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Faster random generation of linear extensions

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Abstract

This paper examines the problem of sampling (almost) uniformly from the set of linear extensions of a partial order, a classic problem in the theory of approximate sampling. Previous techniques have relied on deep geometric arguments, or have not worked in full generality. Recently, focus has centred on the Karzanov and Khachiyan Markov chain. In this paper, we define a slightly different Markov chain, and present a very simple proof of its rapid mixing, using the method of path coupling. We show that this chain has mixing time $\mathrm{O}(n^3 \log n)$, which significantly improves the previous best bound for this problem, which was a bound of $\mathrm{O}(n^5 \log n)$, for the Karzanov and Khachiyan chain.

We also show how a classical metric, Spearman's footrule, may be reformulated in terms of transpositions.

1. Introduction

Let $N = \{1,2,\ldots,n\}$, and $P = (N, \preccurlyeq)$ be a partial order. A *linear extension* of P is a total order $X = (N, \sqsubseteq)$ which respects P, i.e. for all i, $j \in N$, $i \preccurlyeq j$ implies $i \sqsubseteq j$. Let $\Omega = \Omega(P)$ denote the set of all linear extensions of P.

Being able to sample from Ω has a variety of applications, since various other combinatorial structures exhibit a natural isomorphism to Ω for a particular family of partial orders, e.g. multiset permutations. In addition there are more direct applications to near-optimal sorting, and to decision theory.

There has been much research on the problem of listing all linear extensions; in fact, Pruesse and Ruskey [16] have shown that this may be accomplished in constant amortized time.

Brightwell and Winkler [3] showed that determining $|\Omega|$ is $\#P$-complete. The existence of a fully polynomial randomized approximation scheme (*fpras*) for $|\Omega|$ followed from the work of Dyer et al. [9] on volume approximation. Their method is based on the *rapid mixing* of a particular geometric Markov chain. See Jerrum and Sinclair [12] for a

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recent survey of this approach to approximation problems. Subsequently, Matthews [14] gave a somewhat different geometric approach.

Using geometric and conductance arguments [17], Karzanov and Khachiyan [13] showed the rapid mixing of a *combinatorial* Markov chain on Ω. Dyer and Frieze [8] improved the conductance estimate, and hence the bound on the mixing time, of this chain. These results all rely on a relationship between Ω and the geometry of a certain polytope in $\mathbb{R}^n$.

Felsner and Wernisch [11] showed how the Karzanov–Khachiyan chain may be used to sample exactly from Ω in the very restricted case of two-dimensional partial orders, using the technique of coupling from the past [15].

In this paper, we significantly reduce the generation time for random linear extensions. We achieve this via the first non-geometric proof of rapid mixing of a Markov chain on Ω, employing the method of *path coupling* [4]. We define a new Markov chain on Ω, and show that this has a mixing rate of $O(n^3 \log n\varepsilon^{-1})$, which significantly improves the best bound previously known for this problem (a bound on the Karzanov and Khachiyan chain of $O(n^4 \log |\Omega|\varepsilon^{-1}) = O(n^5 \log n + n^4 \log \varepsilon^{-1})$ [8]). As a consequence, we note that the mixing rate for the Karzanov and Khachiyan chain can, in fact, be reduced to $O(n^4 \log^2 n + n^3 \log n \log \varepsilon^{-1})$.

2. Notation and preliminaries

Let $\sigma(i,j)$ $(1 \leqslant i < j \leqslant n)$ denote the *transposition* operators on total orders of N. Thus, if $Y = \sigma(i,j)X$, we have

$$X = (a_1\, a_2 \cdots a_{i-1}\, a_i \cdots a_j\, a_{j+1} \cdots a_n), \qquad Y = (a_1\, a_2 \cdots a_{i-1}\, a_j \cdots a_i\, a_{j+1} \cdots a_n).$$

If $j = i+1$, we will call $\sigma(i,j)$ a *close* transposition. The integer $(j-i)$ will be called the *width* of the transposition $\sigma(i,j)$. Thus close transpositions have unit width.

