Sampling Lattice Points

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Abstract

When is the volume of a convex polytope in $\boldsymbol{R}^n$ close to the number of lattice points in the polytope? We show that if the polytope contains a ball of radius $n\sqrt{\log m}$, where m is the number of facets, then the volume approximates the number of lattice points to within a constant factor. This general condition is then specialized to derive polynomial time sampling and counting algorithms for various combinatorial problems whose solutions can be viewed as lattice points of convex polytopes. We also show, via tight examples, that our condition is essentially the best possible.

1 Introduction

In this paper we consider the problem of counting approximately the number of lattice points in an $n-$dimensional polytope of the form

$$P = \{x \in \mathbf{R}^n : Ax \leq b\},$$

where A is an $m \times n$ matrix of nonnegative reals and b is an $m-$ vector of nonnegative reals. Letting $\mathbf{Z}^n$ denote the set of integer points (points with all integer coordinates), we are interested in the problem of estimating $|P \cap \mathbf{Z}^n|$ given A, b. Closely related to it is the problem of sampling nearly uniformly from the set $P \cap \mathbf{Z}^n$ [10].

This problem includes as a special case several combinatorial counting problems that have been studied - like that of estimating the permanent of a 0-1 matrix [9], the number of contingency tables [6], solutions to knapsack problems [5] etc.. It is well-known that the finding $|P \cap \mathbf{Z}^n|$ exactly is # P-hard [14]. It is also easy to show that it is NP-hard to estimate $|P \cap \mathbf{Z}^n|$ to any polynomial (in input length) factor. For completeness, we include a proof of this folklore result here.

An approach to the problem is to reduce it to the tractable problem of estimating the volume of P or a related polytope (see [4]). Intuitively, it is easy to argue that if each entry of b is sufficiently large, then the number of integer points in the polytope is close to the volume of the polytope. In fact, this general principle can be dated back to Gauss, and has been the subject of many fascinating studies (see e.g. [7]).

In this paper, we prove that if the polytope contains a ball of radius $\Omega(n\sqrt{\log m})$, then the volume of P approximates $|P \cap \mathbf{Z}^n|$ well. We also show that this is essentially tight. The proof is relatively simple and is algorithmic, so it actually yields an algorithm to sample nearly uniformly from $P \cap \mathbf{Z}^n$ under the condition. We give a simple class of examples to show that the bound is tight to within constants.

From this general result, several interesting special cases follow.

One interesting case is that of sampling uniformly from the set of nonnegative integer matrices with specified row and column sums (called "contingency tables"). Specifically, the problem is the following : for natural numbers m, n, we are given "row sums" $r_1, r_2, \dots r_m$ and column sums $c_1, c_2, \dots c_n$ which are all nonnegative integers with $\sum r_i = \sum c_j$. We are to pick a sample nearly uniformly from the integer points in the polytope

$$P = \{x \in \mathbf{R}_+^{mn} : \sum_j x_{ij} = r_i \quad \text{for } i = 1, 2, \dots m \quad \sum_i x_{ij} = c_j \quad \text{for } j = 1, 2 \dots n\}.$$

This problem arises in Statistics and Combinatorics [2, 3]. Dyer, Kannan and Mount [6] gave a polynomial time algorithm for this problem provided $r_i \in \Omega(mn^2)$ and $c_j \in \Omega(nm^2)$. Our general result here implies the earlier result, with a simple proof (and with slightly weaker assumptions).

A second special case is that of sampling nearly uniformly from the set of integral $s - t$ flows in a network $G = (V, E)$. We show that if each edge capacity is at least $|E|\sqrt{|E|}$, we can do the sampling in polynomial time and hence also solve approximately the problem of counting the number of integral flows. In contrast, we recapitulate the folklore result that it is NP-hard to estimate the number of integral flows when the capacities are all 1. It is an interesting open problem to reduce this gap.

