The birthday problem and Markov chain Monte Carlo

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Abstract

We study the problem of generating a sample from the stationary distribution of a Markov chain, given a method to simulate the chain. We give an approximation algorithm for the case of a random walk on a regular graph with n vertices that runs in expected time $O^*(\sqrt{n} \tau_{\text{mix}})$, where $\tau_{\text{mix}}$ is the mixing time of the chain in $L^2$. This is close to the best possible, since $\sqrt{n}$ is a lower bound on the worst-case expected running time of any algorithm.

Keywords: randomized algorithms, Markov chain

1 Introduction

Often the only feasible method for sampling from a complex distribution is to simulate a suitably chosen Markov chain for sufficiently many steps. Procedures based on this idea, called Markov chain Monte Carlo, have been applied to a number of problems such as approximating the permanent [7], computing volumes [8] and integrals [9], and approximate counting [10]. In order to find out how many steps one needs to simulate the chain, it is necessary to determine the mixing time, i.e., the number of steps necessary to bring the distribution close to stationary. This analysis is often complex and has to be tailored to the specific type of Markov chain under consideration.

Another, related line of research has been pursued (see [12] for background and see also [3, 11]): the Markov chain is generic, its transition probabilities are not known, and the algorithm is given a procedure to generate the next state of the chain based on the current state. Since the chain is arbitrary, the algorithm cannot have any advanced knowledge of the mixing time. Aldous [11], comes by time $O(\tau \text{Poly}(1/\epsilon))$ to within $\epsilon$ from the stationary distribution in total variation. This was improved by the “cycle popping” algorithm invented by Propp and Wilson [12], which runs in expected time $O(\tau)$, where $\tau$ is the mean hitting time (expected number of steps the chain takes to get from $X$ to $Y$ if $X$ and $Y$ are chosen independently according to the stationary distribution). In [11] a random stopping rule for exact sampling from an unknown Markov chain is given where the expected number of steps is $6\tau^4$. It is easy to see that any algorithm for an arbitrary $n$-state chain must have running time at least $n$: the algorithm must visit every state, since an unvisited state $x$ could potentially have a holding probability $p(x, x)$ very close to 1 and hence a very high stationary probability. In this note, we show that if the chain is a random walk on a regular graph then

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there is an approximation algorithm whose running time can be much less. Our algorithm runs in expected time $O^*(\sqrt{n\tau_{mix}})$, where $\tau_{mix}$ is the $L^2$ mixing time of the chain; this can be much smaller than $n$. We note that our algorithm produces a sample with some error (i.e., the distribution is not exactly stationary, although it can be made arbitrarily close), whereas the algorithms described in [12, 11, 3] produce an exact sample. In a somewhat similar spirit of observing a random walk on an unknown graph, [4] studies what can be learned by knowing polynomially many return times to a fixed vertex of a simple random walk on a regular graph.

Our analysis is based on a variation of the standard birthday problem. Roughly speaking, in a world where there are $n$ possible birthdays, the number of people that you need to pick to be confident that at least two have the same birthday is of the order $\sqrt{n}$. It turns out that in a similar vein, if order $\sqrt{n}$ copies of a Markov chain with uniformly stationary distribution are run for much less than the mixing time then there is likely to be a match, whereas if they are run for much more than the mixing time there is a good chance for no match. (See Section 2 for a precise formulation of this.) This forms the basis for our algorithm. A similar idea was used by Goldreich and Ron [5], as a suggestion for a possible sublinear tester for expansion.

2 Results

2.1 The Problem

The algorithm is given an irreducible, aperiodic $n$ state Markov chain as input. More precisely, the algorithm is given the number of states $n$, a starting state $x_0$, and a procedure $\text{nextstate}()$, which, given a state $x$ of the chain outputs state $y$ which is one step of the chain starting from $x$. The problem is to generate a random state according to the stationary distribution.

We will aim for an $\epsilon$-approximation algorithm, that is, an algorithm that generates a random state within total variation distance $\epsilon$ of the stationary distribution.

