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Fast Unimodular Counting

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This paper describes methods for counting the number of nonnegative integer solutions of the system Ax = b when A is a nonnegative totally unimodular matrix and b an integral vector of fixed dimension. The complexity (under a unit cost arithmetic model) is strong in the sense that it depends only on the dimensions of A and not on the size of the entries of b. For the special case of 'contingency tables' the run-time is $2^{O(\sqrt{d}\log d)}$ (where d is the dimension of the polytope). The method is complementary to Barvinok's in that our algorithm is effective on problems of high dimension with a fixed number of (non-sign) constraints, whereas Barvinok's algorithms are effective on problems of low dimension and an arbitrary number of constraints.

1. Introduction

In this paper we are concerned with determining the number of nonnegative integer solutions, x, to the linear system Ax = b where A is a nonnegative totally unimodular matrix. Even the restricted 'contingency table' version of this problem is #P hard in general [7]. The method applies even when the dimension is not fixed (only the number of equality constraints needs to be fixed). In the application of interest the number of equality constraints and dimension are simultaneously fixed.

It was shown by Barvinok [2, 1] that counting the number of lattice points in an integral polytope is solvable in polynomial time when the dimension is fixed. This method is somewhat difficult to implement (requiring the solution of fixed dimension integer programs and extensive use of triangulations) so there is still some room for specialized techniques for specific problems. We remark that the 4 × 4 transportation (or magic square) polytope is not simple and has a set of vertices that form a non-primitive simplex.

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Since Barvinok's algorithm is based on the additivity of valuations on simple cones, this means Barvinok's algorithm must triangulate and may encounter non-primitive cones.

We also would like to point out the fascinating literature on the dependencies of counting functions (algebraic relations obeyed by the number of nonnegative integer solutions to various linear systems - allowing the computation of solutions for new systems with no additional counting) [4, 17, 18]. While there is a theory of how to solve counting problems directly using algebraic information ('Todd classes' [8]), the less delicate method of using the algebraic dependencies directly on counts (and using brute force to compute the required values) seems fairly effective [13].

Throughout the paper, A is a nonnegative totally unimodular nonnegative m row by ncolumn matrix of full row rank. Without loss of generality we will assume that there is no nonzero nonnegative vector x such that $Ax \leq 0$. We are interested in computing the number of nonnegative integral solutions to Ax = b, $b \in \mathbb{Z}^m \ge 0$. Set $B = \max_i b_i$, and let $\sharp(\{\ldots\})$ denote the number of items in the set $\{\ldots\}$.

2. Method

We are striving for a 'strong' solution to the counting problem; that is, an algorithm with run-time, under the unit cost arithmetic model on numbers of size commensurate with the desired answer, depending only on the order of A and not on the magnitude of the

We show that for a fixed matrix A the function $f_A(b): \mathbb{Z}^m \to \mathbb{Z}$ that computes the number of nonnegative integral solutions to the system Ax = b is a piecewise polynomial in b with degree n-m and no more than $\left(m\binom{n}{m}\right)^m$ pieces. Our method is as follows: for a given b determine the piece and derive the polynomial p on that section. We then evaluate p(b) to get the desired value of $f_A(b)$. Determining which polynomial to use is simple: our decomposition is into polyhedral cones, each defined by no more than $m\binom{n}{m}$ linear inequalities. To find the cone our problem falls in we do not need to compute the entire decomposition (or 'fan'), but only inspect the $m\binom{n}{m}$ linear inequalities. The required polynomial is derived by solving $\binom{n}{m}$ counting problems involving numbers of size no more than $m^{m/2}$ and then applying an interpolation formula.

To solve the $\binom{n}{m}$ smaller problems required by the interpolation formula we exhibit two methods that have proved useful in practice. The first method is a divide and conquer approach that has proved useful for problems where b has small norm. The other method we call the 'even/odd' approach and can solve the needed sub-problems in time $2^{O(m \log m)}$ in general. For the 'magic square' case which has dimension $d = O(m^2)$ this yields a run-time of $2^{O(\sqrt{d}\log d)}\log B$ using the 'even/odd' approach directly and a run-time of $2^{O(\sqrt{d}\log d)}$ using the interpolation approach outlined above (even after allowing for the time to identify which cone we are in and perform the interpolation).