For a concave probability distribution, f, on $\{1,2,\ldots,n-1\}$, define the Markov chain $\mathcal{M}_f$, on $\Omega(P)$: if the current state is $X_t \in \Omega$, then the next state, X_{t+1}, is determined by the following experiment.

1. Choose $p \in \{1,2,\ldots,n-1\}$ according to the distribution f, and $c \in \{0,1\}$ uniformly at random.
2. If $c = 0$ or $\sigma(p,p+1)X_t \notin \Omega$, then $X_{t+1} = X_t$. Otherwise $X_{t+1} = \sigma(p,p+1)X_t$.

The symmetry of the transitions implies that the equilibrium distribution, π, is the uniform distribution. We show below, by using the method of path coupling [4], that $\mathcal{M}_f$ is rapidly mixing, i.e. μ_t, the distribution of X_t, 'quickly' approaches π.

When f is the uniform distribution, we shall abbreviate $\mathcal{M}_f$ to $\mathcal{M}$. Observe that $\mathcal{M}$ is simply the original Karzanov–Khachiyan Markov chain.

For notational convenience we shall assume that f is also defined on 0 and n, and that $f(0) = f(n) = 0$.

Let a *transposition sequence* from X to Y, for any $X, Y \in \Omega$, be any sequence $Z_0, Z_1, \ldots, Z_r$, where $X = Z_0$ and $Y = Z_r$, such that $Z_k \in \Omega$ and $Z_k = \sigma(i_k, j_k)Z_{k-1}$ $(k = 1,$

$2,\dots,r)$. The integer r is the length of the sequence, and its *weight* is its total width, $\sum_{k=1}^{r}(j_k - i_k)$. The *transposition distance* $\delta(X,Y)$ is then the least weight of any transposition sequence from X to Y. Clearly δ is a metric on Ω. The diameter $D = \max_{X,Y\in\Omega}\delta(X,Y)$ is bounded above by the number of incomparable pairs in P, since there is a sequence of close transpositions of at most this length, and thus $D \leqslant {}^nC_2$.

It transpires that we may, in fact, find a tighter upper bound on D than this, since it turns out that the transposition distance metric is equivalent to a classical metric on total orders: Spearman's footrule [18]. Suppose X is a total order; we shall use the notation $X(i)$ to denote the ith element of the total order, X. Then Spearman's footrule, $\delta_S(X,Y) = \frac{1}{2}\sum_{i=1}^{n}|X(i) - Y(i)|$. We prove in Appendix A that $\delta_S = \delta$. It is well known that $\delta_S(X,Y) \leqslant \lfloor n^2/4 \rfloor$ (see, for example, [6]), and thus $D \leqslant \lfloor n^2/4 \rfloor$.

The basic technique we employ is known as *coupling*. We use the following 'Coupling Lemma'. (See, for example, [1].)

Lemma 1 (Coupling). *Let* (X,Y) *be a random process (the* coupling*) such that, marginally,* X *and* Y *are both copies of* $\mathcal{M}_f$. *Moreover, suppose* Y_0 *is chosen from* π, *and* μ_t *is the distribution of* X_t. *Then*

$$\mathrm{d_{TV}}(\mu_t, \pi) \leqslant \boldsymbol{P}(X_t \neq Y_t),$$

where $\mathrm{d_{TV}}$ *is the total variation distance metric on measures.*

When $X_t = Y_t$, we say that X and Y have *coupled.*

3. The coupling

Let X and Y be two copies of $\mathcal{M}_f$ as in the Coupling Lemma. At time t, let $X_t = Z_0, Z_1, \dots, Z_r = Y_t$ be a transposition sequence of minimal weight, d_t. We let the Z_k evolve for a single time step as coupled copies of $\mathcal{M}_f$. Let Z_k' be the state to which Z_k evolves. We couple the Z_k as follows.