2.2 Main Theorem

Let $p^m(\cdot, \cdot)$ be transition probabilities for an irreducible, aperiodic, doubly stochastic $n$-state Markov chain on state space $V$. Let $\mathcal{U}$ denote the uniform distribution over $V$ and for functions $\mu$ on $V$, let $||\mu||_2 = \left(\sum_{x \in V} \frac{1}{n} \mu(x)^2\right)^{1/2}$ denote the norm of $\mu$ in $L^2(\mathcal{U})$. For $\epsilon > 0$, let $\tau(\epsilon) = \min \{n : ||np^n(x_0, \cdot) - 1||_2^2 \leq \epsilon\}$. Denote the mixing time in $L^2$ by

$$\tau_{mix} = \max_g \min\{n : ||np^n(x, \cdot) - 1||_2^2 \leq 1/e\}.$$ 

Our main result is the following theorem.

**Theorem 1** Suppose that the Markov chain is a random walk on a regular, connected graph with degree at most $n$. Then there is an algorithm that returns a sample within total variation distance $\epsilon$ in expected time $O(\sqrt{n\log(n/\epsilon)\tau_{mix}})$.

**Remark:** To obtain a lower bound for the running time, we can consider random walk on the complete graph. If an algorithm simulates the chain for less than order $\sqrt{n}$ steps, it is likely to see only distinct states of the chain, hence it couldn’t “tell the difference” between the chain and random walk on two complete graphs of size $n/2$ joined by a single edge. (Note that in the second
and hence any algorithm needs at least order \( n \sqrt{\tau_{\text{mix}}} \) steps since the mixing time is a constant. We believe that for analogous reasons this would still hold (i.e., any algorithm would need order \( \sqrt{n \tau_{\text{mix}}} \) steps) when the complete graph is replaced by a random \( d \)-regular graph, but it seems harder to prove this.

**Proof:**

The algorithm is as follows. Define \( A_n = n^4 \log(2n/\epsilon) \) and \( l = \lceil 1 + \frac{512 \sqrt{n}}{\epsilon^2} \rceil \). Iterate the following procedure for \( i \in \{1, 2, \ldots \} \) until stopped.

Let \( m = 8 \log(2A_n/\epsilon) \), and perform the following experiment \( m \) times. Simulate \( l \) copies of the Markov chain starting at \( x_0 \) for \( 2^i \) steps, generating \( l \) samples \( X_1, \ldots, X_l \). To avoid the possibility that the Markov chain has an eigenvalue close to \(-1\), we implement a holding probability of \( 1/n \) to each state; i.e., each step we do nothing with probability \( 1/n \), otherwise simulate a step of the chain. This doesn’t change the stationary distribution and ensures that all eigenvalues are at least \(-1 + \frac{2}{n}\). Let \( \delta = \epsilon^2 \). Let

\[
Z = \sum_{k<m} 1(X_k = X_m),
\]

and if \( Z \leq (1 + \delta/2)(\frac{l}{2}) \frac{1}{n} \) then count the experiment as a success; otherwise count it as a failure. If at least \( m/2 \) of the experiments are successful, or if \( i = \lceil \log_2 A_n \rceil \) then stop; otherwise continue with the next value of \( i \).

Let \( i' \) be the value of \( i \) when the above procedure terminates. We claim that with high probability after \( 2^{i'} \) steps the chain is very mixed. Hence the algorithm can run another independent simulation of the chain for \( 2^i \) steps and the result is an almost uniform sample from the state space.

More precisely, let \( \mu(i) = p^2(x_0, \cdot) \). We will show that with probability at least \( 1 - \epsilon/2 \), the value of \( i' \) is large enough so that \( ||n\mu(i') - 1||_2^2 \leq \delta \).

**Analysis of the algorithm.** By a conductance bound (see, e.g., [10]), the spectral gap for the chain must be at least \( 1/n^4 \), and hence \( \tau(\delta/2) \leq n^4 \log(2n/\delta) = A_n \). Thus if \( i' = \lceil \log_2 A_n \rceil \) then \( 2^{i'} \geq A_n \), which implies that \( ||n\mu(i') - 1||_2^2 \leq \delta/2 \).

