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摘　要

對於有線性目標函數的向量分解問題，且每一部份含向量數有規定時，我們給出一只有多項式繁度的解答。

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Linear-shaped partition problems

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Abstract

We establish the polynomial-time solvability of a class of vector partition problems with linear objectives subject to restrictions on the number of elements in each part.

1. Shaped partition problems

The *shaped partition problem* concerns the partitioning of n vectors $A^1,\ldots,A^n$ in d-space into p parts so as to maximize an objective function which is convex on the sum of vectors in each part subject to arbitrary constraints on the number of elements in each part. This class of problems has applications in diverse fields that include circuit layout, clustering, inventory, scheduling and reliability (see [2,3,5,9] and references therein) as well as important recent applications to symbolic computation [11]. In its outmost generality, the shaped partition problem instantly captures NP-hard problems hence is intractable [8]. The purpose of this article is to exhibit polynomial-time solvability for a broad class of shaped partition problems with linear objectives. To define the problem formally, describe our results and raise some remaining questions, we next introduce some notations.

Let $\mathbb{Q}$ and $\mathbb{N}$ denote, respectively, the rational numbers and nonnegative integers. All vectors are columns by default. The vectors of all-ones and all-zeros, of dimension that is clear from the context, are denoted by $\mathbf{1}$ and $\mathbf{0}$, respectively. A *p-partition* of the set $[n]:=\{1,\ldots,n\}$ is an ordered collection $\pi=(\pi_1,\ldots,\pi_p)$ of pairwise disjoint (possibly empty) sets whose union is $[n]$. The *shape* of π is the tuple $|\pi|:=(|\pi_1|,\ldots,|\pi_p|)$ of nonnegative integers which describes the number of elements in each part of π. Let $\mathbb{N}_n^p:=\{\lambda\in\mathbb{N}^p:\mathbf{1}^T\lambda=n\}$ denote the set of all p-shapes of n. The first ingredient of the problem data is a subset $\Lambda\subseteq\mathbb{N}_n^p$ of *admissible* shapes. The feasible solutions to the problem are then all partitions π of $[n]$ of admissible shape $|\pi|\in\Lambda$. The second ingredient of the problem data is a $d\times n$ matrix A whose jth column A^j represents d numerical attributes associated with the jth element of the partitioned set $[n]$. With each p-partition π of $[n]$ we associate the following $d\times p$ matrix whose kth column represents the total

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attribute vector of the kth part,

$$A^{\pi}:=\left[\sum_{j\in\pi_1}A^j,\ldots,\sum_{j\in\pi_p}A^j\right]\in\mathbb{Q}^{d\times p}$$

with $\sum_{j\in\pi_k}A^j:=0$ when $\pi_k=\emptyset$. The third ingredient of the problem data is a convex functional $C:\mathbb{Q}^{d\times l}\to\mathbb{Q}$. The objective value of a partition π is then defined by $C(A^{\pi})$. We consider the following algorithmic problem.

Shaped partition problem Given positive integers d, p, n, matrix $A\in\mathbb{Q}^{d\times n}$, shape set $\Lambda\subseteq\mathbb{N}_n^p$, and convex functional $C:\mathbb{Q}^{d\times p}\to\mathbb{Q}$, either assert that Λ is empty or find a partition π^* of admissible shape $|\pi^*|\in\Lambda$ attaining maximum objective value, that is,

