Generating a random sink-free orientation in quadratic time

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Abstract

A sink-free orientation of a finite undirected graph is a choice of orientation for each edge such that every vertex has out-degree at least 1. Bubley and Dyer (1997) use Markov Chain Monte Carlo to sample approximately from the uniform distribution on sink-free orientations in time $O(m^3 \log(1/\varepsilon))$, where m is the number of edges and ε the degree of approximation. Huber (1998) uses coupling from the past to obtain an exact sample in time $O(m^4)$. We present a simple randomized algorithm inspired by Wilson's cycle popping method which obtains an exact sample in mean time at most O(nm), where n is the number of vertices.

1. Introduction

A common problem is to select a random sample efficiently from a large collection of combinatorial objects. There are many reasons one may wish to do this. One is to obtain an approximate count: Jerrum and Sinclair [JS] showed that if one can generate nearly uniform samples, then for each $\varepsilon > 0$, one can obtain the cardinality of the collection to within a factor of $1 + \varepsilon$ with probability $1 - \varepsilon$, in just a little more time. When counting the collection is #P-hard, as in the case of properly k-coloring a graph, this may be the only reasonable way to count, since it is unlikely that #P-hard counting problems can

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be solved exactly in polynomial time. Another reason to seek a sampling algorithm is that it may shed light on properties of the typical sample. For example, the analysis of typical spanning trees of Cayley graphs [P, BLPS] relies on two algorithms, the first developed by Aldous [A] and Broder [B] and the second by Wilson [W]. The analysis of phase boundaries in typical domino tilings of regions known as Aztec diamonds also relies on a sampling algorithm, known as domino shuffling [CEP]. Finally, sample generation may be a way of producing conjectures about the typical sample via simulation, when no theorem is known (for example, the results in [CEP] were initially discovered this way).

One common way to generate samples is Markov Chain Monte Carlo (MCMC). Here one finds an ergodic Markov chain whose equilibrium measure is the desired distribution μ ; then one runs the chain until the distribution is close to μ . Constructing such a chain is usually easy (often when μ is uniform, there is a natural doubly stochastic transition matrix) and the hard part is knowing how long to run it. This may be established via eigenvalue bounds, or via coupling arguments or stopping times. In cases where the time bounds on the chain are established via coupling, it is often possible to improve on MCMC by using coupling from the past (CFTP) to obtain an exact sample rather than an approximate one [PW1].

In this note we consider the generation of a random sink-free orientation (SFO) of a finite undirected graph. Sink-free orientations were introduced by Bubley and Dyer [BD], who were motivated by an equivalence between counting them and counting satisfying assignments of Boolean formulas in conjunctive normal form in which each variable occurs at most twice (they call this problem Twice-SAT). Bubley and Dyer showed that counting sink-free orientations is #P-complete, so it is unlikely that an exact count can be obtained in polynomial time, and we must use approximate counting techniques based on nearly uniform sampling.

Bubley and Dyer give an MCMC algorithm that produces a sample whose distribution is within ε of uniform (in total variation) in time $O(m^3 \log(1/\varepsilon))$, where m is the number of edges. Huber [H] uses Bubley and Dyer's analysis along with CFTP to produce an exact uniform sample in mean time $O(m^4)$. The purpose of this note is to improve the running time to O(nm), where n is the number of vertices. Instead of MCMC, we use a strong uniform time algorithm inspired by David Wilson's cycle popping algorithm [W] for generating uniform directed spanning trees.

We now describe the problem and our results more precisely. Let G = (V, E) be a finite undirected graph. We allow multiple edges and self-loops (but at most one self-loop per vertex, since multiple self-loops play no useful role in sink-free orientations). We define an n-cycle to be a ring of n vertices v_0, \ldots, v_{n-1} with edges from v_i to v_{i+1} for each i (taken modulo n; note that a 1-cycle is a vertex with a self-loop), and an n-lollipop to be a path consisting of n vertices and n-1 edges, with a self-loop added at one end.

An orientation of an edge between vertices v and w is a mapping of the set {head, tail} onto $\{v, w\}$. Thus, a self-loop has only one orientation, but all other edges have two. To reverse the orientation of an edge, swap its head and tail. An orientation of G is an orientation of each edge. A sink in an orientation is a vertex that is not the tail of any edge (a source is the opposite, i.e., not the head of any edge), and a sink-free orientation

(SFO) of G is an orientation that contains no sinks. If any connected component of G is a tree, then G has no SFO, and vice versa. Henceforth we restrict consideration to the class S of graphs in which no component is a tree. Let μ_G denote the probability measure assigning probability 1/N to each SFO of G, where N is the total number of SFO's of G.