A third special case is the b-matching problem. In this problem, we are given non-negative integers $b(v)$ associated with the vertices of a graph G. A b-matching is an edge-weighted subgraph of G whose degree at vertex v is at most $b(v)$. Optimization over the set of b-matchings of a graph is studied e.g. in [8]. Here we show that if all the $b(v)$'s satisfy $b(v) \geq |E| deg(v)$, where $deg(v)$ is the degree of vertex v in G, then we can sample uniformly from the set of b-matchings.

Another special case is that of the multidimensional knapsack problem. Here the polytope

P is of the form

$$P = \{x \in \mathbf{R}^n : Ax \leq b, 0 \leq x_i \leq d, \quad for \quad i = 1, \ldots, n\},$$

where A is a nonnegative integer matrix and d is a vector of "upper bounds". Without loss of generality, we may assume that $d_j A_{ij} \leq b_i$ for all i, j. It is shown in [5] that if all $d_j \geq n^2$, then there is a polynomial time algorithm to count approximately the number of integer points in P. We show that our general result gives a polynomial time algorithm with slightly better bounds.

2 The Sampling Theorem

We call a point in $\mathbf{R}^n$ with all integer coordinates an integer point. If x is any point, and λ a positive real, we denote by $C(x, \lambda)$ the cube of side 2λ with x as center.

Suppose A is an $m \times n$ matrix of reals and b is an $m \times 1$ of nonnegative reals and

$$P = \{x \in \mathbf{R}^n : Ax \leq b\}.$$

Let r be the maximum number (over integral points x) of facets of P that intersect any $C(x, 1)$ for x an integral point. Let A_i denote the i th row of A. Then our main result can be summarized as follows.

Theorem 1 *For any polytope P satisfying $b_i \in \Omega(n\sqrt{\log r}|A^{(i)}|)$ for all i, there exists a polynomial time algorithm for nearly-uniformly sampling $P \cap \mathbf{Z}^n$.*

The running time of the algorithms will be inversely proportional to the desired accuracy. The rest of this section is devoted to proving this theorem by constructing a sampling algorithm.

Let c be any positive real to be specified later and let b' be a $m-$vector defined by

$$b'_i = b_i + (c + \sqrt{2 \log r})|A_i|.$$

$$\text{Let } P' = \{x : Ax \leq b'\}.$$

Our idea will be to pick a point p from P' from a probability density close to the uniform. We will then "round" p to obtain an integer point; if the integer point is in P, we accept, otherwise, we reject and repeat. We will use a natural probabilistic rounding procedure which we describe presently. This simple rounding procedure used in a different context by Raghavan and Thompson e.g. [13], is the main new ingredient here.

For $p \in \mathbf{R}^n$, we define a vector-valued random variable $X(p)$ by

$$X(p)_i = \begin{cases} \lfloor p_i \rfloor + 1 & \text{with probability} \quad p_i - \lfloor p_i \rfloor \\ \lfloor p_i \rfloor & \text{with probability} \quad 1 - p_i + \lfloor p_i \rfloor \end{cases}$$

where the $X(p)_i, i = 1, 2, \ldots n$ are chosen independently.

Theorem 2 *Suppose p is picked from a probability density $\mathcal{P}$ whose variational distance to the uniform density on P' is at most ε. Then for any $x \in P \cap \mathbf{Z}^n$, we have*

$$\frac{1 - 2e^{-c^2} - \varepsilon}{Vol(P')} \quad \leq \quad \mathbf{Pr}\left(X(p) = x\right) \quad \leq \quad \frac{1}{Vol(P')}.$$

Proof. First we establish the lower bound. The idea is to bound the probability of picking an integer point x in terms of the probability of picking x given that we pick a continuous point in $C(x, 1)$.