$$C(A^{\pi^*})=\max\{C(A^{\pi}):\ |\pi|\in\Lambda\}.$$

A natural example is *clustering*, where n observation points $A^1,\ldots,A^n\in\mathbb{Q}^d$ are to be grouped into p clusters in such a way that the sum of suitably defined cluster variances is minimized. The restriction of shapes to a shape set Λ may allow to reflect a priori information about the anticipated number of data points in different clusters. For instance, when minimizing the sum of the l_2 cluster variances $\sum_{i=1}^{p}(1/|\pi_i|)\sum_{j\in\pi_i}\|A^j-\bar{A}^{\pi_i}\|^2$, with $\bar{A}^{\pi_i}:=(1/|\pi_i|)\sum_{j\in\pi_i}A^j$ the cluster barycenter, and the a priori indication that all clusters have the same number of elements, the clustering problem becomes a shaped partition problem with $\Lambda=\{n/p\cdot\mathbf{1}\}$ and C on a matrix $M\in\mathbb{Q}^{d\times p}$ given by $C(M)=\alpha\cdot\langle M,M\rangle-\beta$, with the constants $\alpha=(p/n)^2$ and $\beta=(p/n)\sum_{j=1}^{n}\|A^j\|^2$, and with $\langle M,M\rangle:=\sum_{i=1}^{d}\sum_{j=1}^{p}M_{i,j}^2$.

The shaped partition problem in its full generality, with d, p, n variable, with Λ arbitrary and possibly presented by a membership oracle, and C arbitrary convex and possibly presented by an evaluation oracle, has a very broad expressive power. In fact, as explained in [8], even with fixed $d=1$ or $p=2$, the problem immediately captures NP-hard problems. A major result of Hwang et al. [8] was that, with both d, p fixed, the problem can be solved in polynomial-time with Λ and C arbitrary and presented by oracles.

In the present article, we restrict the class of convex functionals and assume C to be linear, but allow d and p to vary as part of the input. The functional C is then identified with a matrix $C\in\mathbb{Q}^{d\times p}$, and the objective value of a partition π becomes $\langle C,A^{\pi}\rangle$. We prove in Theorem 1 the polynomial-time solvability of the problem for a broad class of shape sets, which in particular implies:

Corollary 1. *Given d, p, n, matrix $A\in\mathbb{Q}^{d\times n}$, and $C\in\mathbb{Q}^{d\times p}$, the shaped partition problem can be solved in polynomial-time for every shape set Λ of one of the following two types:*

1. *Any set $\Lambda=\mathbb{N}_n^p\cap\{\lambda:\ l\leqslant\lambda\leqslant u\}$ of shapes defined by given lower and upper bounds.*
2. *Any explicitly given set $\Lambda=\{\lambda^1,\ldots,\lambda^m\}\subseteq\mathbb{N}_n^p$ of shapes.*

Note that, while the shaped partition problem is obviously intractable if Λ is presented by a mere membership oracle, Corollary 1 part 2 implies that if p is fixed then it is solvable in polynomial oracle time since an explicit presentation of Λ can be obtained by querying the oracle on each element of $\{0,1,\ldots,n\}^p$. It would be interesting to find more general shape sets under weak presentations for which the shaped partition problem is polynomial-time solvable. In particular, for which of the following presentations (of increasing generality), of shape sets which are *convex* in the sense $\Lambda=\mathbb{N}_n^p\cap\mathrm{conv}(\Lambda)$, is the problem tractable?

- Convex shape sets presented by an inequality system $\mathrm{conv}(\Lambda)=\{\lambda:\ U\lambda\leqslant u\}$?
- Convex shape sets presented by a *separation oracle* (cf. [6]) over $\mathrm{conv}(\Lambda)$?

2. Optimization over shaped partition polytopes

The linear-shaped partition problem can be embedded into the problem of maximizing $C\in\mathbb{Q}^{d\times p}$ over the convex hull of matrices of feasible partitions, defined as follows.

Shaped partition polytope The *shaped partition polytope* of matrix $A\in\mathbb{Q}^{d\times n}$ and shape set $\Lambda\subseteq\mathbb{N}_n^p$ is defined to be the convex hull of all matrices of admissible partitions,

$$P_A^{\Lambda}:=\mathrm{conv}\{A^{\pi}:\ |\pi|\in\Lambda\}\subset\mathbb{Q}^{d\times p}.$$

Shaped partition polytopes form a broad class which captures and generalizes many classical polytopes (see

[2,4,7,8,10] and references therein for more details). Since a shaped partition polytope is defined as the convex hull of an implicitly presented set whose size is typically exponential in the input size even when both p and d are fixed, an efficient representation as the convex hull of vertices or as the intersection of half-spaces is not readily expected. It was shown in [8], however, that if both p and d are fixed then the number of vertices is polynomial in n, which was the key to the polynomial-time solution in [8] of shaped partition problems with fixed d, p. Related bounds were given in [1].