(1) Choose $p \in \{1,2,\dots,n-1\}$ according to the distribution f, and $c_0 \in \{0,1\}$ uniformly at random.

(2) For each $k \in \{1,2,\dots,r\}$: if $j_k - i_k = 1$ and $p = i_k$, then let $c_k = 1 - c_{k-1}$, otherwise let $c_k = c_{k-1}$.

(3) For each $k \in \{0,1,\dots,r\}$: if $c_k = 0$ or $\sigma(p,p+1)Z_k \notin \Omega$, $Z_k' = Z_k$. Otherwise $Z_k' = \sigma(p,p+1)Z_k$.

We will show that $\boldsymbol{E}d_{t+1} < d_t$, for a suitable choice of f (and in fact that $\boldsymbol{E}d_{t+1} \leqslant d_t$ for an arbitrary concave f). For notational simplicity, let us write $A = Z_{k-1}$, $B = Z_k$ and $(i,j) = (i_k, j_k)$. Thus $B = \sigma(i,j)A$, i.e.

$$A = (a_1\, a_2 \cdots a_{i-1}\, a_i \cdots a_j\, a_{j+1} \cdots a_n), \quad B = (a_1\, a_2 \cdots a_{i-1}\, a_j \cdots a_i\, a_{j+1} \cdots a_n).$$

If $p \notin \{i-1, i, j-1, j\}$ then $\delta(A',B') = (j-i) = \delta(A,B)$, since either we do nothing in both A and B, or $\sigma(p,p+1)$ can be successfully applied in both A and B.

If $p=i-1$, then either we do nothing in both A and B with probability $\frac{1}{2}$, or we attempt to make the transposition, $\sigma(i-1,i)$, in both A and B. If this transposition is successful in neither, we will have $\delta(A',B')=\delta(A,B)$; if it is successful in both, then we will have $\delta(A',B')=\delta(A,B)+1$, since A' and B' will differ by a transposition of width $(j-i+1)$. If it is successful in only one of A and B then $\delta(A',B')=\delta_S(A',B')=\delta(A,B)+1$. Thus, conditional on $p=i-1$, or similarly, $p=j$, we have $\boldsymbol{E}\delta(A',B')\leqslant\delta(A,B)+\frac{1}{2}$.

Now consider $p=i$. Suppose first that $i\neq j-1$, i.e. $(j-i)>1$. Then the transposition, $\sigma(i,i+1)$, must succeed in both A and B — for suppose to the contrary that it fails, in A, say. Then $a_i\preccurlyeq a_{i+1}$, but a_i follows a_{i+1} in B, so $B\notin\Omega$, establishing a contradiction. Thus with probability $\frac{1}{2}$ we have $\delta(A',B')=\delta(A,B)-1$, since A', B' will differ by a transposition of width $(j-i-1)$. Thus conditional on $p=i$, or similarly, $p=j-1$, we have $\boldsymbol{E}\delta(A',B')\leqslant\delta(A,B)-\frac{1}{2}$. Therefore, if $i\neq j-1$,

$$\boldsymbol{E}\delta(A',B')-\delta(A,B)\leqslant\tfrac{1}{2}(f(i-1)-f(i)-f(j-1)+f(j)).$$

It remains only to consider the case $p=i=j-1$. Clearly, we can apply $\sigma(i,i+1)$ in both A,B, since $B=\sigma(i,i+1)A$. Moreover, the coupling $c(B)=1-c(A)$ ensures that we do nothing in one and transpose in the other. Thus $B'=A'$ with unit probability, and $\delta(A',B')=\delta(A,B)-1$. Therefore, if $i=j-1$,

$$\begin{aligned}\boldsymbol{E}\delta(A',B')-\delta(A,B)&\leqslant\tfrac{1}{2}(f(i-1)+f(j))-f(i)\\&=\tfrac{1}{2}(f(i-1)-f(i)-f(j-1)+f(j)).\end{aligned}$$

So, in all cases, we have that the unconditioned expectation, $\boldsymbol{E}\delta(A',B')\leqslant\delta(A,B)+\frac{1}{2}(f(i-1)-f(i)-f(j-1)+f(j))$.