Our algorithm, which we call "sink popping," works as follows. Given a graph, orient the edges by independent, fair coin flips. If this orientation has no sinks, then it is the SFO we seek. Otherwise, choose any sink, and randomly re-orient each edge that points into the sink (i.e., all of its edges). We call this popping the sink, for reasons that will become clearer in the next section. Repeat until there are no more sinks.

We now state our main result.

Theorem 1.1. For every graph $G \in \mathcal{S}$, sink popping terminates in finite time with probability 1, regardless of how one chooses which sink to pop, and produces an output whose distribution is precisely μ_G . The average number of sinks that must be popped is at most $\binom{n}{2}$, where n is the number of vertices of G, once again regardless of how one chooses which sink to pop. Equality holds only for the n-cycle or the n-lollipop. The expected number of times each particular vertex is popped is at most n-1.

Sink popping is briefly mentioned at the end of [PW2], where the claims in the first sentence of the theorem are mentioned without detailed proof (and the running time is not analyzed).

To show that sink popping's running time is O(nm), we need to state the algorithm slightly more carefully. The subtle point is avoiding spending lots of time searching for sinks. We will keep a list of all sinks in the graph, and also a table showing the outdegree of every vertex. Generating these initially takes time proportional to the sum of the degrees of the vertices, or O(m) time. Whenever we search for a sink to pop, we simply take the first sink from the list. When we pop the sink, we update the table to reflect the changes to its out-degree, and to those of its neighbors. It neighbors may have become sinks, in which case we append them to the list of sinks. (The purpose of the table is to let us easily see whether the neighbors have become sinks, without having to examine all their edges: in a complete graph, that would waste lots of time.) No sink can be annihilated except the one we popped, since no two sinks can share a common edge (it would have to point to both). Thus, each time we pop a sink at v, re-orienting its edges and updating the list and table requires time $O(\deg(v))$. By Theorem 1.1, the expected number of times v is popped is O(n), so the total expected number of operations is

$$O\left(\sum_{v} n \deg(v)\right) = O(nm).$$

This time bound does not actually estimate the number of bit operations, but instead treats individual graph operations as units.

In the next section we give another description of the sink popping algorithm and explain its connection to cycle popping. We also state some further results about sink popping with arbitrary initial conditions. The third section contains proofs of the diamond

and strong uniformity lemmas, which are analogous to the equivalent lemmas for cycle popping. The fourth section analyzes the running time. The fifth section derives some further facts about the running time. We conclude with some speculations and open questions.

2. Sink popping and cycle popping

Let H = (V, E) be a finite, connected, directed graph, and let v be any fixed vertex of H. A directed spanning tree of (H, v) is a subset of edges so that every vertex other than v has out-degree 1 and v has out-degree 0. Wilson [W, PW2] invented the following algorithm, known as "cycle popping," for generating a uniform random directed spanning tree. For each $w \in V \setminus \{v\}$ and $k \geq 0$, let $X_{w,k}$ be a random edge leading out of w, chosen uniformly from among all edges leading out of w. Let these be independent as w and k vary. For fixed w, imagine the collection $\{X_{w,k}: k \geq 0\}$ as a stack with $X_{w,0}$ on top. Initially, look at the collection $\{X_{w,0}: w \in V \setminus \{v\}\}\$, that is, consider the collection $\{X_{w,f(w)}\}\$ with $f\equiv 0$. If these form a directed spanning tree, stop and set the sample equal to it. If not, there must be a cycle in this collection. Choose a cycle (it doesn't matter which), and increment f(w) by 1 for each w in the cycle. (Imagine popping these edges off the stack so the next element of each stack is now on top.) If the collection $\{X_{w,f(w)}: w \in V \setminus \{v\}\}\$ is now a directed spanning tree, stop and return this for your sample, otherwise continue popping until you do stop. Wilson showed that the set of cycles popped does not depend on which you choose to pop when you have a choice, and that the algorithm stops almost surely at a directed spanning tree with uniform distribution.

