Correlative Sparsity Structures and Semidefinite Relaxations for Concave Cost Transportation Problems with Change of Variables

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Abstract We present a hierarchy of semidefinite programming (SDP) relaxations for solving the concave cost transportation problem (CCTP), which is known to be NP-hard, with p suppliers and q demanders. In particular, we study cases in which the cost function is quadratic or square-root concave. The key idea of our relaxation methods is in the change of variables to CCTPs, and due to this, we can construct SDP relaxations whose matrix variables are of size $O((\min\{p,q\})^{\omega})$ in the relaxation order ω. The sequence of optimal values of SDP relaxations converges to the global minimum of the CCTP as the relaxation order ω goes to infinity. Furthermore, the size of the matrix variables can be reduced to $O((\min\{p,q\})^{\omega-1})$, $\omega \geq 2$ by using Reznick's theorem. Numerical experiments were conducted to assess the performance of the relaxation methods.

Key words: transportation problem, concave cost minimization, SDP relaxation, sparsity, change of variables

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1 Introduction

Suppose that there exist p suppliers and q demanders, and the transportation cost from the ith supplier to the jth demander is concave in the transportation amount x_{ij}. The concave cost transportation problem (CCTP) is a problem of finding the optimal transportation amount from suppliers to demanders such that the total cost is minimized subject to supply-and-demand constraints. The problem is restated as a network flow problem with a concave cost function on a bipartite graph. Let $I := \{1, \ldots, p\}$ be the set of p suppliers and $J := \{1, \ldots, q\}$ be the set of q demanders. The problem is formulated as

$$(\mathbf{Q}) : \left| \begin{array}{ll} \text{Minimize} & \displaystyle\sum_{i \in I} \sum_{j \in J} f_{ij}(x_{ij}) \\ \text{subject to} & \displaystyle\sum_{j \in J} x_{ij} = a_i, \ i \in I, \ \text{and} \ \sum_{i \in I} x_{ij} = b_j, \ j \in J \\ & x_{ij} \geq 0, \ i \in I, \ j \in J, \end{array} \right.$$

where f_{ij} are univariate concave functions in x_{ij}, and a_i and b_j are positive real constants.

The feature of the problem is in the concavity of cost function. In real-world network flow problems, the cost functions are often assumed to be separable concave functions in order to reflect so-called economies of scale; the cost per unit of transportation decreases as the amount increases. Network flow problems arising from practical applications in transportation systems, facility location and production planning can be formulated with such mathematical models. For instance, the paper [6] has considered and solved the network flow problems with a square root concave cost function derived from the Italian road network and the U.S. telephone network. We refer the reader to [9, 17] for further discussions of the applications.

The concavity of the cost function in the minimization problems makes it difficult to solve. In fact, the CCTP is shown to be NP-hard in [9]. In this paper, we consider two cases for the concave function f_{ij}: a quadratic polynomial function and a square root function. The first case is described in the handbook of test problems [3]. The second case has been studied in, for instance, [10, 16, 11, 31, 1]. Many solution methods for CCTPs have been proposed, and these can be mainly categorized into two groups. The first group is a global approach based on branch-and-bound. We can find the related research in [10, 16, 11]. The second group is a local approach based on metaheuristics. The papers [31, 1] present enhanced algorithms based on simulated annealing and tabu search.

For solving CCTPs, we use the hierarchical SDP relaxation method which was developed by Waki et al. in [28] for polynomial optimization problems (POPs). The relaxation method has advantages of convergence and computational efficiency. In particular, efficiency is ensured by using the structure of the POP. The strength of relaxations is characterized by a parameter ω. Under certain assumptions, the sequence of optimal values of SDP relaxations converges to the global optimal value of the POP as ω goes to infinity. An issue arises in which the size of the SDPs increases rapidly as the relaxation order ω increases, but this problem can be resolved. If a POP has a certain type of the sparsity structure, called correlative sparsity, the relaxation method enables us to reduce the size of the SDPs by exploiting the structure.

In general, CCTPs have no preferable sparsity pattern. However, we show that, by applying a change of variables twice, the CCTPs reduce to quadratic programming problems with characteristic correlative sparsity. Since the sparsity structure of the transformed CCTPs is revealed, we can construct hierarchical SDP relaxations with explicitly written forms by analyzing the structure. Thus, it is possible to evaluate the size of the matrix variables, and the maximum size is $O((\min\{p, q\})^{\omega})$ in the relaxation order ω. The hierarchies are guaranteed to converge to the global minimum of the CCTPs by the theorem of Grimm et al. in [8]. Furthermore, we show that the SDP relaxations can be reduced in size by using Reznick's theorem in [25]. In fact, the maximum size of the matrix variables of SDP is reduced to $O((\min\{p, q\})^{\omega-1})$, $\omega \geq 2$ in the relaxation order ω.

The idea of changing variables was inspired by the work of Kim et al. in [12]. They proposed numerical methods for computing a linear transformation of variables so as to produce a correlative sparsity structure for POPs which do not have such a structure. While the methods can be applied to any POP, it may be difficult to evaluate in advance the size of SDP relaxations for the POPs with the linear transformation. We shall compare the sizes of the SDPs constructed from our relaxation and theirs [12] in Subsection 4.3.

We evaluated the relaxation methods through numerical experiments on randomly generated problems. The relaxation methods work well, in particular, if either of p or q is small. For CCTPs with quadratic concave cost functions, the relaxation methods of order $\omega = 2$ provide the approximate solutions with high accuracy even when the size is large, for instance, $(p, q) = (5, 200), (10, 100)$. For CCTPs with square root concave cost functions, it was often observed that the relaxation of order $\omega = 2$ is not strong. Thus, we examined the strength of relaxation with the increase of the order.

The rest of this paper is organized as follows. After introducing the notation and terminology, we review the hierarchical SDP relaxation method of Waki et al. and its convergence theorem in the first half of Section 2. In the second half of Section 2, we describe the properties of the SDP relaxations for a POP with box constraints, which is a general form of CCTPs with changes of variable. Our relaxation methods are presented in Section 3 and 4. We explain how to construct the SDP relaxations and how to reduce the size of the SDPs for cases in which the cost function f_{ij} of CCTPs is a quadratic or a square root concave one. Numerical experiments are reported in Section 5. Section 6 gives concluding remarks.

1.1 Notation and Terminology

We shall consider a polynomial f in n variables $x_1, \dots, x_n$ with real coefficients $f_{\boldsymbol{\alpha}} \in \mathbb{R}$ of the form,

$$f = \sum_{\boldsymbol{\alpha} \in \mathcal{F}} f_{\boldsymbol{\alpha}} \boldsymbol{x}^{\boldsymbol{\alpha}}, \tag{1}$$

and we will denote the set of such real polynomials f as $\mathbb{R}[\boldsymbol{x}]$. In the form of (1), $\mathcal{F}$ is a nonempty finite subset of $\mathbb{Z}_+^n$, called the *support* of f, and $\boldsymbol{x}^{\boldsymbol{\alpha}}$ represents a monomial $x_1^{\alpha_1} \dots x_n^{\alpha_n}$ for $\boldsymbol{x} = (x_1, \dots, x_n)$ and $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_n)$. Here, $\mathbb{Z}_+^n$ denotes the set of n-dimensional nonnnegative integer numbers. Also, we shall sometimes use the symbol $\mathrm{supp}(f)$ to denote the support of polynomial f. The degree of $f \in \mathbb{R}[\boldsymbol{x}]$ with support

$\mathcal{F} \subseteq \mathbb{Z}_+^n$ is $\max\{|\boldsymbol{\alpha}| : \boldsymbol{\alpha} \in \mathcal{F}\}$, where $|\cdot|$ for a vector represents the summation of elements, i.e., $|\boldsymbol{\alpha}| = \sum_{i=1}^n \alpha_i$ for $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_n)$. We shall also use $|\cdot|$ to represent the cardinality of a set. The symbol $\mathbb{R}[\boldsymbol{x}, \mathcal{G}] := \{f \in \mathbb{R}[\boldsymbol{x}] : \text{supp}(f) \subseteq \mathcal{G}\}$ is used to denote the set of polynomials whose supports are contained in a subset $\mathcal{G}$ of $\mathbb{Z}_+^n$.

For $C \subseteq \{1, \ldots, n\}$, we define $\mathcal{A}(C) := \{\boldsymbol{\alpha} \in \mathbb{Z}_+^n : \alpha_i = 0 \text{ if } i \notin C\}$. This symbol is used to represent polynomials f consisting of variables $x_i,\ i \in C$ as $f \in \mathbb{R}[\boldsymbol{x}, \mathcal{A}(C)]$. Also, for $C \subseteq \{1, \ldots, n\}$ and a positive integer ω, we define $\mathcal{A}^\omega(C) := \{\boldsymbol{\alpha} \in \mathbb{Z}_+^n : \alpha_i = 0 \text{ if } i \notin C \text{ and } |\boldsymbol{\alpha}| \leq \omega\}$, which is used to represent polynomials $f \in \mathbb{R}[\boldsymbol{x}, \mathcal{A}(C)]$ of degree less than or equal to ω as $f \in \mathbb{R}[\boldsymbol{x}, \mathcal{A}^\omega(C)]$.

A polynomial $\phi \in \mathbb{R}[\boldsymbol{x}]$ is said to be a *sum of squares*, abbreviated as *SOS*, if it can be written as a sum of squares of polynomials such that $\phi = f_1^2 + \cdots + f_r^2$ for some $f_1, \ldots, f_r \in \mathbb{R}[\boldsymbol{x}]$, and $\Sigma[\boldsymbol{x}]$ denotes the set of such SOS polynomials ϕ. The symbol $\Sigma[\boldsymbol{x}, \mathcal{G}]$ is used to denote the set of SOS polynomials $\phi \in \mathbb{R}[\boldsymbol{x}]$ such that $\phi = f_1^2 + \cdots + f_r^2$ for some $f_1, \ldots, f_r \in \mathbb{R}[\boldsymbol{x}, \mathcal{G}]$.

In this paper, we will use the following well-known result about the SOS representability of polynomials. We refer the reader to [23, 13] for details. For $\mathcal{G} \subseteq \mathbb{Z}_+^n$, we define a $|\mathcal{G}|$-dimensional column vector $\boldsymbol{u}(\boldsymbol{x}, \mathcal{G}) := (\boldsymbol{x}_{\boldsymbol{\alpha}} : \boldsymbol{\alpha} \in \mathcal{G})$ and define a $|\mathcal{G}| \times |\mathcal{G}|$ symmetric matrix $\boldsymbol{M}(\boldsymbol{x}, \mathcal{G}) := \boldsymbol{u}(\boldsymbol{x}, \mathcal{G})\boldsymbol{u}^\top(\boldsymbol{x}, \mathcal{G})$. $\mathbb{S}(\mathcal{G})$ denotes the set of symmetric matrices of size $|\mathcal{G}| \times |\mathcal{G}|$, and $\mathbb{S}_+(\mathcal{G})$ is the set of positive semidefinite matrices in $\mathbb{S}(\mathcal{G})$. Accordingly, we have

$$\phi \in \Sigma[\boldsymbol{x}, \mathcal{G}] \iff \exists \boldsymbol{Y} \in \mathbb{S}_+(\mathcal{G}),\ \phi = \langle \boldsymbol{M}(\boldsymbol{x}, \mathcal{G}), \boldsymbol{Y} \rangle. \tag{2}$$

Here, $\langle \cdot, \cdot \rangle$ denotes the Frobenius inner product of two matrices, i.e., $\langle \boldsymbol{X}, \boldsymbol{Y} \rangle = \text{tr}(\boldsymbol{X}\boldsymbol{Y})$ for symmetric matrices $\boldsymbol{X}, \boldsymbol{Y}$.