Define $\{Y_i\}_{i=1}^n$ to be independent identically distributed real valued random variables each distributed according to the density function $1 - |t|$ on the real interval $t \in [-1\ +1]$. In the calculations below, dp is an infinitesimal n-dimensional volume and $d\mathcal{P}$ is the probability of picking a point from dp. Then for any $x \in P \cap \mathbf{Z}^n$, and $p \in \mathbf{R}^n$, with $|p_i - x_i| \leq 1$, we have that

$$\text{Prob. density } (x + Y = p) = \prod_{i=1}^{n} (1 - |p_i - x_i|).$$

$$\text{Also, } \mathbf{Pr}(X(p) = x | p) = \prod_{i=1}^{n} (1 - |p_i - x_i|).$$

$$\int_{p \in P'} \mathbf{Pr}(X(p) = x|p) d\mathcal{P} = \frac{1}{\mathrm{Vol}(P')} \int_{p \in P'} \mathbf{Pr}(X(p) = x|p) dp + \varepsilon',$$

where $|\varepsilon'| \leq \varepsilon$.

$$\text{Now, } \int_{p \in P'} \text{Prob. density } (x + Y = p) dp =$$

$$\int_{p \in C(x,1)} \text{Prob. density } (x + Y = p) dp - \int_{C(x,1) \setminus P'} \text{Prob. density } (x + Y = p) dp$$

$$\geq 1 - \sum_{i=1}^{r} \mathbf{Pr}(A_i Y \geq b_i' - b_i).$$

Now for a fixed i, consider the random variables

$$Z_j = \sum_{k=1}^{j} A_{ik} Y_k.$$

It is easy to see that $E(Z_j|Z_{j-1}) = Z_{j-1}$, so the $\{Z_j\}$ form a Martingale. Also, $|Z_j - Z_{j-1}| \leq A_{ij}$. So applying Azuma's inequality [1], we get that

$$\mathbf{Pr}(A_i Y \geq b'_i - b_i) \leq 2e^{-c^2}/r.$$

This proves the lower bound in the Theorem.

The upper bound on the probability follows by

$$\int_{p \in C(x,1)} \text{Prob. density } (x + Y = p)dp = 1.$$

We show that each $x \in P \cap \mathbf{Z}^n$ gets picked with about the same probability by the following algorithm.

Sampling Algorithm

Suppose $\epsilon > 0$ is given.

- Pick a point p from P' with $c = \sqrt{\ln \frac{4}{\epsilon}}$, according to a probability density $\mathcal{P}$ whose variational distance to uniform is at most $\frac{\epsilon}{2}$.
- If $X(p)$ is in P, then return it; otherwise reject and repeat.

It remains to show that the probability of rejection is not too high assuming bounds on b_i.

Lemma 1 *If $b_i \geq 8n\sqrt{\log \frac{r}{\epsilon}}|A_i|$ for all i, then the probability of acceptance of the sampling algorithm is at least $\frac{1}{32}$.*

Proof. The probability of acceptance is

$$\sum_{x \in P \cap \mathbf{Z}^n} \mathbf{Pr}(X(p) = x) \geq \frac{1}{4} \frac{|P \cap \mathbf{Z}^n|}{\text{Vol}(P')}.$$

We show that

$$|P \cap \mathbf{Z}^n| \geq \frac{1}{8}\text{Vol}(P').$$

To this end, suppose we pick p from the uniform density from

$$P'' = \{x : A_i x \leq b_i - (c + \sqrt{2\log r})|A_i| \text{for } i = 1, 2, \ldots m\}$$

and let $x = X(p)$. Then by the same argument as before, with probability at least $\frac{1}{4}$, x will be in $P \cap \mathbf{Z}^n$. Also, for a fixed $x \in P \cap \mathbf{Z}^n$, the probability that we get $X(p) = x$ by this process is at most $1/\text{Vol}(P'')$. So,

$$\frac{|P \cap \mathbf{Z}^n|}{\text{Vol}(P'')} \geq \text{ Prob. that } X(p) \in P \geq \frac{1}{4}.$$

Thus, $|P \cap \mathbf{Z}^n| \geq \frac{1}{4}\mathrm{Vol}(P'')$. Now,

$$\frac{\mathrm{Vol}(P')}{\mathrm{Vol}(P'')} \leq \max_i \left(\frac{b_i + (c + \sqrt{2\log r})|A_i|}{b_i - (c + \sqrt{2\log r})|A_i|} \right)^n \leq 2.$$

□

For algorithmic purposes we can weaken the lower bound to be that each component of b is $\Omega(n|A^{(i)}|\frac{\sqrt{\log r}}{\log n})$.