We can describe sink popping in similar terms, which will be useful in the proof of Theorem 1.1. Let G = (V, E) be a finite undirected graph in \mathcal{S} and let $\Omega = \Omega_0^{\mathbb{N}}$, where Ω_0 is the set of orientations of G, i.e., Ω consists of sequences of orientations of G. We endow Ω with the σ -field \mathcal{F} generated by the coordinate functions $X_{e,k}$ for $e \in E(G)$ and $k \geq 0$, which specify the orientation of e in the k-th orientation in the sequence. Endow Ω with the probability measure **P** under which the coordinate functions are independent and each equally likely to yield either orientation. The intuition is that $\{X_{e,k}:k\geq 0\}$ represents a stack of arrows under the edge e. Define a random function $f: E \times \mathbb{N} \to \mathbb{N}$ as follows. Let f(e,0) = 0 for all e. Given f(e,k) for all e, define $f(\cdot,k+1)$ inductively: If the collection $\{X_{e,f(e,k)}: e \in E\}$ is an SFO, then set f(e,k+1) = f(e,k) for all e. If not, choose a sink $v_k \in V$ arbitrarily, i.e., a vertex v_k for which all edges e incident to it are oriented toward it by the orientation $X_{e,f(e,k)}$. Let f(e,k+1)=f(e,k) for e not incident to v_k , and f(e, k+1) = f(e, k) + 1 for e incident to v_k . The dependence of f on the choice rule (for choosing v_k , if there are several sinks) is suppressed in the notation, as is the dependence on the choice of $\omega \in \Omega$ via the variables $\{X_{e,k}\}$. Intuitively, f(e,k)is the original depth of the arrow under e now at the top of the stack at time k. Say that v_k is the sink popped at time k, and let $\tau = \min\{k : \{X_{e,f(e,k)}\}\}$ is an SFO be the number of pops before an SFO is obtained (conceivably $\tau = \infty$), and $\eta = \eta(\omega, \text{choice rule})$ denote the resulting SFO (if any).

Except for its last sentence, Theorem 1.1 is established by showing that $\tau < \infty$ with probability 1, the law of $\{X_{e,f(e,\tau)}\}$ is precisely μ_G , and $\mathbf{E}\tau \leq \binom{n}{2}$, with equality in and only in the cases indicated. The first two lemmas are analogous to those used by Wilson [W] in establishing the validity of the cycle popping algorithm, and the third is the running time analysis.

Lemma 2.2 (Diamond lemma). The number of pops $\tau \leq \infty$ in a maximal popping sequence is independent of the choice rule, as is the multiset $\{v_k : 0 \leq k < \tau\}$. If $\tau < \infty$ then the resulting SFO η is also independent of the choice rule.

The name "diamond" is meant to remind the reader that moving from the top of a diamond to the bottom by going southeast then southwest is equivalent to going southwest then southeast. This terminology comes from the article [E].

Lemma 2.3 (Strong uniform time). Let N be the number of SFO's of G. Then for each $k \geq 0$, and each SFO η ,

$$\mathbf{P}(\tau = k, \{X_{e,f(e,\tau)}\} = \eta) = \frac{\mathbf{P}(\tau = k)}{N}.$$

In other words, τ is a strong uniform time.

Lemma 2.4. If $G \in \mathcal{S}$ has n vertices, then $\mathbf{E}\tau \leq \binom{n}{2}$, with equality only for the n-cycle and the n-lollipop.

We conclude this section by stating two results that shed further light on the running time of the popping algorithm.

Proposition 2.5. The distribution of τ for the n-cycle is exactly the same as the distribution for the n-lollipop.

Proposition 2.6. Let $G \in \mathcal{S}$ be any graph with n vertices and let \mathcal{F}_0 be the σ -field generated by the variables $\{X_{e,0}\}$. Then the conditional mean running time $\mathbf{E}(\tau \mid \mathcal{F}_0)$ is always bounded by n(n-1), and the only case to achieve this is an n-lollipop with all edges oriented opposite to their orientation in the unique SFO.

3. Strong uniformity

We first establish deterministic facts holding for every sample $\omega \in \Omega$. Say that a sequence v_0, \ldots, v_{k-1} with $k \leq \infty$ is a maximal popping sequence for ω if it is legal (i.e., only sinks are popped) and cannot be extended to larger k (thus if $k < \infty$ it results in an SFO). Note that if $k = \infty$, we do not mean our notation to suggest that v_0, v_1, \ldots is followed by a final term $v_{\infty-1}$; instead, $v_0, \ldots, v_{\infty-1}$ denotes the infinite sequence v_0, v_1, \ldots , with no final term.

Let f(e, k) denote the function $f(e, k, \omega, \mathbf{v})$ where ω is a sample point and \mathbf{v} is a specified legal sequence of pops of length at least k. Define an equivalence relation on

finite sequences v_0, \ldots, v_{k-1} of vertices of G by calling two sequences equivalent if one can be changed to the other by a sequence of transpositions of pairs of vertices (v_i, v_{i+1}) that are not neighbors in G. (Note that such a transposition does not change whether a sequence is a legal popping sequence.) The following lemma is useful, though obvious.