2.1. Piecewise polynomiality

Throughout this note, P will be a lattice polytope, that is, a polytope such that all vertices have integer coordinates. A famous theorem of Ehrhart is that, as k ranges over the me showland it

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Theorem 2.1 (McMull integers $k_1, \ldots, k_M \geqslant 0$,

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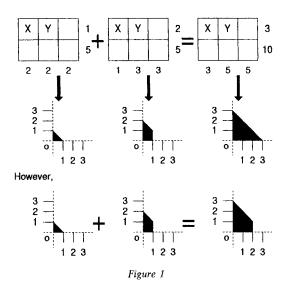
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nonnegative integers, the number of integral points in the polytope kP is a polynomial in k with degree the dimension of the smallest affine space containing P (see [11]).

In fact the result immediately strengthens into an analogue of the so called 'mixed volumes' of convex geometry (the symbol + denotes the Minkowski sum).

Theorem 2.1 (McMullen, Bernštein). For any lattice polytopes $P_1, ..., P_M \subset \mathbb{R}^N$ and integers $k_1, ..., k_M \ge 0$,

$$\sharp (k_1 P_1 + \dots + k_M P_M) = \sum_{r_1 + \dots + r_M \leq N} C(P_1, r_1, \dots, P_M, r_M) k_1^{r_1} \dots k_M^{r_M},$$

where the $C(P_1, r_1, ..., P_M, r_M)$ are constants depending only on $P_1, r_1, ..., P_M, r_M$.

The counting function $f_A(b)$ (mentioned above) is not itself a single polynomial for the simple reason that there are A, b_1 , b_2 such that the polytopes $Ax = b_1$, $x \ge 0$ and $Ax = b_2$, $x \ge 0$ do not Minkowski sum to the polytope $Ax = b_1 + b_2$, $x \ge 0$. An example is the set of contingency tables given by

$$A = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \end{bmatrix}, \quad b = \begin{bmatrix} r_1 \\ r_2 \\ c_1 \\ c_2 \end{bmatrix}.$$

For $\sigma \subset \{1, 2, ..., n\}$ of cardinality m, let A_{σ} be the $m \times m$ matrix formed by the columns of A indexed by σ . Similarly, for any vector v let v_{σ} be the entries of v indexed by σ . Let Γ be the set of σ such that $\det(A_{\sigma}) \neq 0$. Let Ψ be the set of all $r \in \mathbb{R}^m$ such that there exists $\sigma \in \Gamma$ such that r is a row of A_{σ}^{-1} . This divides the positive orthant in \mathbb{R}^m into a collection of equivalence classes such that, for $b_1, b_2 \in \mathbb{R}^m$, we have $b_1 \equiv b_2$ if and only if

 $r \cdot b_1 \geqslant 0 \leftrightarrow r \cdot b_2 \geqslant 0 \ \forall r \in \Psi$. We are interested in the largest dimensional cones in this 'fan'. We say b_1, b_2 are in the same cone if and only if $(r \cdot b_1) \times (r \cdot b_2) \ge 0 \ \forall r \in \Psi$.

Theorem 2.2. If b_1 and b_2 are in the same cone then the Minkowski sum of the polytopes $Ax = b_1, x \ge 0$ and $Ax = b_2, x \ge 0$ is equal to the polytope $Ax = b_1 + b_2, x \ge 0$.

Sketch of proof. We shall use P_b to denote the polytope given by the linear system Ax = b, $x \ge 0$. It is easy to show that $P_{b_1} + P_{b_1} \subseteq P_{b_1 + b_2}$ and that all three of these polytopes are bounded. Also, b_1 and b_2 being in the same cone implies that b_1 , b_2 and $b_1 + b_2$ are all in the same cone (though this is not, in general, a transitive relationship). For $\sigma \in \Gamma$ and $u \in \mathbb{R}^m$ we define $v(\sigma, u)$ to be the vector in \mathbb{R}^n such that $v(\sigma, u)_i = 0 \ \forall i \notin \sigma$ and $v(\sigma, u)_{\sigma} = A_{\sigma}^{-1}u$. All vertices of Ax = b are of the form $v(\sigma, b)$ (though $v(\sigma, b)$ is not always a vertex or even always in P_b).

Let v be an arbitrary vertex of $P_{b_1+b_2}$ and σ be such that $v = v(\sigma, b_1 + b_2)$. We note that $v(\sigma, b_1) + v(\sigma, b_2) = v(\sigma, b_1 + b_2)$ and the 'in the same cone' relationship guarantees that $v(\sigma, b_1) \in P_{b_1}$ and $v(\sigma, b_2) \in P_{b_2}$. The arbitrary choice of v completes the proof.