In the present article we allow d and p to be a variable part of the input. In this situation, the enumerative methods of Hwang et al. [8] fail: indeed, even if one of d and p remains fixed, the number of vertices of the shaped partition polytope may be exponential in n. For instance, if $d = 1$, $p = n$, $A = [1, \ldots, n]$, and $\Lambda = \{\mathbf{1}\}$ then partitions correspond to permutations and P_A^Λ is the permutohedron having $n!$ vertices. If $p = 2$, $d = n$, $A = I$ is the $n \times n$ identity matrix, and $\Lambda = \mathbb{N}_n^2$ then P_A^Λ is affinely equivalent to the cube having 2^n vertices.

We now take a closer look at the shaped partition polytope of the identity I,

$$P^\Lambda := P_I^\Lambda = \operatorname{conv}\{I^\pi : |\pi| \in \Lambda\} \subset \mathbb{Q}^{n \times p}.$$

We aim to derive an inequality description of P^Λ. Consider the polytope T^Λ defined by

$$T^\Lambda := \{X \in \mathbb{Q}^{n \times p} : X \geqslant 0,\ X\mathbf{1} = \mathbf{1},\ \mathbf{1}^{\mathrm{T}} X \in \operatorname{conv}(\Lambda)\}.$$

Since each matrix I^π is $\{0,1\}$-valued with a unique 1 per row, it follows that $P^\Lambda \subseteq T^\Lambda$ for any shape set $\Lambda \subseteq \mathbb{N}_n^p$. The converse is usually false. For instance, let $n = p = 2$ and let $\Lambda = \{(2,0),(0,2)\}$ be a nonconvex set of two shapes. Then the 2×2 identity I lies in T^Λ since $\mathbf{1}^{\mathrm{T}} I = (1,1) \in \operatorname{conv}(\Lambda)$, but

$$I \notin P^\Lambda = \left\{ \begin{bmatrix} \alpha & 1-\alpha \\ \alpha & 1-\alpha \end{bmatrix} : 0 \leqslant \alpha \leqslant 1 \right\}.$$

Next assume that Λ is convex, that is, $\Lambda = \mathbb{N}_n^p \cap \operatorname{conv}(\Lambda)$. If $\operatorname{conv}(\Lambda)$ has the inequality description $\operatorname{conv}(\Lambda) = \{\lambda \in \mathbb{Q}^p : \lambda \geqslant 0,\ \mathbf{1}^{\mathrm{T}}\lambda = n,\ U\lambda \leqslant u\}$ then T^Λ has the description

$$T^\Lambda = \{X \in \mathbb{Q}^{n \times p} : X \geqslant 0,\ X\mathbf{1} = \mathbf{1},\ UX^{\mathrm{T}}\mathbf{1} \leqslant u\}. \quad (1)$$

As demonstrated below in Example 1, convexity is not sufficient for equality $P^\Lambda = T^\Lambda$. We need a more restrictive assumption on Λ that we describe next. Recall from [12] that a matrix is *totally unimodular* if all its subdeterminants, in particular all entries, are $-1, 0, 1$.