Lemma 3.7 (Deterministic strong Markov property). Given an integer j and vertices v_0, \ldots, v_{j-1} , let ω be any initial configuration for which v_0, \ldots, v_{j-1} is a legal popping sequence and let ω' and ω be related by

$$X_{e,k}(\omega') = X_{e,k+f(e,j)}(\omega).$$

That is, ω' looks like ω after v_0, \ldots, v_{j-1} are popped. Then the following deterministic strong Markov property (DSMP) holds. For any $k \leq \infty$, the set of sequences $\{v_{j+i} : 0 \leq i \leq k-1\}$ for which v_0, \ldots, v_{j+k-1} is a legal popping sequence for ω is the same as the set of legal popping sequences of length k for ω' . If v_0, \ldots, v_{j+k-1} is maximal for ω then v_i, \ldots, v_{j+k-1} is maximal for ω' , and leaves the same SFO (if $k < \infty$).

Extend the definition of equivalence to infinite sequences by saying that v_0, v_1, \ldots is equivalent to w_0, w_1, \ldots if, by a sequence of transpositions as above applied to v_0, v_1, \ldots , one can transform v_0, v_1, \ldots so that arbitrarily long initial segments of it match those of w_0, w_1, \ldots . In particular, this implies that the multisets $\{v_k\}$ and $\{w_k\}$ are the same.

Let $l(\omega)$ denote the minimal length of a maximal popping sequence for ω .

Lemma 3.8. The set of maximal popping sequences is an equivalence class.

Proof. Let v_0, \ldots, v_{k-1} be a legal popping sequence for ω with $k < \infty$, and let w_0, \ldots, w_{k-1} be obtained from v_0, \ldots, v_{k-1} by transposing v_i and v_{i+1} which are not neighbors in G. Suppose i = 0. Since the edges incident to v_0 are disjoint from the edges incident to v_1 , we may apply the DSMP to v_0, v_1 and to v_1, v_0 and see that w_0, \ldots, w_{k-1} is legal as well and maximal if v_0, \ldots, v_{k-1} is. If i > 0, first apply the DSMP to v_0, \ldots, v_{i-1} and then use the same argument. This shows that equivalent sequences are either both maximal popping sequences or neither. (The case of $k = \infty$ is trivial, since infinite popping sequences are automatically maximal.)

To prove the lemma, we induct on $l(\omega)$, and then deal with the case of $l(\omega) = \infty$. It is clear when l = 0. Assuming the lemma for $l(\omega) < L$, let $l(\omega) = L$ with maximal popping sequence v_0, \ldots, v_{L-1} . Let w_0, \ldots, w_{k-1} be any other maximal popping sequence. If $w_0 = v_0$, applying the DSMP and the induction hypothesis completes the induction. If not, then consider the least i for which $v_i = w_0$, if any. When we pop v_0, \ldots, v_{L-1} , the orientation $\{X_{e,f(e,j)}: e \in E\}$ has a sink at w_0 for each j < i, since the sink at w_0 exists until one of its edges is popped and no other sink can contain any such edge until w_0 is popped. Thus i exists and v_j cannot be a neighbor of v_i for j < i. Hence, we can move v_i to the first position by a sequence of adjacent transpositions with non-neighbors in G. We have seen that the resulting sequence $v_i, v_0, v_1, v_2, \ldots, v_{i-1}, v_{i+1}, \ldots, v_{L-1}$ is a maximal popping sequence. Now apply the DSMP and the induction hypothesis to conclude that w_0, \ldots, w_{k-1} is equivalent to $v_i, v_1, \ldots, v_{i-1}, v_{i+1}, \ldots, v_{L-1}$, and thus to v_0, \ldots, v_{L-1} .

All that remains is the case of $l(\omega) = \infty$, i.e., the case when all maximal popping sequences are infinite. Given two such sequences v_0, v_1, \ldots and w_0, w_1, \ldots , the argument from the previous paragraph shows that we can transform v_0, v_1, \ldots so that its first element is w_0 . Now applying the DSMP shows that we can bring arbitrarily long initial segments into agreement, which is the definition of equivalence.

Proof of the diamond lemma. From the previous lemma, we know that $\tau = l$, so τ is independent of the choice rule. Furthermore, since all maximal popping sequences are equivalent, the multisets of popped vertices are the same. The assertion about SFO's follows because the SFO depends only on which vertices were popped.

Proof of strong uniform time. We prove by induction that for any SFO η and any finite sequence v_0, \ldots, v_{k-1} , the following event has probability $2^{-m-\sum_{i=0}^{k-1} \deg_0(v_i)}$, where \deg_0 means the degree not counting self-loops: $\tau = k$, and v_0, \ldots, v_{k-1} is a legal popping sequence for ω , and $\eta(\omega) = \eta_0$. This is vacuously true when k = 0. Now the probability that the singleton v_0 is a legal pop is $2^{-\deg_0(v_0)}$, so applying the DSMP we see that the probability of a maximal popping sequence $v_0, v_1, \ldots, v_{k-1}$ with $\eta = \eta_0$ is

$$2^{-\deg_0(v_0)}2^{-m-\sum_{i=1}^{k-1}\deg_0(v_i)}$$

which completes the induction.