2 SDP Relaxations of Waki et al. for POPs

In 2001, Lasserre [18] introduced a globally convergent hierarchy of SDP relaxations for solving a POP. Sparse variants were developed by Waki et al. [28] in 2006; they improve computational efficiency by exploiting structured sparsity in the POP. Lasserre later showed the convergence of their hierarchy in [19]. Similar convergence results were obtained by Grimm et al. [8] in 2007 and Kojima and Muramatsu [14] in 2009 under weaker assumptions. In particular, we shall use the results of Grimm et al. to ensure the convergence of our SDP relaxations for CCTPs.

2.1 Convergence Theorem

Let $f, g_1, \ldots, g_m \in \mathbb{R}[\boldsymbol{x}]$. Consider the POP

$$(\mathbf{P}) : \Big|\ \text{Minimize} \quad f(\boldsymbol{x}) \quad \text{subject to} \quad g_k(\boldsymbol{x}) \geq 0,\ k = 1, \ldots, m. \tag{3}$$

To ensure the global convergence of SDP relaxations of Waki et al., we need to make the following assumptions.

Assumption 1. *Let $C_i,\ i = 1, \ldots, \ell$ be a subset of $\{1, \ldots, n\}$.*

1-1. For each $j = 2, \ldots, \ell$, there exists $C_i,\ i \in \{1, \ldots, j-1\}$ such that $C_i \supseteq C_j \cap (C_1 \cup C_2 \cup \cdots \cup C_{j-1})$.

1-2. $f = \sum_{i=1}^{\ell} f_i$ with $f_i \in \mathbb{R}[\boldsymbol{x}, \mathcal{A}(C_i)]$.

1-3. There exist disjoint sets $K_i,\ i = 1, \ldots, \ell$ such that $\cup_{i=1}^{\ell} K_i = \{1, \ldots, m\}$, and $g_k \in \mathbb{R}[\boldsymbol{x}, \mathcal{A}(C_i)]$ for each $k \in K_i$.

Note that Assumption 1-1 depends on how one arranges $C_1, \ldots, C_\ell$. In graph theory, it is known that the maximal cliques in a chordal graph always satisfy the assumption if we choose an appropriate ordering; it is known as the *running intersection property*. Here, a graph is said to be *chordal* if every cycle of length greater than 4 has a chord. (We refer the reader to [2, 4] for the details.) Throughout this paper, we use the symbol Δ to denote the collection of $C_1, \ldots, C_\ell$, and say that $\Delta = \{C_1, \ldots, C_\ell\}$ is a *qualified collection* if $C_1, \ldots, C_\ell$ satisfy Assumption 1. Also, we call $K_1, \ldots, K_\ell$ of Assumption 1-3 the *associated disjoint partition* of $\{1, \ldots, m\}$ by Δ.

For $C_i \subseteq \{1, \ldots, n\}$ and $K_i \subseteq \{1, \ldots, m\}$, $i = 1, \ldots, \ell$, we define $\mathcal{M}_i := \{\phi_i + \sum_{k \in K_i} \phi_{ik} g_k : \phi_i, \phi_{ik} \in \Sigma[\boldsymbol{x}, \mathcal{A}(C_i)]\}$, which is called the *quadratic module* generated by $g_k,\ k \in K_i$.

Assumption 2. *For each $i = 1, \ldots, \ell$, $\mathcal{M}_i$ is Archimedean. Namely, there exists a positive integer θ_i such that $\theta_i - \sum_{j \in C_i} x_j^2 \in \mathcal{M}_i$.*

In what follows, we construct the form of the hierarchy of SDP relaxations by using the qualified collection $\Delta = \{C_1, \ldots, C_\ell\}$ and the associated disjoint partition $\{K_1, \ldots, K_\ell\}$. Let $\omega_0 = \lceil \deg(f)/2 \rceil$ and $\omega_k = \lceil \deg(g_k)/2 \rceil$. Choose a parameter ω such that $\omega \geq \max\{\omega_0, \omega_1, \ldots, \omega_m\}$. Note that ω determines the strength of the SDP relaxations and serves as a relaxation order for the hierarchical SDPs. To introduce the generalized Lagrangian L, we shall choose an SOS polynomial $\phi_{ik} \in \Sigma[\boldsymbol{x}, \mathcal{A}^{\omega-\omega_k}(C_i)]$ as a multiplier of each constraint polynomial $g_k(\boldsymbol{x})$. Let $\Phi^\omega := \{(\phi_{ik} : k \in K_i,\ i = 1, \ldots, \ell) : \phi_{ik} \in \Sigma[\boldsymbol{x}, \mathcal{A}^{\omega-\omega_k}(C_i)]\}$. The form of L is

$$L(\boldsymbol{x}, \boldsymbol{\phi}) = f(\boldsymbol{x}) - \sum_{i=1}^{\ell} \sum_{k \in K_i} \phi_{ik}(\boldsymbol{x}) g_k(\boldsymbol{x}) \text{ with } \boldsymbol{\phi} \in \Phi^\omega, \tag{4}$$

and gives the Lagrangian dual problem for (**P**),

$$\text{Maximize} \quad \eta \quad \text{subject to} \quad L(\boldsymbol{x}, \boldsymbol{\phi}) - \eta \geq 0 \quad \text{for all } \boldsymbol{x} \in \mathbb{R}^n, \quad \text{and} \quad \boldsymbol{\phi} \in \Phi^\omega.$$

The first constraint of the problem means that the polynomial $L - \eta$ is nonnegative on $\mathbb{R}^n$. We replace it with one in which $L - \eta$ can be written as an SOS of the form $L - \eta = \sum_{i=1}^{\ell} \phi_i,\ \phi_i \in \Sigma[\boldsymbol{x}, \mathcal{A}^\omega(C_i)]$. Thus, we get

$$\text{Maximize} \quad \eta \quad \text{subject to} \quad f(\boldsymbol{x}) - \eta = \sum_{i=1}^{\ell} (\phi_i(\boldsymbol{x}) + \sum_{k \in K_i} \phi_{ik}(\boldsymbol{x}) g_k(\boldsymbol{x})). \tag{5}$$

Note that $L(\boldsymbol{x}, \boldsymbol{\phi}) - \eta = \sum_{i=1}^{\ell} \phi_i$ implies $L(\boldsymbol{x}, \boldsymbol{\phi}) - \eta \geq 0,\ \forall \boldsymbol{x} \in \mathbb{R}^n$ but the converse is not true in general. From (2), SOS polynomials ϕ_i, ϕ_{ik} can be written by using positive semidefinite matrices. Also, the above equality holds for every $\boldsymbol{x} \in \mathbb{R}^n$. Thus, by solving the identity, we obtain the following SDP

$$
(\mathbf{P}^{\omega}) : \left|
\begin{array}{ll}
\text{Maximize} & -\sum_{i=1}^{\ell} \langle \boldsymbol{A}_{\mathbf{0}}^{(i)}, \boldsymbol{X}^{(i)} \rangle - \sum_{i=1}^{\ell} \sum_{k \in K_i} \langle \boldsymbol{A}_{\mathbf{0}}^{(i,k)}, \boldsymbol{X}^{(i,k)} \rangle \\
\text{subject to} & \sum_{i=1}^{\ell} \langle \boldsymbol{A}_{\boldsymbol{\alpha}}^{(i)}, \boldsymbol{X}^{(i)} \rangle + \sum_{i=1}^{\ell} \sum_{k \in K_i} \langle \boldsymbol{A}_{\boldsymbol{\alpha}}^{(i,k)}, \boldsymbol{X}^{(i,k)} \rangle = f_{\boldsymbol{\alpha}}, \quad \boldsymbol{\alpha} \in \widetilde{\mathcal{F}}^{\omega} \setminus \{\mathbf{0}\}, \\
& \boldsymbol{X}^{(i)} \in \mathbb{S}_+(\mathcal{A}^{\omega}(C_i)), \quad i = 1, \ldots, \ell, \\
& \boldsymbol{X}^{(i,k)} \in \mathbb{S}_+(\mathcal{A}^{\omega - \omega_k}(C_i)), \quad k \in K_i,\ i = 1, \ldots, \ell,
\end{array}
\right.
$$

which is essentially the same as (5). In the above, $\boldsymbol{A}_{\boldsymbol{\alpha}}^{(i)}$ and $\boldsymbol{A}_{\boldsymbol{\alpha}}^{(i,k)}$ are symmetric matrices in $\mathbb{S}(\mathcal{A}^{\omega}(C_i))$ and $\mathbb{S}(\mathcal{A}^{\omega-\omega_k}(C_i))$, respectively. $\widetilde{\mathcal{F}}^{\omega}$ represents a monomial set obtained by the union of two sets, respectively corresponding to the set of all monomials in $\phi_i \in \Sigma[\boldsymbol{x}, \mathcal{A}^{\omega}(C_i)]$ and the set of all monomials in $\phi_{ik} g_k$ with $\phi_{ik} \in \Sigma[\boldsymbol{x}, \mathcal{A}^{\omega-\omega_k}(C_i)]$. $f_{\boldsymbol{\alpha}}$ is the coefficient of monomial $\boldsymbol{x}^{\boldsymbol{\alpha}}$ in the cost function f of $(\mathbf{P})$.

The dual problem $(\mathbf{P}_*^{\omega})$ of $(\mathbf{P}^{\omega})$ is

$$
(\mathbf{P}_*^{\omega}) : \left|
\begin{array}{ll}
\text{Minimize} & \sum_{\boldsymbol{\alpha} \in \mathcal{F}} f_{\boldsymbol{\alpha}} x_{\boldsymbol{\alpha}} \\
\text{subject to} & \boldsymbol{A}_{\mathbf{0}}{}^{(i,k)} + \sum_{\boldsymbol{\alpha} \in \widetilde{\mathcal{F}}^{\omega} \setminus \{\mathbf{0}\}} \boldsymbol{A}_{\boldsymbol{\alpha}}^{(i,k)} x_{\boldsymbol{\alpha}} \in \mathbb{S}_+(\mathcal{A}^{\omega-\omega_k}(C_i)), \quad k \in K_i,\ i = 1, \ldots, \ell, \\
& \boldsymbol{A}_{\mathbf{0}}^{(i)} + \sum_{\boldsymbol{\alpha} \in \widetilde{\mathcal{F}}^{\omega} \setminus \{\mathbf{0}\}} \boldsymbol{A}_{\boldsymbol{\alpha}}^{(i)} x_{\boldsymbol{\alpha}} \in \mathbb{S}_+(\mathcal{A}^{\omega}(C_i)), \quad i = 1, \ldots, \ell.
\end{array}
\right.
$$

$\mathcal{F}$ is the support of the cost function f of $(\mathbf{P})$. The above problem can also be obtained by linearizing $\boldsymbol{x}^{\boldsymbol{\alpha}}$ to $x_{\boldsymbol{\alpha}}$ in the following polynomial SDP,

$$
\begin{array}{ll}
\text{Minimize} & f(\boldsymbol{x}) \\
\text{subject to} & g_k(\boldsymbol{x}) \boldsymbol{M}(\boldsymbol{x}, \mathcal{A}^{\omega-\omega_k}(C_i)) \in \mathbb{S}_+(\mathcal{A}^{\omega-\omega_k}(C_i)), \quad k \in K_i,\ i = 1, \ldots, \ell, \\
& \boldsymbol{M}(\boldsymbol{x}, \mathcal{A}^{\omega}(C_i)) \in \mathbb{S}_+(\mathcal{A}^{\omega}(C_i)), \quad i = 1, \ldots, \ell,
\end{array}
$$

which is the equivalent to the $(\mathbf{P})$. Let $\zeta(\mathbf{P}^{\omega})$ and $\zeta(\mathbf{P}_*^{\omega})$ denote the optimal value of $(\mathbf{P}^{\omega})$ and $(\mathbf{P}_*^{\omega})$, respectively. Also, let ζ denote the optimal value of the $(\mathbf{P})$.