Next we have to bound the probability that the algorithm stops early on a value of \( i \) such that \( ||n\mu(i) - 1||_2^2 \geq \delta/2 \). Fix \( i < \lceil \log_2 A_n \rceil \) and let \( p_x \) be the probability that the chain is at \( x \) after \( 2^i \) steps. Cauchy-Schwarz gives \( \sum_x p_x^2 \geq 1/n \). It follows that if \( Z \) is defined as in (1) then

\[
\mathbb{E}(Z) = (\frac{l}{2}) \sum_x p_x^2 \geq \frac{1}{n} (\frac{l-1}{2})^2,
\]

and hence

\[
\frac{1}{\mathbb{E}(Z)} \leq \frac{\delta^2}{512}.
\]

We also have

\[
\frac{2 \sqrt{n}}{l} \leq \frac{\delta^2}{512}.
\]

Note that \( \mathbb{E}(Z) = (\frac{l}{2}) \frac{1}{n} (1 + ||n\mu(i) - 1||_2^2) \). Thus if \( ||n\mu(i) - 1||_2^2 \geq \delta/2 \), then \( \mathbb{E}(Z) \geq (\frac{l}{2}) \frac{1}{n} (1 + \delta/2) \) and hence

\[
P\left(Z \leq (\frac{l}{2}) \frac{1}{n} (1 + \delta/2)\right) \leq P\left(Z \leq \mathbb{E}(Z) \left(\frac{1 + \delta/2}{1 + \delta}\right)\right)
\]
The values of the chain are given as 0-1 strings, whose lengths we treat as constant. If we store the Running time. A running time of \( m/\delta \) time.) Summing this over \( i \) shows that the number of steps corresponding to \( i \leq i^* \) is \( O(l 2^i \log(2A_n/\epsilon)) = O(l \tau_{mix}' \log(2A_n/\epsilon)) \). Suppose that \( i \geq i^* \). Then \( 2^i \geq \tau_{mix}' \) and hence \( |\mu(i') - \mathcal{U}|_2 \leq \delta/4 \). Step \( i + 1 \) occurs only if there are more than \( m/2 \) failures in step \( i \). Note that \( E(Z) \leq \left( \frac{l}{2} \right) 1/(1\delta/4) \) and hence

\[
P\left(Z > \left( \frac{l}{2} \right) \frac{1}{n}(1+\delta/2) \right) \leq P\left(Z > E(Z) \left( \frac{1+\delta/2}{1+\delta/4} \right) \right) \leq P\left(Z > E(Z) \left( 1 + \frac{\delta}{8} \right) \right) \leq \frac{\text{var}(Z)}{\left[ \frac{2}{l} \frac{1}{n} \frac{1}{n} \frac{1}{n} \frac{1}{n} \frac{1}{n} \right] E(Z)^2} \leq \frac{64}{\delta^2} \frac{1 + \frac{2\sqrt{\pi}}{l} E(Z)}{E(Z)} \leq \frac{1}{4},
\]

where the third line is Chebyshev’s inequality and the second line uses the fact that \( 1+\delta/2 \geq 1+\delta/8 \) whenever \( \delta \leq 1 \). Thus Hoeffding’s bounds give \( P(\text{stage } i+1 \text{ occurs}) \leq P(\text{more than } m/2 \text{ failures}) \leq e^{-m/8} \leq \epsilon/2A_n \). Since the maximum number of steps in any stage is \( O(A_n l \log(2A_n/\epsilon)) \), summing the above bound over \( i \) gives an \( O(l \log(2A_n/\epsilon)) \) bound. Adding everything up gives a total expected running time of \( O(l \tau_{mix}' \log(2A_n/\epsilon)) = O(l \tau_{mix} \log(n/\epsilon)) \).
Remarks:

- By running $\sqrt{n}$ samples after the mixing time is estimated instead of just one, the algorithm could actually produce $\sqrt{n}$ samples and the expected running time would still be $O^*(\sqrt{n}T_{mix})$.
- The assumption that the degree is at most $n$ can be relaxed; it is only used to get a poly($n$) upper bound for the mixing time (in order to bound $A_n$).
- In [2] it was observed that a non-backtracking random walk mixes (up to a factor two) faster. Thus, in the setting where the algorithm can determine the set of neighbors of a state $x$, one can very slightly reduce the randomness used, as well as the running time, by replacing the simple random walk with a non-backtracking random walk. Also simulating the $l$ copies of the Markov chain at each stage, can of course be done in parallel.

3 Appendix

The following bound on the variance of $Z$ was needed.

**Lemma 2** Let $X$ be a random variable taking values in $\{1, \ldots, n\}$, and let $p_i = P(X = i)$ for $1 \leq i \leq n$. Let $X_1, \ldots, X_l$ be independent copies of $X$ and let $Z = \sum_{i<j} 1(X_i = X_j)$. Then

1. $E(Z) = \binom{l}{2} \sum_i p_i^2$.
2. $\text{var}(Z) \leq E(Z) \left(1 + 2\sqrt{n} E(Z)\right)$.