To find the probability of both $\tau = k$ and $\eta = \eta_0$ (with no restrictions on the popping sequence), we must sum this probability over all equivalence classes of potential popping sequences of length k. We sum over equivalence classes to avoid double counting, since for any given ω , Lemma 3.8 tells us that the set of maximal popping sequences is an equivalence class. Since neither the summand nor the set of sequences depends on η_0 , we have proved the lemma.

4. Analysis of the running time

We still have not shown that τ is almost surely finite. While this may appear obvious from some kind of Markov property, the choice rule makes things sticky and we find it easiest to conclude this from the existence of a finite upper bound on the expected run time. To bound τ we make repeated use of the following monotonicity principle. We let Q(G, v) denote the random number of times v is popped in a maximal popping sequence (possibly ∞), which, by the diamond lemma, is well defined.

Lemma 4.9 (Monotonicity). Fix $G \in \mathcal{S}$ and let $H \in \mathcal{S}$ be a subgraph of G, that is, $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. For $v \in V(H)$,

$$\mathbf{E}Q(H, v) \ge \mathbf{E}Q(G, v).$$

Proof. This is proved by stochastic domination: we run sink popping simultaneously on H and G, using the same stacks for edges common to both graphs. Every legal popping sequence on G restricts to a legal popping sequence on H as well, so under this coupling $Q(H,v) \geq Q(G,v)$ always.

Remark: Additionally, we see that equality occurs only when no SFO on G can require further popping of v on H.

Proposition 4.10. If G is an n-cycle, then $\mathbf{E}\tau = \binom{n}{2}$. Furthermore, conditioned on starting with j edges oriented clockwise and n-j counterclockwise, the expected value of τ is 2j(n-j).

Proof. At any time, some of the arrows point clockwise and others counterclockwise. Let Y_k be the number of arrows pointing clockwise at time k. Popping at any vertex causes two opposite pointing arrows to be replaced by two random arrows. Thus Y_{k+1} has the distribution of $Y_k + Z$ where $\mathbf{P}(Z = 1) = \mathbf{P}(Z = -1) = 1/4$ and $\mathbf{P}(Z = 0) = 1/2$. Therefore $\{Y_k : k \geq 0\}$ is a simple random walk with delay probability of 1/2 absorbed at 0 and n. The expected absorption time from j is twice that for simple random walk, and thus is 2j(n-j); see equation (3.5) on page 349 of Feller [F]. Hence $\mathbf{E}\tau = 2\mathbf{E}Y_0(n-Y_0)$, which is twice the expected number of ordered pairs of edges where the first is initially clockwise and the second initially counterclockwise. There are n(n-1) ordered pairs of distinct edges, each having these orientations with probability 1/4, so $\mathbf{E}\tau = n(n-1)/2$. \square

Corollary 4.11. Let S_0 denote the class of graphs in which every vertex is in some cycle. For $G \in S_0$ and $v \in V(G)$,

$$\mathbf{E}Q(G, v) < (n-1)/2.$$

Equality holds for all v if and only if G is an n-cycle.

Proof. Fix G and v and let H be a cycle containing v. By monotonicity, $\mathbf{E}Q(G,v) \leq \mathbf{E}Q(H,v)$ which is at most (n-1)/2 by Proposition 4.10 and symmetry. In fact, $\mathbf{E}Q(H,v)$ is strictly less than (n-1)/2 unless H is an n-cycle. By the remark following the proof of the monotonicity lemma, the inequality $\mathbf{E}Q(G,v) \leq \mathbf{E}Q(H,v)$ is strict unless no SFO on G can require further popping of v on H. In our case, H is an n-cycle, and G is an n-cycle with some chords or self-loops added. Then (assuming G is not an n-cycle), there is always an SFO on G that does not restrict to an SFO on H: if G has a self-loop, one can choose an SFO on G such that H has a sink there; if G has a chord, one can use the chord to create a short circuit across H giving a cycle of length less than n, orient this cycle in a loop, and orient the other edges in G towards the cycle. If v is a sink in the restriction to H of such an SFO on G, then strict inequality holds for v (because with positive probability, sink popping on G will produce this SFO, and v will still need to be popped in H).

Lemma 4.12. For every $G \in \mathcal{S}$ with n vertices, and each $v \in V(G)$,

$$\mathbf{E}Q(G,v) \le n-1,$$

and equality holds only when v is the vertex furthest from the self-loop in an n-lollipop.