Note that we assumed as hypothesis that $b_i \in \Omega(n\sqrt{\log r}|A^{(i)}|)$. It is easy to see that this is equivalent to saying that a ball of radius $\Omega(n\sqrt{\log r})$ with the origin as center is contained in P. It is then a simple matter to remove the restriction that the ball have the origin as its center.

The latest algorithms for estimating the volumes of convex sets (or sampling from them) are quite fast: $O^*(n^5)$ [11]. This follows a long series of improvements starting from [4] and [12]. It is worth mentioning that these "continuous" random walks are now provably much faster than their discrete counterparts.

The arguments used in proving Theorem 1 also prove

Theorem 3 *Let P be a polytope in $\boldsymbol{R}^n$ with m facets containing a ball of radius $\Omega(n\sqrt{\log m})$. Then there is a constant c such that*

$$c|P \cap \mathbf{Z}^n| \leq \mathit{Vol}(P) \leq \frac{1}{c}|P \cap \mathbf{Z}^n|.$$

3 Special cases of the theorem

3.1 Contingency tables

The problem is as described in the Introduction. But it will be more convenient to deal with a full dimensional polytope. With some simple manipulation, it is easy to see that as in [6], we can define the polytope P with $\{x_{ij}\}, 1 \leq i \leq m-1 \quad 1 \leq j \leq n-1$ as the variables defined by the following constraints :

$$\sum_{j=1}^{n-1} x_{ij} \leq r_i \quad \forall i$$

$$\sum_{i=1}^{m-1} x_{ij} \leq c_j \quad \forall j$$

$$\sum_{i=1}^{m-1}\sum_{j=1}^{n-1} x_{ij} \geq \sum_{i=1}^{m-1} r_i - c_n \quad x_{ij} \geq 0.$$

In the above, as well as in the rest of the section, i will run through $1, 2, \ldots m-1$ and j will run through $1, 2, \ldots n-1$ unless otherwise specified.

To apply Theorem 1, we will reformulate the problem with the substitution

$$y_{ij} = x_{ij} - mn.$$

Then the polytope P in y-space is defined by

$$\sum_{j=1}^{n-1} y_{ij} \leq r_i - mn(n-1) \quad \forall i$$

$$\sum_{i=1}^{m-1} y_{ij} \leq c_j - mn(m-1) \quad \forall j$$

$$\sum_{i=1}^{m-1}\sum_{j=1}^{n-1} y_{ij} \geq \sum_{i=1}^{m-1} r_i - c_n - mn(n-1)(m-1)$$

$$y_{ij} \geq -mn.$$

Now if $r_i \geq 2mn^2$ for each r_i and $c_j \geq 2nm^2$ for each c_j, P satisfies the theorem's requirements. We can relax these conditions slightly, namely it suffices to have $r_i \geq 2mn^2/\sqrt{\log mn}$ and $c_j \geq 2nm^2/\sqrt{\log mn}$ for each r_i and each c_j respectively.