Theorem 1. *([8, 20]) Under Assumption 1 and 2, $\zeta(\mathbf{P}^{\omega})$ and $\zeta(\mathbf{P}_*^{\omega})$ converge to ζ as $\omega \to \infty$.*

The above theorem follows from Theorem 5 of [8] by Grimm et al. In fact, the proof is in Corollary 8.10 of the survey paper [20]. The assumption of the above theorem is slightly weaker than one of Lasserre in [19]. In that paper, the global convergence property of the SDP relaxation of Waki et al. was shown under the existence of ball constraints $\theta_i - \sum_{j \in C_i} x_j^2 \geq 0,\ i = 1, \ldots, \ell$ in $(\mathbf{P})$. It was also shown that if $(\mathbf{P})$ has a unique global optimal solution $\boldsymbol{x}$, then, $\boldsymbol{x}_{lin}^{\omega} \to \boldsymbol{x}$ as $\omega \to \infty$. Here, $\boldsymbol{x}_{lin}^{\omega} := (x_{\boldsymbol{\alpha}}^{\omega} : |\boldsymbol{\alpha}| = 1)$ for an optimal solution $\boldsymbol{x}^\omega$ of the dual SDP relaxation $(\mathbf{P}^\omega_*)$. We call such a component vector $\boldsymbol{x}^\omega_{lin}$ of $\boldsymbol{x}^\omega$ a *linear part solution* of $(\mathbf{P}^\omega_*)$.

The following simple observation will be used in Subsection 4.2. Suppose that $g_k,\ k = 1,\dots,m$ are linear, i.e., $\deg(g_k) = 1$. Then, the dual SDP relaxation $(\mathbf{P}^\omega_*)$ have $g_k(\boldsymbol{x}) \geq 0,\ k = 1,\dots,m$ as constraints. Thus, the linear part solution $\boldsymbol{y}^\omega_{lin}$ of $(\mathbf{P}^\omega_*)$ is always a feasible solution of $(\mathbf{P})$ for any relaxation order ω.

Remark 1. The SDP relaxations of Lasserre [18] in 2001 can be regarded as the case of $\Delta = \{C\}$ with $C = N$.

2.2 POPs with Box Constraints

We describe the properties of SDP relaxations of Waki et al. for a POP with box constraints in the following lemmas. (We thank the first anonymous referee for bringing them to our attention.) The lemmas will apply to our SDP relaxations of CCTPs with changes of variable. Consider a POP of the form

$$\begin{array}{lll} \text{Minimize} & f(\boldsymbol{x}) & \\ \text{subject to} & g_k(\boldsymbol{x}) \geq 0, & k = 1,\dots,m, \\ & 0 \leq x_j \leq a_j, & j = 1,\dots,n, \end{array} \tag{6}$$

where $f, g_1, \dots, g_m \in \mathbb{R}[\boldsymbol{x}]$ and $a_1, \dots, a_n$ are nonnegative real numbers. Note that all variables of (6) have lower and upper bounds. Such bound constraints are called as *box constraints*.

We shall rewrite the box constraints $0 \leq x_j \leq a_j$ as $h^\ell_j(\boldsymbol{x}) \geq 0$ and $h^u_j(\boldsymbol{x}) \geq 0$ where $h^\ell_j(\boldsymbol{x}) := x_j$ and $h^u_j(\boldsymbol{x}) := a_j - x_j$. Let $\Delta = \{C_1, \cdots, C_\ell\}$ be a qualified collection for (6), and we choose the associated disjoint partition $\{K_1, \dots, K_\ell\}$ of $\{1, \dots, m\}$ which corresponds to $g_1, \dots, g_m$. By adding redundant box constraints to (6) if necessary, we get

$$\begin{array}{lll} \text{Minimize} & f(\boldsymbol{x}) & \\ \text{subject to} & g_k(\boldsymbol{x}) \geq 0, & k = 1,\dots,m, \\ & h^\ell_j(\boldsymbol{x}) \geq 0 \quad \text{and} \quad h^u_j(\boldsymbol{x}) \geq 0, & j \in C_i,\ i = 1,\dots,\ell, \end{array} \tag{7}$$

which is equivalent to (6). As the SDP relaxation $(\mathbf{P}^\omega)$ for (7), we can have

$$\text{Maximize} \quad \eta \quad \text{subject to} \quad f - \eta = \sum_{i=1}^{\ell} (\phi_i + \sum_{k \in K_i} \phi_{ik} g_k + \sum_{j \in C_i} \phi^\ell_{ij} h^\ell_j + \sum_{j \in C_i} \phi^u_{ij} h^u_j),$$

where $\phi_i \in \Sigma[\boldsymbol{x}, \mathcal{A}^\omega(C_i)],\ \phi_{ik} \in \Sigma[\boldsymbol{x}, \mathcal{A}^{\omega-\omega_i}(C_i)]$ and $\phi^\ell_{ij}, \phi^u_{ij} \in \Sigma[\boldsymbol{x}, \mathcal{A}^{\omega-1}(C_i)]$. Here, $\omega_i = \lceil \deg(g_i)/2 \rceil$. Lemma 2 and Lemma 3 follow from the identities in Lemma 1 whose precise form is given in the Appendix. Note that a_i is a constant term in h^u_i.

Lemma 1. *For a real number $\kappa \in \mathbb{R}$,*

1-1. $\kappa x_i + |\kappa| a_i = \phi^\ell h^\ell_i + \phi^u h^u_i$ for some nonnegative real numbers ϕ^ℓ, ϕ^u.

1-2. $\kappa x_i^2 + |\kappa| a_i^2 = \phi^\ell h_i^\ell + \phi^u h_i^u$ *for some* $\phi^\ell, \phi^u \in \Sigma[\boldsymbol{x}, \mathcal{A}^1(\{i\})]$.

1-3. $\kappa x_i x_j + \frac{1}{2}|\kappa|(a_i^2 + a_j^2) = \phi_{ij}^\ell h_i^\ell + \phi_{ij}^u h_i^u + \phi_j^\ell h_j^\ell + \phi_j^u h_j^u$ *for some* $\phi_{ij}^\ell, \phi_{ij}^u \in \Sigma[\boldsymbol{x}, \mathcal{A}^1(\{i,j\})]$ *and some* $\phi_j^\ell, \phi_j^u \in \Sigma[\boldsymbol{x}, \mathcal{A}^1(\{j\})]$.

Lemma 2. *For each* $i = 1, \ldots, \ell$, *the quadratic module* $\mathcal{M}_i$ *of (7) is Archimedean.*

Proof. It follows from Lemma 1-2 with $\kappa = -1$. Namely, there exist $\phi_{ij}^\ell, \phi_{ij}^u \in \Sigma[\boldsymbol{x}, \mathcal{A}(\{j\})]$, $j \in C_i$ such that $\sum_{j \in C_i}(a_j^2 - x_j^2) = \sum_{j \in C_i}(\phi_{ij}^\ell h_j^\ell + \phi_{ij}^u h_j^u)$. ■

Lemma 3. *Let* f *of* (7) *be a quadratic function of the form* $f(\boldsymbol{x}) = \boldsymbol{x}^\top \boldsymbol{C} \boldsymbol{x} + \boldsymbol{d}^\top \boldsymbol{x}$ *where* $\boldsymbol{C} \in \mathbb{R}^{n \times n}$, $\boldsymbol{d} \in \mathbb{R}^n$ *and* $^\top$ *denotes transposition. Let* $(\mathbf{P}^\omega)$ *and* $(\mathbf{P}_*^\omega)$ *be the primal-dual pair of the SDP relaxation of order* ω *for* (7). *Assume that the feasible region of* (7) *has a nonempty interior. Then,* $(\mathbf{P}^\omega)$ *and* $(\mathbf{P}_*^\omega)$ *have a zero duality gap for any positive integer* $\omega \geq 2$.

Proof. $(\mathbf{P}^\omega)$ is feasible for any positive integer ω, since from Lemma 1, there exist $\eta \in \mathbb{R}$ and $\phi_{ij}^\ell, \phi_{ij}^u \in \Sigma[\boldsymbol{x}, \mathcal{A}(C_i)^{\omega-1}]$, $\omega \geq 2$ such that $f - \eta = \sum_{i=1}^\ell \sum_{j \in C_i}(\phi_{ij}^\ell h_j^\ell + \phi_{ij}^u h_j^u)$. Also, from Lemma 4.4 of [20], $(\mathbf{P}_*^\omega)$ is strictly feasible for any relaxation order ω if the feasible region of (7) has a nonempty interior. Thus, the desired result follows from the strong duality theorem of SDP. ■

3 SDP Relaxations for CCTPs

Although Theorem 1 provides a numerical framework for solving POPs, computational issues arise when we implement it in practice. The main obstacle is that the size of SDP relaxations rapidly become large as we increase the relaxation order ω. The variables $\boldsymbol{X}^{(i,k)}$ and $\boldsymbol{X}^{(i)}$ of SDP $(\mathbf{P}^\omega)$ are symmetric matrices of size

$$|\mathcal{A}^{\omega-\omega_k}(C_i)| = \binom{|C_i| + \omega - \omega_k}{\omega - \omega_k} \text{ and } |\mathcal{A}^\omega(C_i)| = \binom{|C_i| + \omega}{\omega}, \tag{8}$$

which are evaluated as $O(|C_i|^{\omega-\omega_k})$ and $O(|C_i|^\omega)$, respectively. We thus know that the size of $\boldsymbol{X}^{(i,k)}$ and $\boldsymbol{X}^{(i)}$ increases exponentially with ω. The key to the practical implementation of Theorem 1 is in finding a qualified collection Δ consisting of small components $C_i \in \Delta$. In this section, we show that a change of variables to the CCTP produces such qualified collections. From (8), we note that the size of matrix variables $\boldsymbol{X}^{(i)}$ is larger than that of $\boldsymbol{X}^{(i,k)}$, and the maximum size of the matrix variables $\boldsymbol{X}^{(i)}$ is given by the maximum size of components C_i of Δ.

Throughout this paper, we make the following assumptions.

Assumption 3. *For CCTP* $(\mathbf{Q})$,

3-1. $a_i, b_j > 0$ *for every* $i \in I$ *and every* $j \in J$.

3-2. $\sum_{i \in I} a_i = \sum_{j \in J} b_j$.