Proof. We induct on G. The base step is $G \in \mathcal{S}_0$, which is immediate from the previous corollary. Assume for induction that the conclusion holds for all subgraphs of G. There are three cases other than the base step.

Case 1. G is not connected. Then the result follows from the induction hypothesis and the monotonicity lemma applied to the component H of G containing v. Equality never occurs.

If G is connected and not in S_0 , then G must contain an isthmus, i.e., an edge whose removal disconnects G.

Case 2. Some edge e disconnects G into two components both in S. Again the result follows from the induction hypothesis applied to the component H of $G \setminus \{e\}$ containing v, and equality never occurs.

Case 3. G has an isthmus and removal of any isthmus always leaves a component that is a tree. Then G has a leaf z. If $v \neq z$ then the result follows immediately from monotonicity with $H = G \setminus \{z\}$. If v is the only leaf, then let w be its neighbor. Choose a popping order that pops v whenever possible, and otherwise executes any choice rule for sink popping on $H := G \setminus \{v\}$. Initially there is a 1/2 chance that v is a sink, in which case it is popped a mean 2 geometric number of times until the edge vw points to w. Then, each time w is popped, the probability is 1/2 that this edge is reversed, in which case it takes another mean 2 geometric number of pops to reverse it again. Thus

$$\mathbf{E}Q(G, v) = 1 + \mathbf{E}Q(H, w).$$

By induction, this is at most 1+(n-2). Equality occurs for v in G if and only if it occurs for w in H, so we see by induction that it holds only at the end of a lollipop. \square

Proof of Lemma 2.4. We prove the lemma by induction, following the pattern of the last proof. The base step is $G \in \mathcal{S}_0$, in which case the lemma follows from Corollary 4.11. In the cases 1 and 2 of the induction, if G is disconnected or the union of two graphs in \mathcal{S} along an added edge, the result is again immediate from the subadditivity of the function $n \mapsto \binom{n}{2}$ and monotonicity. Finally, if G has a leaf v, we set $H := G \setminus \{v\}$ and observe that the number of pops τ_G and τ_H on G and H respectively are related by $\tau_G = \tau_H + Q(G, v)$. Thus

$$\mathbf{E}\tau_G = \mathbf{E}\tau_H + \mathbf{E}Q(G, v) \le \binom{n-1}{2} + (n-1) = \binom{n}{2}.$$

By the previous lemma, the last inequality is strict unless H is an n-lollipop and its vertex of degree 1 is the neighbor of v in G. This completes the induction.

Proof of Theorem 1.1. The theorem follows immediately from combining Lemmas 2.2, 2.3, 2.4, and 4.12.

5. Further proofs

The n-cycle and n-lollipop have the worst mean run times. Here we prove Proposition 2.5, namely that the run time distributions are in fact identical.

Proof of Proposition 2.5. Number the vertices of the n-hollipop $0, \ldots, n-1$ with 0 being the leaf. Always pop the sink with lowest number. Let Y_k denote the sink popped at

time k. Clearly Y_0 is -1 plus a mean 2 geometric random variable, with the proviso that a value of n-1 or higher represents the terminal state in which no sink needs to be popped. Let \mathcal{F}_k be the σ -field generated by Y_0, \ldots, Y_{k-1} . We claim that $\{Y_k : k \geq 0\}$ is a time-homogeneous Markov chain with respect to $\{\mathcal{F}_k\}$ and that from any state j > 0 its increments are -2 plus a mean 2 geometric, jumping to the terminal state if it reaches n-1 or greater, and from state 0 the same thing with -2 replaced by -1 (thus the jump from 0 is resampled if it hits -1). All that is needed to check this is an inductive verification that the orientations of edges between vertices of higher index than Y_k are conditionally i.i.d. fair coin flips given \mathcal{F}_k , which is straightforward.

Now we show that the running time on an n-cycle is also equal to the time for a random walk to hit at least n-1 when its increments are -2 plus a mean 2 geometric, resampled if it hits -1. At time k, let Y_k denote the least index of a sink when the edge from n-1 to 0 is oriented toward 0 and n-1 minus the greatest index of a sink when the edge is oriented toward n-1. In other words, this quantity is the distance from the head of the 0, n-1 edge to the nearest sink in that direction. We always choose the pop that sink. The only time the 0, n-1 edge can change orientations is when $Y_k = 0$, in which case Y_{k+1} will be -1 plus a mean 2 geometric; when $Y_k > 0$ verification of the conditional increment is trivial. The stopping rule is, again, that one must jump to n-1 or greater, and Y_0 has the right distribution for the same reason as before, so the sequence has the same distribution.

Our final result deals with the run time started from an arbitrary state, that is, the conditional distribution of τ given \mathcal{F}_0 (as defined in Proposition 2.6). While this quantity is a hidden variable as far as users of the algorithm are concerned, it has relevance to the distribution of the run time, as well as having some intrinsic interest. We begin again with a result on the n-cycle.

