for sampling from a target distribution $\vec{\tau}$ in a Markov chain P in a number steps that is quadratically smaller than the optimal random walk.

Our two main results are two quantum algorithms. Both algorithms produce a quantum state that approximates the quantum state $|\tau\rangle = \sum_i \sqrt{\tau_i}$ corresponding to the target distribution $\vec{\tau} = (\tau_1, \ldots, \tau_N)$. Here N is the size of the state space of the random walk. Our first quantum algorithm starts in the quantum state $\sum_i \sqrt{\pi_i}|i\rangle$ and uses quadratically fewer steps than the access time from $\vec{\pi}$ to $\vec{\tau}$. Our second quantum algorithm takes as input a marked subset $\mathcal{M}$ and a target distribution $\vec{\tau}$ that is non-zero only on states in $\mathcal{M}$. The algorithm starts in the normalized quantum state corresponding to the states that are not marked, and it also achieves a quadratic speed-up. Our two quantum algorithms are the first general algorithms for sampling quadratically faster from all target distributions in all reversible Markov chains from the stationary distribution.

Our algorithms are based on quantum walks [Sze04, Amb04]. Quantum walks have been studied intensively and led to rich and powerful algorithmic techniques, such as those in [Sze04, Amb04, AKR05, MNRS11, Bel13, BCJ+13, KMOR16, DH17, AS19, AGJK20, AGJ19] and found a myriad of applications such as those in [Amb04, Amb07, BDH+05, MSS07, LG14, LGN15, Mon18]. We introduce and use generalizations of controlled quantum walks [DH17].

The proofs of our quantum walks use a new analytical idea. Associated to any stopping rule is a real-valued non-negative vector $\vec{x}$ called the *exit frequencies* and whose entries equal the expected number of times we exit each state before stopping. We introduce a quantum analogue $|x\rangle$ of the exit frequencies $\vec{x}$, and we use $|x\rangle$ to analyze the behavior and complexity of our quantum walks. We believe that our analytical approach yields simple, transparent and natural proofs, and that our approach has the potential of both simplifying other existing proofs as well as leading to new results.

Our proofs also use and generalize a proof idea used in [DH17]. Given a controlled quantum walk, we construct a related quantum circuit and then prove that the complexity of the original quantum walk can be expressed in terms of the principal eigenvector of this related circuit. We then prove that this principal eigenvector can be expressed in terms of the quantum state $|x\rangle$, which we then relate to the exit frequencies of a stopping rule, permitting us to derive a quadratic speed up over the access time.

We give applications of our quantum walk and our analytical approach. We give a new quantum algorithm for the resampling problem. We prove that controlled quantum walks can emulate quantum walks derived from random walks with self-loops. We give an explicit and exact expression of the hitting time as an access time. We give an explicit and exact expression of the extended hitting time as an access time. We propose self-loops as a potential alternative to stopping rules in random walks.

Our main result is the first known quantum algorithm for generating any desired distribution over states in a Markov chain using quadratically fewer steps than the optimal random walk starting from the stationary distribution.

References

[AGJ19] Simon Apers, András Gilyén, and Stacey Jeffery. A unified framework of quantum walk search, 2019. `arXiv:1912.04233`.

[AGJK20] Andris Ambainis, András Gilyén, Stacey Jeffery, and Martins Kokainis. Quadratic speedup for finding marked vertices by quantum walks. In *Proceedings of the 52nd Annual ACM SIGACT Symposium on Theory of Computing*, STOC'20, pages 412–424, 2020. `doi:10.1145/3357713.3384252`.

[AKR05] Andris Ambainis, Julia Kempe, and Alexander Rivosh. Coins make quantum walks faster. In *Proceedings of the 16th Annual ACM-SIAM Symposium on Discrete Algorithms*, SODA'05, pages 1099–1108, 2005. URL: `http://dl.acm.org/citation.cfm?id=1070432.1070590`, `arXiv:quant-ph/0402107`.

[Amb04] Andris Ambainis. Quantum walk algorithm for element distinctness. In *Proceedings of the 45th IEEE Symposium on Foundations of Computer Science*, FOCS'04, pages 22–31, 2004. `arXiv:quant-ph/0311001`, `doi:10.1109/FOCS.2004.54`.

[Amb07] Andris Ambainis. Quantum walk algorithm for element distinctness. *SIAM Journal on Computing*, 37(1):210–239, 2007. `arXiv:quant-ph/0311001`, `doi:10.1137/S0097539705447311`.

[AS19] Simon Apers and Alain Sarlette. Quantum fast-forwarding: Markov chains and graph property testing. *Quantum Information & Computation*, 19(3–4):181–213, March 2019. `doi:10.26421/QIC19.3-4`.