**Proof:** Part 1 is obvious. For part 2, let $M = \max_i p_i$. Clearly, $\sum_i p_i^2 \geq M^2$, and Cauchy-Schwarz gives $\sum_i p_i^2 \geq \frac{1}{n}$. Hence

$$\sum_i p_i^2 \geq \sqrt{M^2 \cdot \frac{1}{n}} = \frac{M}{\sqrt{n}}.$$ It follows that

$$\sum_i p_i^2 \leq M \sum_i p_i^2 \leq \sqrt{n} \left(\sum_i p_i^2\right)^2.$$ (12)

For $1 \leq i < j \leq n$, let $Z_{i,j} = 1(X_i = X_j)$, so that $Z = \sum_{i<j} Z_{i,j}$. Note that $\text{cov}(Z_{i,j}, Z_{k,l}) = 0$ if $i, j, k, l$ are distinct. Thus,

$$\text{var}(Z) = \text{cov}\left(\sum_{i\neq j} Z_{i,j}, \sum_{i\neq j} Z_{i,j}\right) = \binom{l}{2} \text{cov}(Z_{1,2}, Z_{1,2}) + 2 \binom{l}{3} \text{cov}(Z_{1,2}, Z_{1,3}) \leq \binom{l}{2} E(Z_{1,2}) + 2 \binom{l}{3} E(Z_{1,2} Z_{1,3}) \leq E(Z) + 2 \binom{l}{3} \sum_i p_i^3.$$
Combining this with equation [12] and part 1 of the lemma yields

\[
\text{var}(Z) \leq \mathbb{E}(Z) + \left(\frac{l}{3}\right) \sqrt{n} \left(\sum_i p_i^2\right)^2 = \mathbb{E}(Z) \left(1 + \frac{2\binom{l}{1} \sqrt{n}}{l^2} \mathbb{E}(Z)\right) \leq \mathbb{E}(Z) \left(1 + \frac{2\sqrt{n}}{l} \mathbb{E}(Z)\right),
\]

establishing part 2 of the lemma.

\[\square\]

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References

[1] Aldous, D. On simulating a Markov chain stationary distribution when the transition probabilities are unknown. *Discrete Probability and Algorithms, IMA Volumes in Mathematics and its Applications, 72* Springer-Verlag, (1995), pp. 1–9.

[2] Alon, N. Benjamini, I. Lubetzky, E. and S. Sodin, Non-backtracking random walk mixes faster. Preprint (2006).

[3] Asmussen, S., Glynn, P., and Thorisson, H. Stationary detection in the initial transient problem. *ACM Transactions on Modeling and Computer Simulation. 2* (1992), pp. 130–157.

[4] Benjamini, I. Kozma, G. Lovász , L. Romik, D. and Tardos, G. Waiting for a Bat to Fly By (in Polynomial Time). *Combinatorics, Probability and Computing 15* (2006), pp. 673-683.

[5] Goldreich, O., and Ron, D. On testing expansion in bounded-degree graphs. *ECCC, TR00-020*, (2000).

[6] Jerrum, M. and Sinclair, A. Approximating the permanent. *SIAM Journal on Computing. 18* (1989), pp. 1149–1178.

[7] Jerrum, M., Sinclair, A., and Vigoda, E. A polynomial-time approximation algorithms for the permanent of a matrix with non-negative entries. *Journal of the ACM. 51* (2004), pp. 671–697.

[8] Dyer, M, Frieze, A., and Kannan, R. A random polynomial time algorithm for approximating the volume of convex sets. *Journal of the ACM. 38* (1991), pp. 1–17.

[9] Frieze, A., Kannan, R., and Polson, N. Sampling from log-concave distributions. *Annals of Applied Probability. 4* (1994), pp. 812–837.

[10] Jerrum, M., Valiant, L., and Vazirani, V. Random generation of combinatorial structures from a uniform distribution. *Theoretical Computer Science. 43* (1986), pp.169–188.
[11] Lovász, L. and Winkler, P. Exact mixing in an unknown Markov chain. *Electronic Journal of Combinatorics*. 2 (1995). Paper #R15.

[12] Propp, J. and Wilson, D. How to get a perfectly random sample from a generic Markov chain and generate a random spanning tree of a directed graph. *Journal of Algorithms*. 27 (1998), pp.170–217.