Proposition 5.13. Let G be an n-cycle. Then for every $v \in V(G)$,

$$\mathbf{E}(Q(G, v) \mid \mathcal{F}_0) \le 3n/4,$$

with equality if and only if n is even and all edges are oriented along the direction of shortest travel to v.

Proof. Number the vertices $0, \ldots, n-1 \mod n$. We first establish that the discrete Laplacian of $\mathbf{E}(Q(G, v) | \mathcal{F}_0)$ depends on the initial orientation of G via

$$\mathbf{E}\left[Q(G,v) - \frac{Q(G,v+1) + Q(G,v-1)}{2} \middle| \mathcal{F}_0\right] = \begin{cases} 1 & \text{if } v \text{ is a sink,} \\ -1 & \text{if } v \text{ is a source, and} \\ 0 & \text{otherwise.} \end{cases}$$
(5.1)

To see this, choose any popping order and let Y(v, k) denote the in-degree of v at time k, that is, the number of $e \in E(G)$ adjacent to v for which $X_{e,f(e,k)}$ is oriented toward v. Then, conditionally on anything up to time k,

$$\mathbf{E}Y(v, k+1) = \mathbf{E}Y(v, k) - \mathbf{P}(v_k = v) + \frac{\mathbf{P}(v_k = v+1) + \mathbf{P}(v_k = v-1)}{2},$$

since any pop at v reduces the expected in-degree by mean 1 and any pop at a neighbor of v increases it by mean 1/2. Summing over k, conditioning on \mathcal{F}_0 and using $Y(v,\tau) \equiv 1$ proves (5.1).

From Proposition 4.10 we know that $\mathbf{E}(\tau \mid \mathcal{F}_0) = 2Y_0(n - Y_0)$ where Y_0 is the number of initial clockwise arrows (edges oriented from i + 1 to $i \mod n$ for some i). This, along with (5.1), determines $\mathbf{E}(Q(G, \cdot) \mid \mathcal{F}_0)$, since the difference of any two candidates for this function would be a harmonic function on the cycle, and hence constant.

In general,

$$\mathbf{E}(Q(G,v) \mid \mathcal{F}_0) = \frac{k}{n} \left(1 + 3n - 2k - \frac{2}{k} \sum_{j=1}^k a_j \right), \tag{5.2}$$

if there are k clockwise edges pointing from $v + a_j$ to $v + a_j - 1$ for a set $\{a_1, \ldots, a_k\} \subseteq \{1, \ldots, n\}$ (addition taken mod n). To prove this formula, we need only prove that the right hand side satisfies the two properties that characterize the left hand side. The sum over all v (i.e., $\mathbf{E}(\tau \mid \mathcal{F}_0)$) is easy, since it equals

$$k(1+3n-2k) - \frac{2}{n} \sum_{j=1}^{k} \sum_{i=1}^{n} i,$$

which does indeed simplify to 2k(n-k). To check that the right hand side of (5.2) works in (5.1), we proceed as follows. Let f(v) be the right hand side of (5.2). Then

$$g(v) \stackrel{\text{def}}{=} f(v+1) - f(v) = -\frac{2}{n} \left(-k + n \delta_{\min\{a_j\},1} \right),$$

where δ is the Kronecker delta. Hence,

$$-\frac{g(v) - g(v - 1)}{2} = \begin{cases} 1 & \text{if } v \text{ is a sink,} \\ -1 & \text{if } v \text{ is a source, and} \\ 0 & \text{otherwise,} \end{cases}$$

as desired.

Equation (5.2) makes it easy to see when $\mathbf{E}(Q(G, v) | \mathcal{F}_0)$ is maximized: that can occur only when $\{a_1, \ldots, a_k\} = \{1, \ldots, k\}$, in which case $\mathbf{E}(Q(G, v) | \mathcal{F}_0)$ equals 3n(k/n)(1 - k/n). This quantity is bounded above by 3n/4, with equality if and only if n = 2k.

Proof of Proposition 2.6. Induct again, as in the proof of Lemma 4.12 and the main theorem. Simultaneously, we show by induction that $\mathbf{E}(Q(G,v) | \mathcal{F}_0) \leq 2(n-1)$, with equality only for the leaf of an *n*-lollipop and initial conditions $X_{e,0}$ all pointing toward v. Note that the previous proposition proves this bound for all $G \in \mathcal{S}_0$, if we use monotonicity (which also holds conditioned on the initial orientation).