The first assumption holds for (**Q**) without loss of generality since $a_i = 0$ or $b_j = 0$ imply $x_{i1} = \cdots = x_{iq} = 0$ or $x_{1j} = \cdots = x_{pj} = 0$, respectively, and thus we can remove such variables. The second one guarantees the feasibility of (**Q**); if we do not have it, (**Q**) is infeasible. In fact, for $\xi = \sum_{i \in I} a_i = \sum_{j \in J} b_j$, let $\tilde{x}_{ij} = a_i b_j / \xi$ and let $\tilde{\boldsymbol{x}} = (\tilde{x}_{ij} : i \in I, j \in J)$. Then, it is easy to check that $\tilde{\boldsymbol{x}}$ is a feasible solution of (**Q**).

3.1 Observations on the Simplified Problems

In general, CCTPs (**Q**) have no preferable sparsity pattern, and hence, the size of the SDP relaxations of Waki et al. becomes large. In fact, the paper [12] reports that it is difficult to solve the SDP relaxations for (**Q**) with quadratic concave functions even when $(p, q) = (5, 15)$ and $\omega = 2$. In the following subsections, we see that a characteristic correlative sparsity pattern can be produced by applying a change of variables to (**Q**).

First, let us consider a simplified version of CCTPs (**Q**) without the second equality constraint and plot the resulting CSP graphs in order to illustrate our idea.

$$\begin{array}{lll} \text{Minimize} & \displaystyle\sum_{i \in I} \sum_{j \in J} f_{ij}(x_{ij}) & \\ \text{subject to} & \displaystyle\sum_{j \in J} x_{ij} = a_i, & i \in I \\ & x_{ij} \geq 0, & i \in I, \ j \in J. \end{array} \tag{9}$$

Assume for simplicity that f_{ij} of problem (9) is a polynomial in x_{ij}. It is ideal to have a qualified collection consisting of small components when we construct a hierarchy of SDP relaxations for (9) according to Theorem 1. Although the search for such a collection is not easy, the correlative sparsity pattern (CSP) graph proposed by Waki et al. in [28] is a useful tool for it.

For the POP (**P**), the CSP graph $G = (V, E)$ with a vertex set V and edge set E is defined as follows. V is $\{1, \dots, n\}$ and each vertex $i \in V$ corresponds to a variable x_i in (**P**). There exists an edge $(i, j) \in E$ with $i \neq j$ if some monomial of the cost polynomial function f has variables x_i and x_j, or if some constraint polynomial $g_k, \ k = 1, \dots, m$ has variables x_i and x_j. Each variable appearing in a monomial of f or each variable appearing in the polynomial g_k corresponds to the vertex of some clique in G. Hence, Assumption 1-2 and 1-3 are satisfied if we regard the maximal cliques of G as C_i. Furthermore, as stated in Section 2, if G is a chordal graph, the maximal cliques arranged in appropriate order satisfy Assumption 1-1.

We know that the CSP graph G for the problem (9) is a disconnected graph composed of p complete graphs, each of which has q vertices. Obviously, G is chordal, and the maximal cliques of G are the p complete graphs. Thus, we obtain a qualified collection consisting of $C_1, \cdots, C_p$ of size q whose elements are the vertices of the complete graphs. Figure 1 illustrates the CSP graph for (9) with $p = 2, q = 4$. In the figure, each node label corresponds to a subscript (i, j) of x_{ij}.

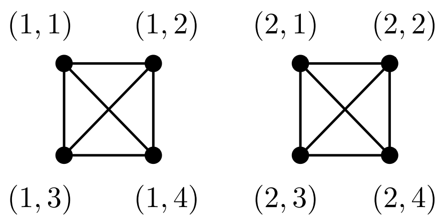

Figure 1: CSP graph for the problem (9) with $p = 2, q = 4$.

For (9) we perform a change of variables from $\boldsymbol{x} = (x_{ij} : i \in I,\ j \in J) \in \mathbb{R}^{pq}$ to $\boldsymbol{y} = (y_{ij} : i \in I,\ j \in J) \in \mathbb{R}^{pq}$,

$$\begin{cases} x_{ij} = y_{ij} - y_{i,j+1}, & i \in I,\ j \in J \setminus \{q\}, \\ x_{iq} = y_{iq}, & i \in I. \end{cases} \tag{10}$$

Note that this transformation is invertible since

$$(10) \Longleftrightarrow y_{ij} = x_{ij} + \cdots + x_{iq}, \quad i \in I,\ j \in J.$$

Accordingly, we obtain the equivalent problem,

$$\begin{array}{ll} \text{Minimize} & \displaystyle\sum_{i \in I} \sum_{j \in J \setminus \{q\}} f_{ij}(y_{ij} - y_{i,j+1}) + \sum_{i \in I} f_{iq}(y_{iq}) \\ \text{subject to} & y_{i1} = a_i, \quad i \in I, \\ & y_{ij} - y_{i,j+1} \geq 0, \quad i \in I,\ j \in J \setminus \{q\}, \\ & y_{iq} \geq 0, \quad i \in I. \end{array} \tag{11}$$

The CSP graph G for (11) is a disconnected graph composed of p line segments, each of which has q vertices aligned in a straight line. Hence, G is chordal, and the maximal cliques correspond to the graphs consisting of two vertices with an edge. The left side of Figure 2 illustrates the CSP graph for (11) with $p = 2, q = 4$ and the right side shows the maximal cliques. In the figure, each node label corresponds to a subscript (i, j) of variable y_{ij}. Thus, we can construct a qualified collection using $C_1, \cdots, C_{p(q-1)}$ of size 2. The sets are much smaller size than those from (9).

We saw that the change of variables to problem (9) works well to obtain a qualified collection consisting of small components. The key is in a separable structure of the problem; each equality constraint does not share the same variables, and each monomial of cost function consists of a single variable. Such an observation was made by Kim et al. in [12], and they proposed numerical methods for computing a linear transformation of variables to find qualified collections with small components. Although CCTP (**Q**) does not have such a separable structure in general, we show in the following subsections that a characteristic CSP graph can be obtained by performing a change of variables twice.

We shall briefly mention an efficient numerical method in [28] to find qualified collections. We refer the reader to [2, 4] for the theoretical background. Suppose that G is a CSP graph

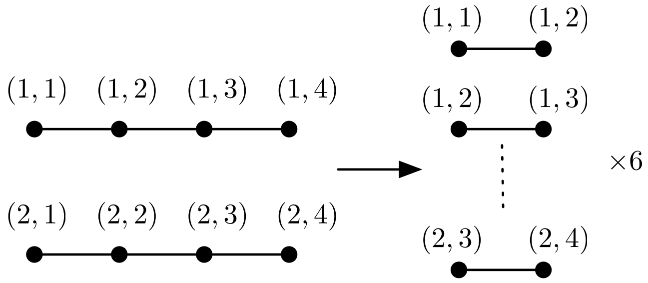

Figure 2: CSP graph for the problem (11) with $p = 2, q = 4$ and its maximal cliques. The left side is the CSP graph, and the right side shows the maximal cliques.

of a POP, and it is not necessarily chordal. We apply Cholesky factorization to the adjacency matrix of G, called the *CSP matrix* in [28]. From the sparsity pattern of the Cholesky factor, we can construct a chordal extension $\bar{G}$ of G, and as a result, find the maximal cliques for $\bar{G}$. A graph $\bar{G} = (V, \bar{E})$ with $\bar{E} \supseteq E$ is called a *chordal extension* of $G = (V, E)$ if $\bar{G}$ is chordal. Thus, the family of maximal cliques becomes a qualified collection for the POP.

The following facts should be noted. The size of components in the resulting qualified collection is determined by the sparsity pattern of the Cholesky factor. The sparsity pattern varies according to the ordering of the row and column indices of the CSP matrix. In general, it is difficult to find the best ordering that minimizes component sizes of the qualified collection. Thus, a practical implementation often uses heuristic methods such as minimum degree ordering and reverse Cuthill-McKee ordering [7].

The following is an outline of the methods presented in [28] for solving a POP $(\mathbf{P})$. A qualified collection Δ is obtained by applying Cholesky factorization to the CSP matrix for $(\mathbf{P})$. Then, an SDP relaxation of the form $(\mathbf{P}^{\omega})$ is constructed using the Δ, and it is solved. These methods are implemented in the MATLAB package SparsePOP in [29].

3.2 Applying Change of Variables to CCTPs

Let us focus on the first and second equality constraints of $(\mathbf{Q})$,

$$(\mathbf{T}) : \begin{cases} \displaystyle\sum_{j \in J} x_{ij} = a_i, & i \in I, \\ \displaystyle\sum_{i \in I} x_{ij} = b_j, & j \in J. \end{cases}$$

Note that the other constraints in $(\mathbf{Q})$ have a separable structure. For the variable $\boldsymbol{x} = (x_{ij} : i \in I,\ j \in J)$ of $(\mathbf{T})$, we perform a variable transformation (10) and obtain

$$\begin{cases} y_{i1} = a_i, & i \in I, \\ \displaystyle\sum_{i \in I} (y_{ij} - y_{i,j+1}) = b_j, & j \in J \setminus \{q\}, \text{ and } \textstyle\sum_{i \in I} y_{iq} = b_q. \end{cases}$$

The second equalities can be rewritten as $\sum_{i\in I} y_{ij} = \bar{b}_j,\ j \in J,$ where $\bar{b}_j := \sum_{k=j}^{q} b_k$. Therefore, the following form is obtained,

$$(\mathbf{T}1): \begin{cases} y_{i1} = a_i, & i \in I, \\ \sum_{i\in I} y_{ij} = \bar{b}_j, & j \in J, \end{cases}$$

which is equivalent to $(\mathbf{T})$ under the variable transformation (10).

We again perform a change of variables to $(\mathbf{T}1)$ from $\boldsymbol{y} = (y_{ij} : i \in I,\ j \in J) \in \mathbb{R}^{pq}$ to $\boldsymbol{z} = (z_{ji} : i \in I,\ j \in J) \in \mathbb{R}^{pq}$,

$$\begin{cases} y_{ij} = z_{ji} - z_{j,i+1}, & i \in I \setminus \{p\},\ j \in J, \\ y_{pj} = z_{jp}, & j \in J, \end{cases} \tag{12}$$

or equivalently, $z_{ji} = y_{ij} + \cdots + y_{pj},\ i \in I,\ j \in J$. $(\mathbf{T}1)$ is then transformed into

$$\begin{cases} z_{1i} - z_{1,i+1} = a_i, & i \in I \setminus \{p\}, \text{ and } z_{1p} = a_p, \\ z_{j1} = \bar{b}_j, & j \in J, \end{cases}$$

and the first equalities are rewritten as $z_{1i} = \bar{a}_i,\ i \in I$ where $\bar{a}_i := \sum_{k=i}^{p} a_k$. Consequently, we get

$$(\mathbf{T}2): \begin{cases} z_{1i} = \bar{a}_i, & i \in I, \\ z_{j1} = \bar{b}_j, & j \in J, \end{cases}$$

which is equivalent to $(\mathbf{T})$ under

$$(u_{ji}(\boldsymbol{z}) =)\ x_{ij} = \begin{cases} (z_{ji} - z_{j,i+1}) - (z_{j+1,i} - z_{j+1,i+1}), & i \in I \setminus \{p\}, & j \in J \setminus \{q\}, \\ z_{qi} - z_{q,i+1}, & i \in I \setminus \{p\}, & j = q, \\ z_{jp} - z_{j+1,p}, & i = p, & j \in J \setminus \{q\}, \\ z_{qp} & i = p, & j = q. \end{cases}$$

Let $u_{ji}(\boldsymbol{z})$ denote the right-hand linear functions in $\boldsymbol{z}$. Then, we have the equivalent problem for the CCTP $(\mathbf{Q})$,

$$\begin{array}{ll} \text{Minimize} & \sum_{j\in J} \sum_{i\in I} f_{ij}(u_{ji}(\boldsymbol{z})) \\ \text{subject to} & z_{j1} = \bar{b}_j, \quad j \in J, \\ & z_{1i} = \bar{a}_i, \quad i \in I, \\ & u_{ji}(\boldsymbol{z}) \geq 0, \quad j \in J,\ i \in I. \end{array} \tag{13}$$

We can evaluate the range of variables z_{ji} in (13). The x_{ij} of $(\mathbf{Q})$ satisfy $\sum_{j\in J} x_{ij} = a_i$ and $x_{ij} \geq 0$. The y_{ij} are obtained by applying the variable transformation of (10) to x_{ij} of $(\mathbf{Q})$. Hence, y_{ij} are in $0 \leq y_{ij} \leq a_i$. From (12), we know that z_{ji} are in $0 \leq z_{ji} \leq \bar{a}_i$.