Note that this shows that the transposition distance does not increase in expectation under this coupling for *any* concave probability distribution f. It is possible to prove rapid mixing in this general setting, resulting in a mixing time of $O(n^5)$, however we do not do this here. Instead, we fix on a particular choice of f and show that, for this f, $\mathcal{M}_f$ has a mixing time of $O(n^3\log n)$.

Our choice of concave probability distribution is $F(i)=i(n-i)/K$, where K is the normalizing constant. It is easy to verify that $K=\frac{1}{6}(n^3-n)$. We choose F as quadratic, since we observe that to minimize $\max_{i<j}\{(f(i-1)-f(i)-f(j-1)+f(j))/(j-i)\}$, we should use a function with a constant second difference.

Then, for all i, $F(i)-F(i-1)=(n+1-2i)/K$, and thus $\frac{1}{2}(F(i-1)-F(i)-F(j-1)+F(j))=(i-j)/K$.

Now recall that $\delta(A,B)=j-i$, and thus $\boldsymbol{E}(\delta(A',B'))\leqslant(1-(1/K))\delta(A,B)$.

Following [4] we have

$$\boldsymbol{E}d_{t+1}\leqslant\boldsymbol{E}\left(\sum_{k=1}^{r}\delta\left(Z'_{k-1},Z'_k\right)\right)\leqslant(1-(1/K))\sum_{k=1}^{r}\delta(Z_{k-1},Z_k)=(1-(1/K))d_t.$$

Thus $d_t\leqslant(1-(1/K))^tD$, and since d_t is a non-negative integer valued variable, $\boldsymbol{P}(X_t\neq Y_t)\leqslant(1-(1/K))^tD$. Applying the Coupling Lemma, we see that $\mathrm{d}_{\mathrm{TV}}(X_t\neq Y_t)\leqslant$

$(1-(1/K))^t D$. Taking logarithms, and rearranging, we see that in order to ensure that $d_{TV}(X_t \neq Y_t) \leqslant \varepsilon$ we need only simulate $\mathcal{M}_F$ for $K \ln D\varepsilon^{-1}$ steps.

Recalling that $D \leqslant \lfloor n^2/4 \rfloor$, we see that this shows that the mixing rate of $\mathcal{M}_F$ is bounded above by $\lceil \frac{1}{6}(n^3-n)\ln(n^2\varepsilon^{-1}/4) \rceil$, establishing the claimed result.

4. Lower bounds and related chains

It is well-known (see e.g. Aldous [1]), that for the Karzanov and Khachiyan chain on the set of all total orders, the mixing time is $\Omega(n^3)$, and $O(n^3 \log n)$, and thus the mixing time for $\mathcal{M}$, is in general $\Omega(n^3)$, based on experimental data.

Consider the partial order consisting of a chain of length $n-1$, and one independent element. This would have only n linear extensions: the chain, with the independent element inserted at each point. $\mathcal{M}_f$, would thus in this case be equivalent to a random walk on $\{1,2,\dots,n\}$, denoting the position of the random element, and moving with probabilities given by f. Since f is a concave probability distribution, its maximum is at most $2/n$. To see this, suppose the maximum is $f(k)=h$. Then $f(i) \geqslant hi/k$ for $i \leqslant k$ and $f(i) \geqslant h(n-i)/(n-k)$ for $i > k$. Thus

$$1 = \sum_{i=1}^{n-1} f(i) \geqslant \sum_{i=1}^{k} hi/k + \sum_{i=k+1}^{n-1} h(n-i)/(n-k) = hn/2,$$

from which the assertion follows. Thus the expected time before $\mathcal{M}_f$ could perform a non-null transition is $\Omega(n)$. Since a simple random walk on $\{1,2,\dots,n\}$ has mixing time $\Theta(n^2)$, we see that for any concave choice of f, $\mathcal{M}_f$ has a mixing time that is $\Omega(n^3)$ in the worst case.