There are no more than $m\binom{n}{m}$ elements in Ψ so the orthant is split into no more than $(m\binom{n}{m})^m$ cones. By combining Theorem 2.1 with Theorem 2.2 we see that the restriction of the counting function $f_A(b)$ to any of these cones is a polynomial of degree no more than n-m [4, 17, 18].

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2.2. Interpolation

We now have a decomposition of the positive orthant into cones such that $f_A(b)$ restricted to any cone is an unknown polynomial of degree n-m. For a given cone, it remains to derive the polynomial. The method we use is to find an integral point y in the interior of the cone. The polynomial for a cone is completely determined by the values of $f_A((n-m)y + \Delta)$ where Δ runs over all $\binom{n}{m}$ nonnegative integral vectors in the simplex S_{n-m} in \mathbb{Z}^m such that $1 \cdot \Delta \leq n-m$. We call the required $f_A((n-m)y + \Delta)$ 'small sub-problems' and describe how to solve them in the next section. With the small subproblem solutions in hand, the interpolation can be done very quickly. We introduce the multivariate 'Lagrange polynomial' $l_{b,x,d}(\cdot)$ which allows us to perform the interpolation without having to (computationally) invert a $\binom{n}{m}$ by $\binom{n}{m}$ matrix. In this notation we call $b \in \mathbb{Z}^m$ the 'base', $x \in \mathbb{Z}^m$ is such that $x - b \in S_d$ and d is the degree. We define $l_{b,x,d}(\cdot)$ as the unique polynomial map from $\mathbb{Z}^m \to \mathbb{R}$ of degree d such that $l_{b,x,d}(x) = 1$ and $l_{b,y,d}(y) = 0$ when y is integral and $y - b \in S$ and $y \neq x$. These polynomials have a very simple explicit formula:

$$l_{b,x,d}(v) \stackrel{\text{def}}{=} \left\{ \begin{array}{ll} \prod_{i=1}^d (1 + (1 \cdot b - 1 \cdot v)/i), & x = b, \\ \frac{(v_i - b_i)}{(x_i - b_i)} l_{b + E^i, x, d - 1}(v), & x_i > b_i, \ x_j = b_j \ \forall j < i. \end{array} \right.$$

Then the desired polynomial is

$$p(v) \stackrel{\text{def}}{=} \sum_{\Delta \in S} f_A((n-m)y + \Delta) l_{(n-m)y,(n-m)y+\Delta,n-m}(v).$$

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(v).

The sum can be evaluated symbolically with v as an indeterminate vector or can be evaluated very quickly using almost no space if $v \in \mathbb{Z}^m$ is given explicitly.

2.3. Size of sub-problems

By Hadamard's inequality [14] the system $Cy \ge 0$, $y \ge 0$ (where the rows of C are elements of Ψ or their opposites) representing an arbitrary cone of the type mentioned above has an integral interior point y such that $y_i \leq m^{m/2+1}$ (remember, because A is totally unimodular all vectors in Ψ are $0,\pm 1$). Graham and Sloane studied the equality version of this problem [10] and Văn H. Vũ of Yale has shown [19] that the $m^{O(m)}$ bound is essentially best possible

2.4. Divide and conquer

For small problems (many of those arising from magic square problems) we have devised a specialized decomposition which we call 'divide and conquer'. This method is similar to that of Chan and Robbins [3] who used it to compute the volume of the order 7 and order 8 Birkhoff polytopes. To count the number of nonnegative integral solutions to Ax = b we divide the columns of A into two sets of size about n_1, n_2 $(n_1 + n_2 = n, n_1 = \lfloor n/2 \rfloor)$: A_1, A_2 and then explicitly enumerate all possible b_1, b_2 such that $A_1x_1 = b_1, x_1 \geqslant 0$ and that $A_2x_2 = b_2$, $x_2 \ge 0$ are feasible and $b_1 + b_2 = b$. We have a recursive expansion of the form

$$\sharp(\lbrace x|Ax = b, \ x \geqslant 0, \ x \in \mathbb{Z}^n\rbrace) = \sum_{b_1,b_2 \ b_1+b_2=b,b_1,b_2 \in \mathbb{Z}^m \geqslant 0} \quad \sharp(\lbrace x_1|A_1x_1 = b_1, \ x \geqslant 0, \ x \in \mathbb{Z}^{n_1}\rbrace) \times \\ \quad \sharp(\lbrace x_2|A_2x_2 = b_2, \ x \geqslant 0, \ x \in \mathbb{Z}^{n_2}\rbrace).$$