The variables $z_{j1},\ j \in J$ and $z_{1i},\ i \in I$ can be eliminated from the problem since they are now constant. Also, for the subscripts j and i of the variable z_{ji}, we shift each value of j and i by -1. In so doing, the above problem can be rewritten as

$$\begin{array}{ll} \text{Minimize} & \sum_{j\in J} \sum_{i\in I} f_{ij}(v_{ji}(\boldsymbol{z})) \\ \text{subject to} & v_{ji}(\boldsymbol{z}) \geq 0, \quad j \in J,\ i \in I, \\ & 0 \leq z_{ji} \leq \delta_{ji}, \quad j \in J',\ i \in I', \end{array} \tag{14}$$

where δ_{ji} are positive numbers such that $\delta_{ji} > \bar{a}_i$ and

$$v_{ji}(\boldsymbol{z}) := \begin{cases} z_{(1,1)} + c, & j = 1, \quad i = 1, \\ -z_{(j-1,1)} + z_{(j,1)} + b_j, & j \in J' \setminus \{1\}, \quad i = 1, \\ -z_{(1,i-1)} + z_{(1,i)} + a_i, & j = 1 \quad i \in I' \setminus \{1\}, \\ (z_{(j-1,i-1)} - z_{(j-1,i)}) - (z_{(j,i-1)} - z_{(j,i)}), & j \in J' \setminus \{1\}, \quad i \in I' \setminus \{1\}, \\ -z_{(1,p-1)} + a_p, & j = 1, \quad i = p, \\ z_{(j-1,p-1)} - z_{(j,p-1)}, & j \in J' \setminus \{1\}, \quad i = p, \\ -z_{(q-1,1)} + b_q, & j = q, \quad i = 1, \\ z_{(q-1,i-1)} - z_{(q-1,i)}, & j = q, \quad i \in I' \setminus \{1\}, \\ z_{(q-1,p-1)}, & j = q, \quad i = p. \end{cases}$$

In this formulation, we use $c := \bar{a}_1 - \bar{a}_2 - \bar{b}_2$, $J' := \{1, \ldots, q-1\}$ and $I' := \{1, \ldots, p-1\}$. The variable z_{ji} is written as $z_{(j,i)}$ to be clearly readable. The above problem has $(q-1)(p-1)$ variables. Note that the global optimal value of the CCTP $(\mathbf{Q})$ coincides with that of problem (14), and the global optimal solution of the $(\mathbf{Q})$ can be constructed from that of (14) through a linear transformation.

Let $\mathcal{V}$ be the feasible region of (14). The reason we chose $\delta_{ji} > \bar{a}_i$ above is to make $\mathcal{V}$ have an interior.

Lemma 4. *Under Assumption 3, $\mathcal{V}$ has a nonempty interior.*

Proof. From Assumption 3-2, we have $(\xi :=) \sum_{i \in I} a_i = \sum_{j \in J} b_j$ for $(\mathbf{Q})$, and let ξ be the value of the sum. Let $\tilde{x}_{ij} = a_i b_j / \xi$, $i \in I$, $j \in J$ and let $\tilde{\boldsymbol{x}} = (\tilde{x}_{ij} : i \in I, j \in J)$. Then, $\tilde{\boldsymbol{x}}$ satisfies all constraints of $(\mathbf{Q})$. Also, from Assumption 3-1, the $\tilde{x}_{ij}$ are all positive. From the variable transformation of (10) and (12), there exists a linear transformation $\boldsymbol{H} : \mathbb{R}^{qp} \to \mathbb{R}^{(q-1)(p-1)}$ which maps the feasible solution $\tilde{\boldsymbol{x}}$ of $(\mathbf{Q})$ into the feasible solution $\boldsymbol{H}\tilde{\boldsymbol{x}} = \tilde{\boldsymbol{z}}$ of (14). In particular, each element $\tilde{z}_{ji}$ of $\tilde{\boldsymbol{z}}$ is $\bar{a}_i \bar{b}_j / \xi$, and from Assumption 3-1, the $\tilde{z}_{ji}$ are all positive. For all constraints of (14), strict inequalities hold for $\tilde{\boldsymbol{z}}$. Since $v_{ji}(\boldsymbol{z}) = x_{ij}$, $\tilde{\boldsymbol{z}}$ satisfies $v_{ji}(\tilde{\boldsymbol{z}}) = \tilde{x}_{ij} > 0$. We already know that $\tilde{z}_{ji} > 0$. Since $\bar{b}_j / \xi \leq 1$, we have $\tilde{z}_{ji} = \bar{a}_i \bar{b}_j / \xi \leq \bar{a}_i < \delta_{ji}$. Hence, $\mathcal{V}$ has a nonempty interior. ■

3.3 SDP Relaxations for Transformed CCTPs

3.3.1 Case: Quadratic Concave Function

Let us consider the case in which f_{ij} of CCTP $(\mathbf{Q})$ is a quadratic concave function of the form,

$$f_{ij}(x_{ij}) = \mu_{ij} x_{ij}^2 + \nu_{ij} \text{ with } \mu_{ij} < 0. \tag{15}$$

This case is described in the handbook of test problems [3]. The transformed CCTP of (14) is

$$(\mathbf{R}_q) : \left| \text{ Minimize } \sum_{j \in J} \sum_{i \in I} \mu_{ij} v_{ji}^2(\boldsymbol{z}) + \nu_{ij} \quad \text{subject to} \quad \boldsymbol{z} \in \mathcal{V}. \right.$$

The following should be noted. $(\mathbf{R}_q)$ is a special case of a POP with box constraints (6). Hence, we can use Lemma 2 to ensure Assumption 2 of Theorem 1. Also, since the cost function is quadratic and the feasible region $\mathcal{V}$ has an interior by Lemma 4, we can use Lemma 3.

Below, we show that $(\mathbf{R}_q)$ has qualified collections Δ and $\widetilde{\Delta}$, each of which consists of the components of size $q+1$ and $p+1$, respectively. Figure 3 shows the CSP graph G for the problem. We define $J'' := \{1, \ldots, q-2\}$ and $I'' := \{1, \ldots, p-2\}$. Let

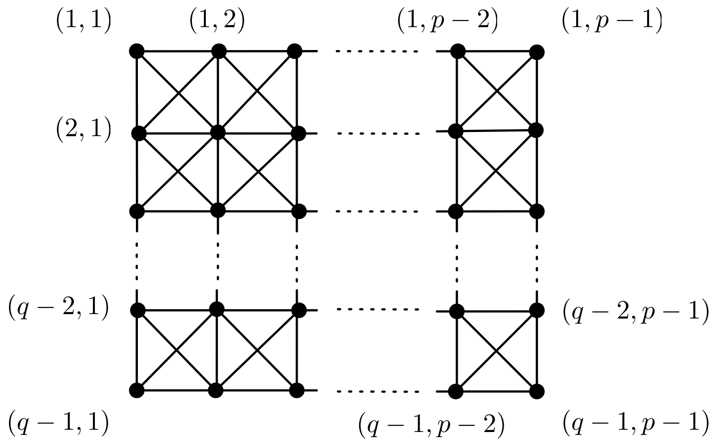

Figure 3: CSP graph G for $(\mathbf{R}_q)$.

$$\Delta = \{C_{ji} : j \in J'',\ i \in I''\} \tag{16}$$

where

$$C_{ji} = \{(j,i), (j+1,i), \ldots, (q-1,i), (1,i+1), (2,i+1), \ldots, (j+1,i+1)\}, \tag{17}$$

and

$$\widetilde{\Delta} = \{\widetilde{C}_{ji} : j \in J'',\ i \in I''\} \tag{18}$$

where

$$\widetilde{C}_{ji} = \{(j,i), (j,i+1), \ldots, (j,p-1), (j+1,1), (j+1,2), \ldots, (j+1,i+1)\}. \tag{19}$$

Note that $|C_{ji}| = q+1$ and $|\widetilde{C}_{ji}| = p+1$. Figure 4 shows the subgraphs $G(C_{ji})$ and $G(\widetilde{C}_{ji})$ of G induced by C_{ji} and $\widetilde{C}_{ji}$. The observations about $G(C_{ji})$ and $G(\widetilde{C}_{ji})$ may help us to understand the proof of the following lemma.

Lemma 5. *Let Δ and $\widetilde{\Delta}$ as* (16) *and* (18)*, respectively. Then, each of Δ and $\widetilde{\Delta}$ is a qualified collection for* $(\mathbf{R}_q)$.

Proof. It is enough to check that Δ satisfies Assumption 1 since $\widetilde{\Delta}$ can be identified as Δ if we rotate the CSP graph G for the problem by interchanging j with i in the vertex label (j,i) of G. We have $C_{ji} \supseteq (C_{ji} \cap C_{j+1,i})$ for each $j = 1, \ldots, q-2$ and $C_{q-2,i} \supseteq (C_{q-2,i} \cap C_{1,i+1})$, so that Assumption 1-1 is satisfied in the following order

$$C_{11}, C_{21}, \ldots, C_{q-2,1}, C_{12}, C_{22}, \ldots, C_{q-2,2}, \ldots, C_{1,p-2}, C_{2,p-2}, \ldots, C_{q-2,p-2}.$$

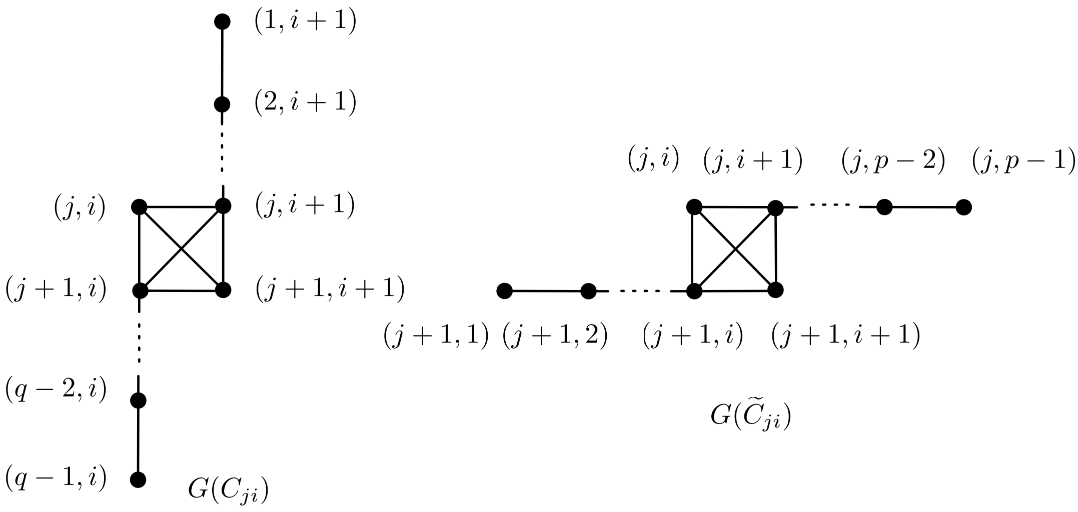

Figure 4: Induced subgraphs $G(C_{ji})$ and $G(\widetilde{C}_{ji})$ of G.