Proposition 1. *Let $\Lambda = \mathbb{N}_n^p \cap \{\lambda : U\lambda \leqslant u\}$ be a convex shape set with U being an integer matrix and u an integer vector. If the matrix $a(U) := [\mathbf{1}\ U^{\mathrm{T}}]^{\mathrm{T}}$ is totally unimodular then*

$$\operatorname{conv}(\Lambda) = \{\lambda \in \mathbb{Q}^p : \lambda \geqslant 0,\ \mathbf{1}^{\mathrm{T}}\lambda = n,\ U\lambda \leqslant u\}. \quad (2)$$

Proof. Clearly $\operatorname{conv}(\Lambda)$ is contained on the right-hand side of (2). Now, since $a(U)$ is totally unimodular, it follows (cf. [12]) that all vertices of the right-hand side of (2) are integers. But Λ is precisely the set of integer points on the right hand side of (2) since $\Lambda = \mathbb{N}_n^p \cap \{\lambda : U\lambda \leqslant u\}$. Hence, all vertices of the right-hand side of (2) lie in Λ and the proposition follows. □

However, as the following example shows, P^Λ may be strictly contained in T^Λ even if Λ is convex and $a(U)$ (and hence U) is totally unimodular.

Example 1. Let $n = p = 4$ and let $\Lambda = \{(2,0,0,2), (1,1,1,1), (0,2,2,0)\}$ be a convex shape set with $\Lambda = \mathbb{N}_4^4 \cap \{\lambda : U\lambda \leqslant 2 \cdot \mathbf{1}\}$, where $a(U)$ is totally unimodular with

$$U = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}.$$

Then both T^Λ and P^Λ are 10-dimensional polytopes in the space $\mathbb{Q}^{4\times 4}$ of 4×4 matrices. However, P^Λ has 24 facets and 36 vertices which are the $\{0,1\}$-matrices I^π, whereas T^Λ has 16 facets and 84 vertices. The only integer vertices of T^Λ are the 36 matrices I^π. To verify directly that P^Λ is indeed strictly contained in T^Λ, define two identical matrices

$$V := C := \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0.5 & 0.5 & 0 \\ 0.5 & 0 & 0 & 0.5 \\ 1 & 0 & 0 & 0 \end{bmatrix}.$$

Then V satisfies the inequalities defining T^Λ but attains the value $\langle C, V\rangle = \sum_{i,j} C_{i,j} V_{i,j} = 3$ under the functional C, which is strictly larger than the value $\langle C, I^\pi\rangle$ for any π with $|\pi| \in \Lambda$.

Let $U = [U^1, \ldots, U^p]$ be an $m \times p$ matrix, let $[U^1\mathbf{1}^{\mathrm{T}}, \ldots, U^p\mathbf{1}^{\mathrm{T}}]$ be the $m \times pn$ matrix obtained

from U by replicating each column n times, and let I be the $n \times n$ identity matrix. Define the following $(n+m) \times pn$ matrix:

$$n(U) := \begin{bmatrix} I & I & \cdots & I \\ U^1\mathbf{1}^T & U^2\mathbf{1}^T & \cdots & U^p\mathbf{1}^T \end{bmatrix}.$$

We then have the following sufficient condition for equality $P^\Lambda = T^\Lambda$ to hold.

Lemma 1. *Let $\Lambda = \mathbb{N}_n^p \cap \{\lambda: U\lambda \leqslant u\}$ be a convex shape set with U an integer matrix and u an integer vector. If the matrix $n(U)$ is totally unimodular then $P^\Lambda = T^\Lambda$.*

Proof. We use the total unimodularity of $n(U)$ twice. First, if $n(U)$ is totally unimodular then so is $a(U) = [\mathbf{1}\ U^T]^T$; indeed, $a(U)$ is the submatrix of $n(U)$ corresponding to rows $(n+i: i = 0,\ldots,m)$ and columns $(j \cdot n: j = 1,\ldots,p)$. Thus, by Proposition 1, $\mathrm{conv}(\Lambda)$ has the description in (2), hence T^Λ has the description in (1). Now, identifying $\mathbb{Q}^{n\times p} \cong \mathbb{Q}^{pn}$ via $X \mapsto [X_{1,1},\ldots,X_{n,1},\ldots,X_{1,p},\ldots,X_{n,p}]$, this inequality description of T^Λ becomes

$$T^\Lambda = \left\{X \in \mathbb{Q}^{pn}: X \geqslant 0, \begin{bmatrix} -I & \cdots & -I \\ I & \cdots & I \\ U^1\mathbf{1}^T & \cdots & U^p\mathbf{1}^T \end{bmatrix} \cdot X \leqslant \begin{bmatrix} -\mathbf{1} \\ \mathbf{1} \\ u \end{bmatrix}\right\}. \quad (3)$$