[BCJ+13] Aleksandrs Belovs, Andrew M. Childs, Stacey Jeffery, Robin Kothari, and Frédéric Magniez. Time-efficient quantum walks for 3-distinctness. In *Proceedings of the 40th International Colloquium on Automata, Languages, and Programming*, ICALP'13, pages 105–122, 2013. `arXiv:1302.7316`, `doi:10.1007/978-3-642-39206-1_10`.

[BDH+05] Harry Buhrman, Christoph Dürr, Mark Heiligman, Peter Høyer, Frédéric Magniez, Miklos Santha, and Ronald de Wolf. Quantum algorithms for element distinctness. *SIAM Journal on Computing*, 34(6):1324–1330, 2005. `arXiv:quant-ph/0007016`, `doi:10.1137/S0097539702402780`.

[Bel13] Aleksandrs Belovs. Quantum walks and electric networks, 2013. `arXiv:1302.3143`.

[DH17] Cătălin Dohotaru and Peter Høyer. Controlled quantum amplification. In *Proceedings of the 44th International Colloquium on Automata, Languages, and Programming*, volume 80 of *ICALP'17*, pages 18:1–18:13, Dagstuhl, Germany, July 2017. Schloss Dagstuhl–Leibniz-Zentrum für Informatik. `doi:10.4230/LIPIcs.ICALP.2017.18`.

[KMOR16] Hari Krovi, Frédéric Magniez, Māris Ozols, and Jérémie Roland. Quantum walks can find a marked element on any graph. *Algorithmica*, 74(2):851–907, 2016. `arXiv:1002.2419`, `doi:10.1007/s00453-015-9979-8`.

[LG14] François Le Gall. Improved quantum algorithm for triangle finding via combinatorial arguments. In *Proceedings of the 55th IEEE Symposium on Foundations of Computer Science*, FOCS'14, pages 216–225, 2014. `arXiv:1407.0085`, `doi:10.1109/FOCS.2014.31`.

[LGN15] François Le Gall and Shogo Nakajima. *Quantum algorithm for triangle finding in sparse graphs*, volume 9472 of *Lecture Notes in Computer Science*, pages 590–600. Springer Berlin Heidelberg, 2015. arXiv:1507.06878, doi:10.1007/978-3-662-48971-0_50.

[LW95] László Lovász and Peter Winkler. Efficient stopping rules for Markov chains. In *Proceedings of the 27th Annual ACM Symposium on Theory of Computing*, STOC'95, pages 76–82, New York, NY, USA, June 1995. Association for Computing Machinery (ACM). doi:10.1145/225058.225086.

[MNRS11] Frédéric Magniez, Ashwin Nayak, Jérémie Roland, and Miklos Santha. Search via quantum walk. *SIAM Journal on Computing*, 40(1):142–164, 2011. arXiv:quant-ph/0608026, doi:10.1137/090745854.

[Mon18] Ashley Montanaro. Quantum-walk speedup of backtracking algorithms. *Theory of Computing*, 14(15):1–24, 2018. URL: http://www.theoryofcomputing.org/articles/v014a015, doi:10.4086/toc.2018.v014a015.

[MRR+53] Nicholas Metropolis, Arianna W. Rosenbluth, Marshall N. Rosenbluth, Augusta H. Teller, and Edward Teller. Equation of state calculations by fast computing machines. *Journal of Chemical Physics*, 21(6):1087–1092, 1953.

[MSS07] Frédéric Magniez, Miklos Santha, and Mario Szegedy. Quantum algorithms for the triangle problem. *SIAM Journal on Computing*, 37(2):413–424, 2007. arXiv:quant-ph/0310134, doi:10.1137/050643684.

[ORR13] Māris Ozols, Martin Rötteler, and Jérémie Roland. Quantum rejection sampling. *ACM Transactions on Computation Theory*, 5(3):11:1–33, August 2013. doi:10.1145/2493252.2493256.

[Pit77] Jim W. Pitman. Occupation measures for Markov chains. *Advances in Applied Probability*, 9(1):69–86, 1977. doi:10.2307/1425817.

[Sze04] Mario Szegedy. Quantum speed-up of Markov chain based algorithms. In *Proceedings of the 45th IEEE Symposium on Foundations of Computer Science*, FOCS'04, pages 32–41, 2004. doi:10.1109/FOCS.2004.53.

[TOV+11] Kristan Temme, Tobias J. Osborne, Karl G. Vollbrecht, David Poulin, and Frank Verstraete. Quantum Metropolis sampling. *Nature*, 471(7336):87–90, March 2011. doi:10.1038/nature09770.

[YA12] Man-Hong Yung and Alán Aspuru-Guzik. A quantum–quantum Metropolis algorithm. *Proceedings of the National Academy of Sciences*, 109(3):754–759, 2012. doi:10.1073/pnas.1111758109.