For any fixed $\breve{j} \in J''$ and any fixed $\breve{i} \in I''$, all the supports of $v_{\breve{j}\breve{i}}(\boldsymbol{z})$ are contained in a set $\{(j,i),(j+1,i),(j,i+1),(j+1,i+1)\}$ for some $j \in J''$ and some $i \in I''$, and the set is contained in C_{ji}. This shows that Assumptions 1-2 and 1-3 are satisfied. ■

Note that $(\mathbf{R}_q)$ can have qualified collections other than Δ of (16) and $\widetilde{\Delta}$ of (18). Thus, qualified collections may exist whose component sizes are smaller than those of Δ or $\widetilde{\Delta}$. In Subsection 5.1, we experimentally evaluate the component sizes of Δ and $\widetilde{\Delta}$ by comparing them with those determined by the numerical method of [28].

Define Δ_q° such that $\Delta_q^\circ = \Delta$ if $q \leq p$, otherwise, $\Delta_q^\circ = \widetilde{\Delta}$, and modify $(\mathbf{R}_q)$ to the form (7) by adding redundant box constraints. Using Δ_q°, we construct SDP relaxations of Waki et al. for the modified problem based on the discussion in Section 2. Let $(\mathbf{R}_q^\omega)$ be the SDP of relaxation order ω and $(\mathbf{R}_{q,*}^\omega)$ be its dual. Assumption 1 holds by Lemma 5, and Assumption 2 holds by Lemma 2. In addition, $\mathcal{V}$ has a nonempty interior by Lemma 4. Thus, Theorem 1 and Lemma 3 can be applied to $(\mathbf{R}_q^\omega)$ and $(\mathbf{R}_{q,*}^\omega)$. Let ζ be the global optimal value of $(\mathbf{R}_q)$. Let $\zeta(\mathbf{R}_q^\omega)$ and $\zeta(\mathbf{R}_{q,*}^\omega)$ be the optimal values of $(\mathbf{R}_q^\omega)$ and $(\mathbf{R}_{q,*}^\omega)$, respectively.

Proposition 1. *For any positive integer $\omega \geq 2$, we have $\zeta(\mathbf{R}_q^\omega) = \zeta(\mathbf{R}_{q,*}^\omega)$. Furthermore, $\lim_{\omega\to\infty} \zeta(\mathbf{R}_q^\omega) = \lim_{\omega\to\infty} \zeta(\mathbf{R}_{q,*}^\omega) = \zeta$.*

We know from (8) that the maximum size of the matrix variables in $(\mathbf{R}_q^\omega)$ is

$$\begin{pmatrix} \min\{p+1, q+1\} + \omega \\ \omega \end{pmatrix},$$

which is evaluated as $O((\min\{p,q\})^\omega)$.

3.3.2 Case: Square Root Concave Function

The next case is that f_{ij} of CCTPs ($\mathbf{Q}$) is a square root concave function of the form,

$$f_{ij}(x_{ij}) = \mu_{ij} x_{ij}^{1/2} \text{ with } \mu_{ij} > 0. \tag{20}$$

This case has been intensively studied (for instance, see [10, 16, 11, 31, 1]). Since f_{ij} of (20) is not a polynomial, we cannot deal with the transformed problem (14) as a POP. Thus, we should introduce a new variable w_{ji} to represent $v_{ji}^{1/2}(\boldsymbol{z})$ such that

$$v_{ji}^{1/2}(\boldsymbol{z}) = w_{ji} \Longleftrightarrow v_{ji}(\boldsymbol{z}) = w_{ji}^2 \text{ and } w_{ji} \geq 0, \tag{21}$$

and rewrite it as a quadratic programming problem,

$$\begin{array}{lll} \text{Minimize} & \displaystyle\sum_{j \in J} \sum_{i \in I} \mu_{ij} w_{ji} & \\ \text{subject to} & w_{ji}^2 - v_{ji}(\boldsymbol{z}) = 0, & j \in J,\ i \in I, \\ & v_{ji}(\boldsymbol{z}) \geq 0, & j \in J,\ i \in I, \\ & 0 \leq z_{ji} \leq \delta_{ji}, & j \in J',\ i \in I', \\ & 0 \leq w_{ji} \leq \gamma_{ji}, & j \in J,\ i \in I, \end{array} \tag{22}$$

where γ_{ji} are positive numbers such that $\gamma_{ji} > a_i^{1/2}$. The bounds for w_{ji} are derived from the fact that the x_{ij} of ($\mathbf{Q}$) satisfy $0 \leq x_{ij} \leq a_i$ and $x_{ij} = v_{ji}(\boldsymbol{z})$. We relax the equality of the first constraint of (22) into an inequality as follows:

$$(\mathbf{R}_s): \left| \begin{array}{lll} \text{Minimize} & \displaystyle\sum_{j \in J} \sum_{i \in I} \mu_{ij} w_{ji} & \\ \text{subject to} & w_{ji}^2 - v_{ji}(\boldsymbol{z}) \geq 0, & j \in J,\ i \in I, \\ & v_{ji}(\boldsymbol{z}) \geq 0, & j \in J,\ i \in I, \\ & 0 \leq z_{ji} \leq \delta_{ji}, & j \in J',\ i \in I', \\ & 0 \leq w_{ji} \leq \gamma_{ji}, & j \in J,\ i \in I. \end{array} \right. \tag{23}$$

In fact, (23) is equivalent to (22). If we assume that strict inequality holds for some inequality constraint $(w_{ji}^*)^2 - v_{ji}(\boldsymbol{z}^*) \geq 0$ at the optimal solution $(\boldsymbol{z}^*, \boldsymbol{w}^*)$ of (23), it contradicts the fact that $(\boldsymbol{z}^*, \boldsymbol{w}^*)$ is the optimal solution. Thus, we have

Lemma 6. *The problems* (22) *and* (23) *have the same optimal value and solution.*

Let $\mathcal{W}$ be the feasible region of (23). $\mathcal{W}$ has an interior due to the choice of $\gamma_{ji} > a_i^{1/2}$.

Lemma 7. *Under Assumption 3, $\mathcal{W}$ has a nonempty interior.*

Proof. In the same way of Lemma 4, we consider the feasible solution $\tilde{x}_{ij} = a_i b_j / \xi$ of ($\mathbf{Q}$) and the feasible solution $\tilde{z}_{ji} = \bar{a}_i \bar{b}_j / \xi$ of problem (14) whose vector $\tilde{\boldsymbol{x}} = (\tilde{x}_{ij} : i \in I, j \in J)$ and $\tilde{\boldsymbol{z}} = (\tilde{z}_{ji} : j \in J', i \in I')$ satisfy the relation $\boldsymbol{H}\tilde{\boldsymbol{x}} = \tilde{\boldsymbol{z}}$ for some $\boldsymbol{H} \in \mathbb{R}^{qp \times (q-1)(p-1)}$. There exist $\epsilon_{ji} > 0$ such that $a_i^{1/2} + \epsilon_{ji} < \gamma_{ji}$ since $\gamma_{ji} > a_i^{1/2}$. Using such ϵ_{ji}, we set $\tilde{w}_{ji} = a_i^{1/2} + \epsilon_{ji}$ and then we have $0 < \tilde{w}_{ji} < \gamma_{ji}$. Let $\tilde{\boldsymbol{w}} = (\tilde{w}_{ji} : j \in J, i \in I)$. For all constraints of (23), strict inequalities hold for $(\tilde{\boldsymbol{z}}, \tilde{\boldsymbol{w}})$. Indeed, we already know that the statement is true for the second, third and fourth constraints. For the first constraints, we have

$$\begin{aligned} \tilde{w}_{ji}^2 - v_{ji}(\tilde{\boldsymbol{z}}) &= \tilde{w}_{ji}^2 - \tilde{x}_{ij} \\ &= (a_i^{1/2} + \epsilon_{ji})^2 - a_i b_j/\xi \\ &= a_i(1 - b_j/\xi) + 2a_i^{1/2}\epsilon_{ji} + \epsilon_{ji}^2 > 0. \end{aligned}$$

Hence, $\mathcal{W}$ has a nonempty interior. ■

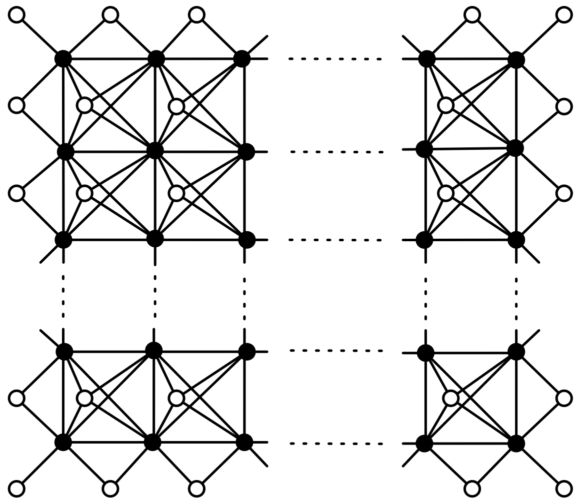

Figure 5: CSP graph G for $(\mathbf{R}_s)$. Black vertices correspond to z_{ji}, and white ones correspond to w_{ji}.

We shall use the symbol $(\mathbf{R}_s)$ to represent the problem (23). We shall also write the variable of $(\mathbf{R}_s)$ as $\bar{\boldsymbol{z}} := (\boldsymbol{z}, \boldsymbol{w}) \in \mathbb{R}^{(q-1)(p-1)} \times \mathbb{R}^{qp}$ such that

$$\bar{z}_{ji} := z_{ji} \text{ for } j \in J',\ i \in I', \text{ and } \bar{z}_{q'+j,p'+i} := w_{ji} \text{ for } j \in J,\ i \in I, \tag{24}$$

where $q' := q - 1$ and $p' := p - 1$. The CSP graph G for $(\mathbf{R}_s)$ is in Figure 5. In the figure, black vertices correspond to z_{ji} and white ones correspond to w_{ji}.