For the base case, $G \in \mathcal{S}_0$ and Proposition 5.13 shows that in fact $\mathbf{E}(\tau \mid \mathcal{F}_0) < 3n^2/4$. There is strict inequality because equality in Proposition 5.13 cannot hold simultaneously for all vertices in a cycle. It follows that $\mathbf{E}(\tau \mid \mathcal{F}_0) < n(n-1)$ unless $n \leq 3$. The cases with $n \leq 3$ are easily dealt with: those with n = 2 are trivial, and for n = 3 the worst case contains a 3-cycle, which can be analyzed using the sharper bounds in the proof of Proposition 5.13.

When G is not connected or is the union of two graphs in \mathcal{S} along an added isthmus, the n(n-1) bound is immediate from subadditivity of n(n-1) and monotonicity, and the 2(n-1) bound follows from monotonicity. Finally, when G has a leaf v, set $H := G \setminus \{v\}$ as before. This time, in the worst case we know that v is a sink initially, so $\mathbf{E}(Q(G,v) \mid \mathcal{F}_0)$ is bounded by $2 + \mathbf{E}(Q(H,w) \mid \mathcal{F}_0)$. This verifies the conclusion that $\mathbf{E}(Q(G,v) \mid \mathcal{F}_0) \le 2(n-1)$, and adding this to $\mathbf{E}\tau_H$ gives, by induction, at most (n-1)(n-2)+2(n-1)=n(n-1), which completes the proof of the upper bound; the conditions for equality are clear from the proof.

6. Questions

It is tempting to view both cycle popping and sink popping as special cases of what might be called "partial rejection sampling:" to generate a random structure, choose a random candidate, and if it has any flaws, locally rerandomize until it is flawless. Does partial rejection sampling apply to other natural combinatorial problems? Can one develop a general theory? Note that Fill and Huber's randomness recycler [FH] also uses the idea of rejecting only part of a structure, although in a different way.

Cycle popping was applied to the study of random spanning trees on \mathbb{Z}^d , as well as some more general graphs, in [BLPS]. It would be interesting if sink popping could be used similarly. Do random sink-free orientations on \mathbb{Z}^d exhibit any interesting or surprising structure?

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References

- [A] D. Aldous, A random walk construction of uniform spanning trees and uniform labelled trees, SIAM Journal of Discrete Mathematics 3 (4) (1990), 450–465.
- [BLPS] I. Benjamini, R. Lyons, Y. Peres, and O. Schramm, *Uniform spanning forests*, Ann. Probab. **29** (2001), no. 1, 1–65.
- [B] A. Broder, Generating random spanning trees, Proceedings of 30th Annual Symposium on Foundations of Computer Science (Research Triangle Park, NC, 1989), 442–447, IEEE, 1989.

- [BD] R. Bubley and M. Dyer, Graph orientations with no sink and an approximation for a hard case of #SAT, Proceedings of the Eighth Annual ACM-SIAM Symposium on Discrete Algorithms (New Orleans, LA, 1997), 248–257, ACM, New York, 1997.
- [CEP] H. Cohn, N. Elkies, and J. Propp, Local statistics for random domino tilings of the Aztec diamond, Duke Math. J. **85** (1996), no. 1, 117–166, arXiv:math.CO/0008243.
- [E] K. Eriksson, Strong convergence and the polygon property of 1-player games, Discrete Math. **153** (1996), no. 1–3, 105–122.
- [F] W. Feller, An introduction to probability theory and its applications, Volume I, third edition, John Wiley & Sons, Inc., New York, 1968.
- [FH] J. Fill and M. Huber, The randomness recycler: a new technique for perfect sampling, Proceedings of the Forty-first Annual Symposium on Foundations of Computer Science (Redondo Beach, CA, 2000), 503–511, IEEE, 2000.
- [H] M. Huber, Exact sampling and approximate counting techniques, Proceedings of the Thirtieth Annual ACM Symposium on the Theory of Computing (Dallas, TX, 1998), 31–40, ACM, New York, 1998.
- [JS] M. Jerrum and A. Sinclair, Approximate counting, uniform generation and rapidly mixing Markov chains, Inform. and Comput. 82 (1989), no. 1, 93–133.
- [P] R. Pemantle, Choosing a spanning tree for the integer lattice uniformly, Ann. Probab. **19** (1991), no. 4, 1559–1574.
- [PW1] J. Propp and D. Wilson, Exact sampling with coupled Markov chains and applications to statistical mechanics, Random Structures and Algorithms 9 (1996), no. 1–2, 223–252.
- [PW2] J. Propp and D. Wilson, 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), 170–217.
- [W] D. Wilson, Generating random spanning trees more quickly than the cover time, Proceedings of the Twenty-eighth Annual ACM Symposium on the Theory of Computing (Philadelphia, PA, 1996), 296–303, ACM, New York, 1996.