3.2 Integral flows

In this section we consider the problem of sampling (nearly) uniformly from the set of integral $s-t$ flows in a network. Although our approach could be used for directed graphs, for simplicity we assume here that we are given an undirected graph $G = (V, E)$ with capacities on the edges $C : E \to \boldsymbol{R}^+$, and two distinguished vertices $s, t \in V$ called the source and the sink respectively. An *integral flow* is an assignment of integers to the edges corresponding to a flow from s to t. Such an assignment must respect the capacity constraints, namely the flow through an edge must be less than the capacity, and the conservation constraints, namely the net flow at a vertex must be zero. To set up the problem as a polytope, we make two modifications to G. First we add the edge (t, s) to the graph (if it is not present) so that we can enforce the conservation constraints at all vertices (i.e. including s and t). Then we arbitrarily direct every edge so that E is now a set of directed edges. The resulting polytope of feasible solutions, P, has the following constraints:

$$-C(i,j) \leq x_{ij} \leq C(i,j) \quad \forall (i,j) \in E$$
$$\sum_{j:(i,j)\in E} x_{ij} = \sum_{j:(j,i)\in E} x_{ji} \quad \forall i \in V.$$

This polytope is not full-dimensional in $\boldsymbol{R}^{|E|}$. It will be more convenient to work with a full-dimensional polytope, so we apply some further transformations. Choose a spanning tree T of G (such a spanning tree exists because in order to have a non-zero flow we can assume that s and t are in the same connected component; any component that does not contain s or t is irrelevant and can be deleted). For simplicity, we can assume that T is an arborescence, rooted at s (say), by directing the edges of T first, when we chose directions, and then the rest of the edges. Number the vertices in postfix order along T, so that each vertex gets a higher number than any descendant of it. Consider the conservation constraint for a leaf vertex i, let $(k,i) \in T$ be the leaf edge.

$$x_{ki} = \sum_{j:(i,j)\in E\setminus T} x_{ij} - \sum_{j:(j,i)\in E\setminus T} x_{ji}.$$

By substituting these expressions for leaf edges in the conservation constraints for next-to-leaf vertices, and recursing, we get the following equations, one for each tree edge (k,l):

$$x_{kl} = \sum_{i\in S(l)} \left(\sum_{j:(i,j)\in E\setminus T} x_{ij} - \sum_{j:(j,i)\in E\setminus T} x_{ji} \right) \quad \forall (k,l) \in T$$

Here $S(l)$ denotes the set of vertices in the subtree rooted at l in T. So the polytope P can be reformulated in $\boldsymbol{R}^{|E|-|V|+1}$ space as

$$-C(i,j) \leq x_{ij} \leq C(i,j) \quad \forall (i,j) \in E \setminus T$$
$$-C(k,l) \leq \sum_{i\in S(l)} \left(\sum_{j:(i,j)\in E\setminus T} x_{ij} - \sum_{j:(j,i)\in E\setminus T} x_{ji} \right) \leq C(k,l) \quad \forall (k,l) \in T.$$

Since each constraint trivially has at most E variables, if each capacity is at least $|E|^{\frac{3}{2}}$ then we can apply the theorem to sample the integer points of P nearly uniformly (and thus also count the number of integral flows). Note that a simple modification will allow us to sample the number of flows of a specified value f.

3.3 Hardness of counting flows

To contrast with the above result, we recount the folklore result that it is NP-hard to count approximately the number of flows. We do this by reducing the NP-complete problem of deciding whether a graph has a Hamilton cycle to this approximate counting problem.

Theorem 4 *It is NP-hard to count the number of $s-t$ simple paths in a graph with n vertices to any $poly(n)$ factor.*

Proof. Let $k, l \in \mathbf{Z}_+$ be two numbers which we will fix later. We replace each edge of G by lk edges: first divide the edge into l edges by introducing $l-1$ new vertices, and then replace each resulting edge with k parallel edges.

The number of cycles in the new graph G' will tell us if the original graph G is hamiltonian. If G is Hamiltonian then G' has at least $(k^l)^n = k^{ln}$ cycles (corresponding to a single Hamilton cycle). On the other hand, if G has no cycles of length n, an upper bound on the number of cycles in G' is $k^{l(n-1)}2^n n!$ because there are fewer than $2^n n!$ cycles in G and each has at most $k^{l(n-1)}$ representatives in G'. By a suitable choice of k, l with each only $O(n)$, we can make the first number higher than any fixed $poly(n)$ times the second number. Thus counting the number of cycles in G' up to any $poly(n)$ factor would let us decide if G is Hamiltonian.