Below, we show that $(\mathbf{R}_s)$ with a variable $\bar{\boldsymbol{z}} \in \mathbb{R}^{(p-1)(q-1)+pq}$ has qualified collections Δ and $\widetilde{\Delta}$ whose maximum component sizes are $q + 1$ and $p + 1$, respectively. Let

$$\Delta = \{C_{ji}^{(1)}, C_j^{(21)}, C^{(22)}, C^{(23)}, C_{ji}^{(31)}, C_i^{(32)}, C_i^{(33)}, C_j^{(41)}, C^{(42)}, C^{(43)} : j \in J'',\ i \in I''\} \tag{25}$$

where

$$\begin{aligned}
C_{ji}^{(1)} &= \{(j,i),(j+1,i),\dots,(q-1,i),(1,i+1),(2,i+1),\dots,(j+1,i+1)\},\\
C_{j}^{(21)} &= \{(j,1),(j+1,1),(q'+j+1,p'+1)\},\\
C^{(22)} &= \{(1,1),(q'+1,p'+1)\},\\
C^{(23)} &= \{(q-1,1),(q'+q,p'+1)\},\\
C_{ji}^{(31)} &= \{(j,i),(j+1,i),(j,i+1),(j+1,i+1),(q'+j+1,p'+i+1)\},\\
C_{i}^{(32)} &= \{(1,i),(1,i+1),(q'+1,p'+i+1)\},\\
C_{i}^{(33)} &= \{(q-1,i),(q-1,i+1),(q'+q,p'+i)\},\\
C_{j}^{(41)} &= \{(j,p-1),(j+1,p-1),(q'+j+1,p'+p)\},\\
C^{(42)} &= \{(1,p-1),(q'+1,p'+p)\},\\
C^{(43)} &= \{(q-1,p-1),(q'+q,p'+p)\}.
\end{aligned}$$

Figure 6 presents the subgraphs $G(C)$ of the CSP graph G induced by the components $C \in \Delta$. Also, in a similar way as the case of a quadratic cost function f_{ij} in Subsection

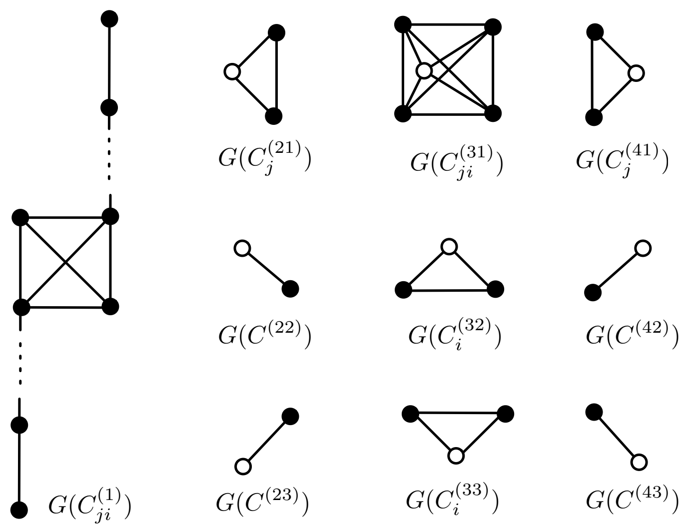

Figure 6: Induced subgraphs $G(C)$ of G by components $C \in \Delta$ of (25). Black vertices correspond to z_{ji}, and white ones correspond to w_{ji}.

3.3.1, we construct

$$\widetilde{\Delta} = \{\widetilde{C}_{ji}^{(1)}, \widetilde{C}_{j}^{(21)}, \widetilde{C}^{(22)}, \widetilde{C}^{(23)}, \widetilde{C}_{ji}^{(31)}, \widetilde{C}_{i}^{(32)}, \widetilde{C}_{i}^{(33)}, \widetilde{C}_{j}^{(41)}, \widetilde{C}^{(42)}, \widetilde{C}^{(43)} : j \in J'',\ i \in I''\}. \quad (26)$$

This corresponds to Δ for the graph obtained by interchanging j with i in the vertex label (j,i) of the CSP graph G for $(\mathbf{R}_s)$. Namely, $\widetilde{C}_{ji}^{(1)}$ of $\widetilde{\Delta}$ coincides with $\widetilde{C}_{ji}$ of (19), and the other components $\widetilde{C} \in \widetilde{\Delta} \setminus \{\widetilde{C}_{ji}^{(1)} : j \in J'', i \in I''\}$ are made by interchanging the first and second position of elements in the corresponding components $C \in \Delta \setminus \{C_{ji}^{(1)} : j \in J'', i \in I''\}$.

Note that the maximum sizes of the components in Δ and $\widetilde{\Delta}$ are $C_{ji}^{(1)}$ of size $q+1$ and $\widetilde{C}_{ji}^{(1)}$ of size $p+1$, respectively.

We first show that Δ satisfies Assumption 1-1 in Lemma 8. We shall use the following notation in the proof. Let $\Gamma := \{C_{ji}^{(1)} : j \in J'', i \in I''\}$. Here, $|\Gamma| = (q-2)(p-2)$. For simplicity, we denote an element $C_{ji}^{(1)} \in \Gamma$ as C_k where $k = (q-2)(i-1)+j$. From Lemma 5, the elements $C_1, \ldots, C_{(q-2)(p-2)} \in \Gamma$ satisfy Assumption 1-1 in this order.

Let $\Gamma^c := \Delta \setminus \Gamma$. Here, $|\Gamma^c| = qp$. We arbitrarily choose an ordering of elements in Γ^c, and arrange them in this order. The ordered elements of Γ^c are denoted as $D_1, \ldots, D_{qp}$. Define $\mathcal{T} := \{(q'+j, p'+i) : j \in J, i \in I\}$; the elements correspond to the white vertices in Figure 5 and 6. Here, $|\mathcal{T}| = qp$. Then, any $D_s \in \Gamma^c$, $s \in \{1, \ldots, qp\}$ can be written as $D_s = \bar{C}_k \cup \{t_s\}$ for some $\bar{C}_k \subseteq C_k \in \Gamma$ and some $t_s \in \mathcal{T}$. For instance, $\Gamma^c \ni C_{11}^{(31)} = \{(1,1),(2,1),(1,2),(2,2)\} \cup \{(q'+2, p'+2)\}$ where $\{(1,1),(2,1),(1,2),(2,2)\} \subseteq C_{11}^{(1)}$ and $\{(q'+2, p'+2)\} \in \mathcal{T}$. Note that the elements $D_s \in \Gamma^c$ are in one-to-one correspondence with the elements $t_s \in \mathcal{T}$.

Lemma 8. *Δ of (25) satisfies Assumption 1-1 in the order $C_1, \ldots, C_{(q-2)(p-2)}, D_1, \ldots, D_{qp}$.*

Proof. We have

$$\begin{aligned} & C_1 \cup \cdots \cup C_{(q-2)(p-2)} \cup D_1 \cdots \cup D_{s-1} \\ = \; & C_1 \cup \cdots \cup C_{(q-2)(p-2)} \cup \{t_1, \ldots, t_{s-1}\} \end{aligned}$$

since $C_1 \cup \cdots \cup C_{(q-2)(p-2)}$ does not contain any element of $\mathcal{T}$. Also, $D_s = \bar{C}_k \cup \{t_s\}$ for some $\bar{C}_k \subseteq C_k \in \Gamma$ and some $t_s \in \mathcal{T}$. Thus,

$$D_s \cap (C_1 \cup \cdots \cup C_{(q-2)(p-2)} \cup D_1 \cdots \cup D_{s-1}) = \bar{C}_k \subseteq C_k.$$

■

Lemma 9. *Let Δ and $\widetilde{\Delta}$ be as in (25) and (26), respectively. Then, each Δ and $\widetilde{\Delta}$ is a qualified collection for the problem $(\mathbf{R}_s)$.*

Proof. It is enough to check that Δ satisfies Assumption 1 for the same reason as the proof of Lemma 5. As stated in the above, Assumption 1-1 holds for Δ from Lemma 5 and 8. Also, for any fixed $\breve{j} \in J$ and any fixed $\breve{i} \in I$, both of the polynomials $w_{\breve{j}\breve{i}}$ and $w_{\breve{j}\breve{i}}^2 - v_{\breve{j}\breve{i}}(\boldsymbol{z})$ are contained in $\mathbb{R}[\bar{\boldsymbol{z}} = (\boldsymbol{z}, \boldsymbol{w}), \mathcal{A}(C)]$ with one of components $C \in \Delta \setminus \{C_{ji}^{(1)} : j \in J'',\ i \in I''\}$. Thus, Assumption 1-2 and 1-3 hold for Δ. ■

The remaining discussion is similar to the one of the previous subsection. For Δ of (25) and $\widetilde{\Delta}$ of (26), we define Δ_s° such that $\Delta_s^\circ = \Delta$ if $q \leq p$; otherwise, $\Delta_s^\circ = \widetilde{\Delta}$. Also, we modify $(\mathbf{R}_s)$ into the form (7) by adding redundant box constraints. Using Δ_s°, we construct SDP relaxations for the modified problem. Let $(\mathbf{R}_s^\omega)$ be the SDP of the relaxation ω and $(\mathbf{R}_{s,*}^\omega)$ be its dual. We know from Lemmas 2, 7, and 9 that Theorem 1 and Lemma 3 can be applied to $(\mathbf{R}_s^\omega)$ and $(\mathbf{R}_{s,*}^\omega)$. Let ζ be the global optimal value of $(\mathbf{R}_s)$. Let $\zeta(\mathbf{R}_s^\omega)$ and $\zeta(\mathbf{R}_{s,*}^\omega)$ be the optimal values of $(\mathbf{R}_s^\omega)$ and $(\mathbf{R}_{s,*}^\omega)$, respectively.

Proposition 2. *For any positive integer $\omega \geq 2$, we have $\zeta(\mathbf{R}_s^\omega) = \zeta(\mathbf{R}_{s,*}^\omega)$. Furthermore, $\lim_{\omega\to\infty} \zeta(\mathbf{R}_s^\omega) = \lim_{\omega\to\infty} \zeta(\mathbf{R}_{s,*}^\omega) = \zeta$.*

The maximum component of Δ_s° is $C_{ji}^{(1)}$ of size $q+1$ if $q \leq p$; otherwise, it is $\widetilde{C}_{ji}^{(1)}$ of size $p+1$. Therefore, the maximum size of the matrix variables of $(\mathbf{R}_s^\omega)$ is

$$\binom{\min\{p+1, q+1\} + \omega}{\omega}.$$

4 Reducing the Size of the SDP Relaxations

In the previous section, we saw that the transformed CCTPs have qualified collections consisting of small components. These collections give a hierarchy of SDP relaxations, and their optimal values converge to the global optimal value of CCTP as the relaxation order increases. In this section, we show that the size of the matrix variables of the SDP relaxations can be reduced by using Reznick's theorem, which is a statement about the support size of polynomials used in the SOS representation.