Second, since $n(U)$ is totally unimodular, so is the coefficient matrix of (3); hence, it follows (cf. [12]) that all vertices of T^Λ are integers. But the integer points in T^Λ are precisely all $\{0,1\}$-matrices which equal I^π for some π with $|\pi| \in \Lambda$. Thus $T^\Lambda = \mathrm{conv}\{I^\pi: |\pi| \in \Lambda\} = P^\Lambda$ as claimed. □

Note that a necessary condition for $n(U)$ to be totally unimodular is that U itself is, which implies at once that the same holds for the replicated matrix $[U^1\mathbf{1}^T,\ldots,U^p\mathbf{1}^T]$. However, this condition is not sufficient in general: the matrix U in Example 1 (and $a(U)$, moreover) is totally unimodular but $n(U)$ is not.

Using Lemma 1 and Proposition 1 we obtain the following statement.

Theorem 1. *The shaped partition problem can be solved in polynomial-time for any d, p, n, matrix $A \in \mathbb{Q}^{d\times n}$, linear functional $C \in \mathbb{Q}^{d\times p}$, and shape set $\Lambda = \mathbb{N}_n^p \cap \{\lambda: U\lambda \leqslant u\}$ with U and u being integers and $n(U)$ totally unimodular.*

Proof. Define $W := A^T C \in \mathbb{Q}^{n\times p}$. By Lemma 1 we have $P^\Lambda = T^\Lambda$, which, by Proposition 1, has the inequality description (1). Therefore, we can solve the maximization problem $\max\{\langle W,X\rangle: X \in P_I^\Lambda\}$ of W over $P_I^\Lambda = P^\Lambda$ in polynomial-time by linear programming over T^Λ using the description in (1), and obtain an optimal vertex which equals I^{π^*} for some π^* with $|\pi^*| \in \Lambda$. For any partition π, we have $\langle C, A^\pi\rangle = \langle C, AI^\pi\rangle = \langle W, I^\pi\rangle$. Therefore, π^* is an optimal solution to the shaped partition problem, and it can be uniquely recovered from I^{π^*} by $\pi_j^* := \{i: I_{i,j}^{\pi^*} = 1\}$ for $j = 1,\ldots,p$. □

We can now demonstrate Corollary 1 stated in Section 1.

Proof of Corollary 1. Part 1, where $\Lambda = \mathbb{N}_n^p \cap \{\lambda: l \leqslant \lambda \leqslant u\}$, is a direct consequence of Theorem 1. To see part 2, let $\Lambda = \{\lambda^1,\ldots,\lambda^m\} \subseteq \mathbb{N}_n^p$ be an explicitly given shape set. For $i = 1,\ldots,m$, solve a shaped partition problem with $\Lambda^i := \{\lambda^i\}$ using part 1 with the lower and upper bounds $l^i := u^i := \lambda^i$ and obtain an optimal partition π^i of shape λ^i. Any best partition among the π^i is an optimal solution to the shaped partition problem with Λ. □

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國外出差心得報告

黃光明

赴美的主要目的是去位在 New Jersey 州的離散數學中心(DIMACS)和 U. G. Rothblum 教授會合討論我們合寫書(Partition: Optimality and Clustering)的事宜。我本年度的國科會計畫「和分解問題」將是這書中的一個部門。我們並完成了兩篇論文[1,2]的定稿，和討論了將來研究的一些藍圖。

我也訪問了 AT&T Shannon Labs 的 Neil Sloane 博士和 Rutgers 大學 RUTCOR 負責人 Peter Hammer 教授，敲定了他們五月來台開會講學事宜(Hammer 教授在最後一刻未能成行)。

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