Finally, the number of cycles involving a particular edge (u, v) is just the number of paths/flows from u to v in the graph with the edge deleted and all capacities set to 1. $\square$

3.4 b-matchings

Given an undirected graph, $G = (V, E)$, and a function $b : V \to \mathbf{Z}^+$, a *b-matching* is an assignment of positive integers to edges, $x : E \to \mathbf{Z}^+$, so that the sum of the weights on edges incident at a vertex v is at most $b(v)$. A b-matching is *perfect* if it has a weight of exactly $b(v)$ at every vertex. A perfect b-matching can be found in polynomial time (if one exists) using the ellipsoid algorithm [8]. Here we consider the problem of sampling from the set of b-matchings uniformly at random.

Let P be the polytope defined by the following constraints.

$$x(e) \geq 0 \quad \forall e \in E$$

$$x(\delta(v)) \leq b(v) \quad \forall v \in V$$

In the second set of constraints, $\delta(v)$ represents the edges incident to v and $x(\delta(v))$ is the sum of the weights on these edges. Any integer solution satisfying the above constraints is a valid b-matching of G.

Let $|E| = m$, and $d(v)$ be the degree of a vertex v. To apply the theorem, we use the following substitution,

$$y(e) = x(e) - m.$$

Then in y-space, we have the following polytope

$$y(e) \geq -m$$

$$y(\delta(v)) \leq b(v) - md(v).$$

Now for any b such that $b(v) \geq 2md(v)$ for all $v \in V$, and in particular for b such that each $b(v) \geq 2mn$, we can sample b-matchings of G nearly uniformly. This can be extended to sampling capacitated b-matchings, where there are additional constraints on the maximum weights assigned to edges [8].

4 Tight examples

In this section we give examples to show that our bound on the components of b is tight (up to a $\sqrt{\log r}$ factor). Consider the simplex in n dimensions,

$$P = \{x \in \mathbf{R}^n : \sum_{i=1}^{n} x_i \leq b, \quad x_i \geq 0 \quad \forall i\}$$

To derive an upper bound, we can reformulate P (thereby centering it around the origin). We substitute,

$$y_i = x_i - n.$$

Then in y-space, P becomes,

$$\sum_{i=1}^{n} y_i \leq b - n^2, \quad y_i \geq -n \quad \forall i.$$

So now for $b \geq n^2 + n\sqrt{n}$, P satisfies the conditions of the theorem.

Let us examine what happens if b is slightly smaller. The volume of the simplex is $b^n/n!$ and the number of lattice points in P, i.e., the number of ways of dividing b into n or fewer parts is $\binom{b+n-1}{n-1}$. So the ratio of the number of lattice points to the volume is

$$\frac{n(b+n-1)!}{b^n b!}$$

which is the same as

$$\frac{n}{b}(1+\frac{n-1}{b})(1+\frac{n-2}{b})..(1+\frac{1}{b}).$$

The latter is lower bounded by

$$\frac{n}{b}(1+\frac{n-1}{2b})^{\frac{n}{2}}.$$

For any c such that $b \leq cn^2$, this is exponential in $1/c$ (the ratio is about $e^{\frac{1}{c}}$), showing that the volume is no longer a good approximation to the number of lattice points.

5 Conclusion and open problems

Is the dependence of our main theorem on m, the number of facets, necessary? It would be nice to get rid of it.

Although we have presented a (nearly) tight condition for sampling lattice points, it is possible that a different point of view would yield more general algorithms. For example, for *lattice point based random walks*, what are some simple, easy-to-verify conditions that guarantee rapid-mixing?

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