This divides an m by n counting problem into no more than B^m sub-problems. We combine this with dynamic programming, meaning that we take care never to solve any sub-problem twice. There are no more than $n \log nB^m$ possible sub-problems, which is sufficient to yield a run-time of $n \log nB^{2m}$.

where R_A is the set $\{Az|z\in\{0,1\}^n\}$. We apply this decomposition recursively to the nonzero/one problems until we have driven all the entries of b to zero. Again, for efficiency we use a dynamic programming to avoid recalculating the value of any sub-problem. We note that in this recursion a limited number of right-hand sides (of the form (b-r)/2) are formed. In fact we solve no more than $n^m \log B$ nonzero/one sub-problems. $\leftarrow ?$

The zero/one problems themselves can be solved using either a specialization of the divide and conquer counter to zero/one problems or another application of dynamic

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programming using the recursive formula

$$\sharp(\{z|Az = b, z \in \{0,1\}^n\}) = \sharp(\{z_1|\tilde{A}z_1 = b, z_1 \in \{0,1\}^{n-1}\}) + \sharp(\{z_2|\tilde{A}z_2 = b - A^1, z_2 \in \{0,1\}^{n-1}\}),$$

where A^1 is the first column of A and \tilde{A} is the matrix formed by all columns of A except the first. Either method yields a run-time no worse than $2^{O(m \log n)}$.

Combining these observations lets us conclude that the zero/one counter can be implemented in $2^{O(m \log n)} \log B$ time. Given our problem size bounds above, this is sufficient to run the entire interpolation method in time $2^{O(m \log n)}$.

3. Contingency tables

A special problem is to find the number of nonnegative matrices that sum to given row and column totals. Such matrices are called contingency tables [6]. If the matrices are square and all rows and columns are constrained to sum to the same value then the matrices are called 'magic squares' [15]. As mentioned before, counting contingency tables is $\sharp P$ hard. Counting or uniformly generating contingency tables has applications in statistics [5].

The generating function for $h \times w$ contingency tables is the following:

$$\prod_{i=1\dots h,\ j=1\dots w}\frac{1}{1-x_iy_j}.$$

Even for magic squares (h = w, B = each row/column total, m = h + w - 1, n = (h-1)(w-1)) the counting can be troublesome (though no complexity result is known). Complete expansion of the generating function can require B^{2h} space and similar time. Dynamic programming methods [9] can perform the calculation using hB^{h-1} space. This still yields a rough run-time of B^{2h} as each entry in the dynamic programming table depends on $O(B^h)$ previous entries. Young/Ferris diagram-based methods [12] roughly need to store all Young/Ferris diagrams on hB dots with $\leq h$ rows (yielding $\approx B^{h-1}$ storage). Once B is as big as order h^2 it can be shown that there are at least $(B/(2h))^{h-1}$ diagrams that are connected to roughly $(B/(2h))^{h-1}$ diagrams each yielding $\approx (B/2h)^{2h-2}$ work.

The divide and conquer approach, mentioned above, can be specialized to this problem and compares favourably to these methods, if performed with care. If A is the matrix representing the contingency table counting problem, one can always split the columns of A approximately in half in such a way that both the sub-problems are contingency table problems with either the width or height halved. By combining with the dynamic programming technique, we get a run-time of $B^{3h/2}$ using B^h storage.

This run-time is noticed by computing the work done at each stage of a dynamic programming implementation of divide and conquer. Table 1 shows how many problems occur at each level, what their width and height is, how many sub-problems each problem needs from the next level, and how much work is done at each level (nodes times connections).

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4.1. Zero/one results

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4.3. Magic squares

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Table 1 3 1 2 level $B^{\frac{1}{2}h}$ $B^{\frac{3}{8}h}$ $B^{\frac{3}{4}h}$ B^h B^h nodes 1 h/4h/2width h/8height h h/2h/2h/4 $B^{h/8}$ $B^{h/2}$ $B^{h/2}$ B^h edges/node $B^{\frac{3}{2}h}$ $B^{\frac{3}{4}h}$ $B^{\frac{1}{2}h}$

 B^h

work

For $B \in o(h^{8/3})$ the divide and conquer counter is faster than the even/odd counter and for $B \in o(h^{4/3})$ the divide and conquer counter takes fewer steps than there are terms in the multivariate counting polynomial.