There is therefore no substantial complexity gap between the mixing time proved in this paper and the theoretical optimum for this class of chains. Any significant improvement over the results of this paper would have to be made by turning to different Markov chains.

A corollary of the mixing rate proved in this paper, together with some work of Dyer and Greenhill [10] on eigenvalue comparisons, is that the mixing rate of the Karzanov and Khachiyan chain is worse than that of $\mathcal{M}_F$ by no more than a factor of $O(\log|\Omega|) = O(n \log n)$; i.e. that the mixing rate of $\mathcal{M}$ is $O(n^3 \log n \log|\Omega|\varepsilon^{-1})$ (an improvement on the bound previously known of $O(n^4 \log|\Omega|\varepsilon^{-1})$ [8]), and furthermore, that the Karzanov and Khachiyan chain has a *relaxation time* that is worse than that of $\mathcal{M}_F$ by no more than a constant factor — both are $\Theta(n^3)$ and therefore optimal on this criterion. (The *relaxation time* is essentially the time needed to get second and subsequent random samples from Ω, see e.g. Aldous and Fill [2].)

An obvious candidate for an improved chain would be that which performs transitions by choosing a random transposition rather that merely a random close transposition. On the set of all total orders this is known to have mixing time of only $\Theta(n \log n)$ [5]. Currently, the best-known bound on the mixing time of this chain in general, is $O(n^4 \log n \log|\Omega|\varepsilon^{-1})$, and the relaxation time is $O(n^4)$. (This fact is derived from the mixing rate proved in this paper, again together with some work of Dyer and Greenhill [10]). This approach cannot succeed however, for the relaxation time (and hence the mixing time) of this chain is *in general* $\Omega(n^4)$ (consider again the partial order than consists of a chain and an element; here the probability of a transition being non-null is $O(1/n^2)$).

A more promising candidate is the chain that performs transitions by choosing a random element to delete and a random position for its subsequent reinsertion. This has a mixing time of $\Theta(n \log n)$ on the set of all total orders. Again, the mixing rate proved in this paper together with [10] shows an upper bound on the mixing rate of this chain of $O(n^4 \log n \log |\Omega| \varepsilon^{-1})$, and relaxation time of $O(n^4)$. In general, however, we may show a lower bound of $\Omega(n^2)$ for the mixing time of this chain. Consider the partial order that is formed from two independent chains, A and B, each of size $2n+1$. Let a and b, respectively, be the middle elements of the two chains. If we were to start this Markov chain with the ordering in which all elements of A are ranked before all elements of B, then the initial distance between a and b is $n+1$. Consider how this distance may decrease. In order for it to decrease we would first have to select either the least element of A, or the largest element of B, between a and b. The expected time before this occurs is $\Theta(n)$. Since the initial distance between a and b is $\Theta(n)$, the expected time before we may have b before a is $\Omega(n^2)$ — but since there are as many linear extensions with b before a as b after a, we see that $\Omega(n^2)$ is a lower bound on the mixing time.

One of the major applications of the generation of random linear extensions is to approximate the *number* of linear extensions. Calculating this number exactly is #P-complete [3]. Brightwell and Winkler [3] illustrate an fpras for approximating this number, i.e. an algorithm that approximates the exact number to within a multiplicative factor of $1+\varepsilon$ with probability at least 3/4: this uses an almost uniform sampler as a subroutine; the running time of this algorithm, using the original bounds on the Karzanov–Khachiyan chain is $O(n^9 \log^6 n \varepsilon^{-2} \log \varepsilon^{-1})$. Dyer and Frieze [8], as well as improving the bound on the mixing rate of the Karzanov–Khachiyan chain, use an improved algorithm for the approximate counting problem that runs in time $O(n^6 \log^2 n \varepsilon^{-2} \log(n\varepsilon^{-1})$. Using what are now standard techniques (see e.g. [2,12]), if we have a Markov chain with stationary distribution the uniform distribution on the set of linear extensions, we may use this to generate an algorithm for approximating the number of linear extensions that will run in time $O(n^2 \log^2 n\varepsilon^{-2} \log(n\varepsilon^{-1}) \times$ relaxation time $+ \tau(\varepsilon/n \log n))$, where $\tau(x)$ is a bound on the time for the Markov chain to come within a variation distance of x of the stationary distribution. In particular, for $\mathcal{M}$, or $\mathcal{M}_F$, this translates to an approximation scheme that runs in time $O(n^5 \log^2 n\varepsilon^{-2} \log(n\varepsilon^{-1}))$.

5. Conclusions

We have shown a significantly improved bound on the mixing rate of Markov chains for generating random linear extensions of a partial order. We have also indicated that our results are close to optimal for a family of chains which includes the Karzanov–Khachiyan chain as a special case. The convergence proof is non-geometric, in sharp contrast to all earlier approaches to this problem, and serves well to illustrate the utility of the path coupling method developed in [4].

Appendix A. Equivalence of transposition distance to Spearman's footrule

Recall that when we refer to a total order (or permutation) this is implicitly on the set $\{1,2,\dots,n\}$. Furthermore, if X is a permutation, then $X(i)$ denotes the position that i is moved to under the permutation. Thus the identity permutation, I, could be written as $I(i)=i$. When we compose permutations, we mean $XY(i)=X(Y(i))$.

We defined *Spearman's footrule* as a metric on total orders:

$$\delta_S(X,Y)=\sum_{i=1}^{n}|X(i)-Y(i)|.$$

It should be noted that this definition of Spearman's footrule is in accord with Spearman's usage [18], and that recommended by [7]; other authors (e.g. [5]) drop the half from the definition.

Theorem 1. *Suppose X and Y are distinct total orders. Suppose further that they differ by more than a single transposition (i.e. there is no transposition T, such that $X=TY$), and that both X and Y are linear extensions of a partial order, P. Then there exists a transposition T' such that $X'=T'X$ is a linear extension of P distinct from X and Y, and $\delta_S(Y,X')+\delta_S(X',X)=\delta_S(Y,X)$.*

Proof. We may assume, without loss of generality (by relabelling, say), that $Y=I$. Suppose we have i and j, such that $i\leqslant X(j)<X(i)\leqslant j$. Recall that one can write a permutation as the product of disjoint cycles. In any cycle we may find such an i and j. If we have the further condition that for all k such that $X(j)<k<X(i)$, $X(k)=k$, then we are done, for we may take $X'=\sigma(X(i),X(j))X$.

Suppose that we do not have this condition. Then either there is an entire cycle with all its elements between $X(j)$ and $X(i)$, in which case we may start again with this cycle, or there is either an i' such that $i'<X(j)$ or $i'>X(i)$, and $X(j)<X(i')<X(i)$, in which case we may start again with one of i and i' or j and i'.

This completes the proof by the classical method of infinite descent. □

Corollary 1. *Spearman's footrule is identical to transposition distance.*

Proof. Let X and Y be arbitrary linear extensions of a partial order. If $X=Y$, or X and Y differ by exactly one transposition, then the equivalence of the two metrics follows easily. If, instead, X and Y differ by more than a single transposition, then we may proceed by repeated application of the above theorem. We may use the theorem to construct a transposition sequence. The minimality of δ then guarantees that $\delta \leqslant \delta_S$. Conversely, we may argue by induction on the length of the minimum transposition sequence. If $Z \neq X, Y$ is a member of this sequence, then

$$\delta(Y,X) = \delta(Y,Z) + \delta(Z,X) = \delta_S(Y,Z) + \delta_S(Z,X) \geqslant \delta_S(Y,X),$$

respectively, by induction and the triangle inequality. Thus $\delta_S \leqslant \delta$. □

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