4. Computational results

4.1. Zero/one results

The following single 5×4 problem was solved in 20 minutes using the zero/one method (a previous solution by the interpolation method took just over one week). There are exactly 23196436596128897574829611531938753 ($\approx 2.3 * 10^{34}$) nonnegative 5 by 4 integer matrices whose rows sum to [182, 778, 3635, 9558, 11110] and columns sum to [3046, 5173, 6116, 10928].

4.2. 4 by 4 contingency tables

The 4×4 contingency table problem (after some symmetries are removed) splits into $\underline{3694}$ cones such that the counting function restricts to a degree 9 polynomial in 7 variables in each cone. This means each polynomial is determined by 11440 coefficients so can be interpolated from 11440 sufficiently general evaluations. Each of the 3694 tasks seems to represent about 3 hours of Pmax CPU time (using the divide and conquer counter), so the total job represented about 1.5 Pmax CPU years. This task was completed in just over 6 weeks using Peter Stout's WAX [16] system, which effectively simulates a coarsegrain parallel supercomputer (employing the numerous idle workstations at CMU). This polynomial was stored on disk and was able to solve typical 4 × 4 contingency tables (with margins around a couple of hundred) in 3 seconds. This was made available on the World Wide Web in the form of an online calculator. 7

4.3. Magic squares

We know [15] that the number of nonnegative integral points in the $n \times n$ Birkhoff polytope (i.e., the number of magic squares) is a polynomial of degree $(n-1)^2$ in r (r an integer). Denote this polytope by $H_n(r)$. In fact, the stronger result is known that

$$\sum_{r\geqslant 0} H_n(r)\lambda^r = \frac{h_0 + h_1\lambda + \cdots + h_d\lambda^d}{(1-\lambda)^{(n-1)^2+1}}$$

where $d = n^2 - 3n + 2$ and the h_i are nonnegative integers such that $h_i = h_{d-i}$, i = 0, 1, ... d. This means that $H_7(r)$ is completely determined by the values of $H_7(1)$ through $H_7(15)$

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Table 2

$H_8(r)$	$H_7(r)$
40320	5040
545007960	9135630
1579060246400	4662857360
1455918295922650	936670590450
569304690994400256	94161778046406
114601242382721619224	5562418293759978
13590707419428422843904	215717608046511873
1046591482728407939338275	5945968652327831925
56272722406349235035916800	123538613356253145400
2233160342369825596702148720	2023270039486328373811
68316292103293669997188919040	27046306550096288483238
1667932098862773837734823042196	303378141987182515342992
33427469280977307618866364694400	2920054336492521720572276
562798805673342016752366344185200	24563127009195223721952590
8115208977465404874100226492575360	183343273080700916973016745
101857066150530294146428615917957029	
1128282526405022554049557329097252992	
11161302946841260178530673680176000200	
99613494890126594335550124219924540800	
809256770610540675454657517194018680846	
6031,107,989,875,562,751,266,116,901,999,327,710,720	

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and $H_8(r)$ is completely determined by the values of $H_8(1)$ through $H_8(21)$. Other authors have reported similar results [3]. These values were computed by the divide and conquer technique, and are shown in Table 2.

With these valuations it is trivial to determine both the polynomials $H_7(r)$, $H_8(r)$ and all the coefficients in the numerators of the generating functions given above. To derive the polynomials we use $H_n(0) = 1$, $H_n(-1) = H_n(-2) = \cdots H_n(-n+1) = 0$ and $H_n(-n-r) = (-1)^{n-1}H_n(r)$. Note that the data given here for $H_7(r)$ and $H_8(r)$ obey conjecture (v) on page 26 of [15].

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40320 545007960

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90994400256

82721619224

28422843904

07939338275

35035916800

96702148720

97188919040

34823042196

56364694400

56344185200

26492575360

15917957029

29097252992

30176000200

19924540800

94018680846

99327710720

 $H_8(21)$. Other authors e divide and conquer

nomials $H_7(r)$, $H_8(r)$ ons given above. To $H_n(-n+1) = 0$ and f(r) and $H_8(r)$ obey

al points in polyhedra omputer Science, IEEE

ttice polytope. Discrete

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