4.1 Reznick's Theorem for SOS Representation of Polynomials

Recall that the SDP relaxation $(\mathbf{P}^\omega)$ of a POP $(\mathbf{P})$ is derived from representing a polynomial $L - \eta$ as SOS, where L is the generalized Lagrangian for $(\mathbf{P})$ of the form (4) and η is a real constant. Namely, for a qualified collection $\Delta = \{C_1, \dots, C_\ell\}$, the representation is

$$L - \eta = \sum_{i=1}^{\ell} (f_{i1}^2 + \cdots + f_{ir_i}^2) \quad \text{for some } f_{i1}, \dots, f_{ir_i} \in \mathbb{R}[\boldsymbol{x}, \mathcal{A}^\omega(C_i)],\ i = 1, \dots, \ell. \tag{27}$$

$(\mathbf{P}^\omega)$ is gotten by solving the above identity. The variable $\boldsymbol{X}^{(i)}$ in $(\mathbf{P}^\omega)$ is a symmetric matrix of size $|\mathcal{A}^\omega(C_i)|$, and the set $\mathcal{A}^\omega(C_i)$ comes from the support of polynomials $f_{i1}, \dots, f_{ir_i}$. Here, for the SOS representation of $L - \eta$ in (27), we use the polynomials $f_{i1}, \dots, f_{ir_i}$ whose support size reaches $|\mathcal{A}^\omega(C_i)|$ at maximum. However, since the number of monomials in $L - \eta$ is not so many in practice, we may wonder whether it is possible to reduce the elements of $\mathcal{A}^\omega(C_i)$. Reznick's theorem in [25] gives one way to do it.

For $\mathcal{F} \subseteq \mathbb{Z}_+^n$, let $\mathcal{F}^e := \{\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_n) \in \mathcal{F} : \alpha_1, \dots \alpha_n \text{ are even}\}$; we call it an *even subset* of $\mathcal{F}$. $\frac{1}{2}\text{co}(\mathcal{F}^e)$ denotes the convex hull of $\{\frac{1}{2}\boldsymbol{\alpha} : \boldsymbol{\alpha} \in \mathcal{F}^e\}$.

Theorem 2. *(Theorem 1 of [25]) If a polynomial $f \in \mathbb{R}[\boldsymbol{x}]$ with support $\mathcal{F} \subseteq \mathbb{Z}_+^n$ can be written as $f = \sum_{i=1}^r f_i^2$ using a polynomial $f_i \in \mathbb{R}[\boldsymbol{x}]$ with support $\mathcal{F}_i \subseteq \mathbb{Z}_+^n$, then, $\mathcal{F}_i \subseteq \frac{1}{2}co(\mathcal{F}^e)$ for $i = 1, \dots, r$.*

We refer to the related study of Kojima et al. in [13]. They propose numerical methods to reduce the size of $\mathcal{A}^\omega(C_i)$ in (27). One of the techniques developed in the paper is implemented in SparsePOP [29].

4.2 Size Reduction of $(\mathbf{R}_q^\omega)$ and $(\mathbf{R}_s^\omega)$

4.2.1 Case: $(\mathbf{R}_q^\omega)$

Let us consider a POP $(\mathbf{P})$ that consists of a quadratic cost function $f \in \mathbb{R}[\boldsymbol{x}]$ with $\deg(f) = 2$ and linear constraints $g_k \in \mathbb{R}[\boldsymbol{x}]$ with $\deg(g_k) = 1,\ k = 1, \ldots, m$. It contains $(\mathbf{R}_q)$ as a special case. The generalized Lagrangian L for the POP is

$$L = f - \sum_{i=1}^{\ell} \sum_{k \in K_i} \phi_{ki} g_k \text{ with } \phi_{ki} \in \Sigma[\boldsymbol{x}, \mathcal{A}^{\omega-1}(C_i)], \tag{28}$$

where $\{C_1, \ldots, C_\ell\}$ is a qualified collection, $\{K_1, \ldots, K_\ell\}$ is the disjoint partition of $\{1, \ldots, m\}$ obtained from the qualified collection, and ω is a positive integer. Note that $\deg(L) = 2\omega - 1$ when $\omega \geq 2$ since $\deg(\phi_{ki}) = 2\omega - 2$.

Proposition 3. *Assume that $\omega \geq 2$. If L of (28) is an SOS polynomial such that $L \in \Sigma[\boldsymbol{x}, \mathcal{G}]$ for $\mathcal{G} \subseteq \mathbb{Z}_+^n$, then, we have $|\boldsymbol{\alpha}| \leq \omega - 1$ for any $\boldsymbol{\alpha} \in \mathcal{G}$.*

Proof. Let $\mathcal{F}$ be the support of L, and $\mathcal{F}^e$ be the even subset of $\mathcal{F}$. From the assumption $\omega \geq 2$, $\boldsymbol{\beta} \in \mathcal{F}$ satisfies $|\boldsymbol{\beta}| \leq 2\omega - 1$. Also, $\boldsymbol{\beta} \in \mathcal{F}$ with $|\boldsymbol{\beta}| = 2\omega - 1$ has at least one odd element. Thus, we have $|\boldsymbol{\beta}| \leq 2\omega - 2$ for any $\boldsymbol{\beta} \in \mathcal{F}^e$. From Theorem 2, we have $\mathcal{G} \subseteq \frac{1}{2}\mathrm{co}(\mathcal{F}^e)$. Let $\boldsymbol{\alpha} \in \mathcal{G} \subseteq \frac{1}{2}\mathrm{co}(\mathcal{F}^e)$. $\boldsymbol{\alpha}$ can be represented as a convex combination of $\boldsymbol{\beta}_1, \ldots, \boldsymbol{\beta}_\tau \in \mathcal{F}^e$. Namely, $\boldsymbol{\alpha} = \kappa_1 \bar{\boldsymbol{\beta}}_1 + \cdots + \kappa_\tau \bar{\boldsymbol{\beta}}_\tau$, where $\kappa_1, \ldots, \kappa_\tau \geq 0,\ \sum_{i=1}^{\tau} \kappa_i = 1$ and $\bar{\boldsymbol{\beta}}_i = \boldsymbol{\beta}_i/2$. Since $|\boldsymbol{\beta}_i| \leq 2\omega - 2$, that is, $|\bar{\boldsymbol{\beta}}_i| \leq \omega - 1$, we have

$$\begin{aligned} |\boldsymbol{\alpha}| &= |\kappa_1 \bar{\boldsymbol{\beta}}_1 + \cdots + \kappa_\tau \bar{\boldsymbol{\beta}}_\tau| \\ &\leq (\kappa_1 + \cdots + \kappa_\tau)(\omega - 1) = \omega - 1. \end{aligned}$$

■

Now we consider a POP $(\mathbf{P})$ with a quadratic cost function f and linear constraints $g_1, \ldots, g_m$. Thus, from Proposition 3, the representation of $L - \eta$ in (27) for a general POP $(\mathbf{P})$ can be rewritten as $L - \eta = \sum_{i=1}^{\ell} (f_{i1}^2 + \cdots + f_{ir_i}^2)$ for some $f_{i1}, \ldots, f_{ir_i} \in \mathbb{R}[\boldsymbol{x}, \mathcal{A}^{\omega-1}(C_i)],\ i = 1, \ldots, \ell$ when $\omega \geq 2$. Consequently, the size of the matrix variable $\boldsymbol{X}^{(i)}$ in the obtained SDP relaxations $(\mathbf{P}^\omega)$ can be reduced from $|\mathcal{A}^\omega(C_i)|$ to $|\mathcal{A}^{\omega-1}(C_i)|$.

Recall that $(\mathbf{R}_q)$ has a qualified collection, Δ_q°, defined in Subsection 3.3.1; it is written as Δ of (16) if $q \leq p$, otherwise, $\widetilde{\Delta}$ of (18). From the above discussion, it is apparent that the maximum size of the matrix variables in the SDP relaxation $(\mathbf{R}_q^\omega)$ can be reduced to

$$\binom{\min\{p+1, q+1\} + \omega - 1}{\omega - 1} \quad \text{for } \omega \geq 2, \tag{29}$$

which is evaluated as $O((\min\{p, q\})^{\omega-1})$. To distinguish from $(\mathbf{R}_q^\omega)$, we use the symbol $(\hat{\mathbf{R}}_q^\omega)$ to represent such a size-reduced SDP relaxation for $(\mathbf{R}_q)$, and the symbol $(\hat{\mathbf{R}}_{q,*}^\omega)$ for its dual.

Obviously, Proposition 1 holds for the primal-dual pair of $(\hat{\mathbf{R}}_q^\omega)$ and $(\hat{\mathbf{R}}_{q,*}^\omega)$. Namely, let $\zeta(\hat{\mathbf{R}}_q^\omega)$ and $\zeta(\hat{\mathbf{R}}_{q,*}^\omega)$ be the optimal values of $(\hat{\mathbf{R}}_q^\omega)$ and $(\hat{\mathbf{R}}_{q,*}^\omega)$, respectively. Let ζ be the global optimal value ζ of $(\mathbf{R}_q)$. Then, we have $\lim_{\omega\to\infty}\zeta(\hat{\mathbf{R}}_q^\omega) = \lim_{\omega\to\infty}\zeta(\hat{\mathbf{R}}_{q,*}^\omega) = \zeta$. Also, as the last of Section 2 shows, the linear part solution $\boldsymbol{z}_{lin}^\omega$ of $(\hat{\mathbf{R}}_{q,*}^\omega)$ is the feasible solution of $(\mathbf{R}_q)$, since all the constraints are linear. Let $f(\boldsymbol{z}_{lin}^\omega)$ denote the cost function value of $(\mathbf{R}_q)$ at $\boldsymbol{z}_{lin}^\omega$. Accordingly, we have the relation

$$\zeta(\hat{\mathbf{R}}_q^\omega) = \zeta(\hat{\mathbf{R}}_{q,*}^\omega) \le \zeta \le f(\boldsymbol{z}_{lin}^\omega) \quad \text{for any positive integer } \omega \ge 2.$$

4.2.2 Case: $(\mathbf{R}_s^\omega)$

The key to the proof of Proposition 3 is that the constraints are linear; thus, the degree of the Lagrangian is odd. The transformed CCTP with a square root concave cost function $(\mathbf{R}_s)$ has quadratic constraints. Thus, we cannot apply the proposition to the problem. We consider the following problem with a variable $(\boldsymbol{x}, \boldsymbol{y}) \in \mathbb{R}^n \times \mathbb{R}^m$:

$$\begin{array}{lll} \text{Minimize} & f(\boldsymbol{y}) & \\ \text{subject to} & y_k^2 - g_k(\boldsymbol{x}) \ge 0, & k = 1,\dots,m, \\ & h_j(\boldsymbol{x},\boldsymbol{y}) \ge 0, & j = 1,\dots,s, \end{array} \tag{30}$$

where $f \in \mathbb{R}[\boldsymbol{y}]$ with $\deg(f) = 1$, $g_k \in \mathbb{R}[\boldsymbol{x}]$ with $\deg(g_k) = 1,\ k = 1,\dots,m$, and $h_j \in \mathbb{R}[\boldsymbol{x},\boldsymbol{y}]$ with $\deg(h_j) = 1,\ j = 1,\dots,s$. It contains $(\mathbf{R}_s)$ as the special case. Here, let us look at the structure of the constraints; the quadratic terms consist of variables y_k and the other terms are all linear in the variable $\boldsymbol{x}$. By exploiting the structure, we can obtain a result similar to Proposition 3 for (30). The generalized Lagrangian L for (30) is

$$L(\boldsymbol{x},\boldsymbol{y}) = f(\boldsymbol{y}) - \sum_{i=1}^{\ell}\sum_{k\in K_i}\phi_{ik}^{(1)}(\boldsymbol{x},\boldsymbol{y})(y_k^2 - g_k(\boldsymbol{x})) - \sum_{i=1}^{\ell}\sum_{j\in J_i}\phi_{ij}^{(2)}(\boldsymbol{x},\boldsymbol{y})h_j(\boldsymbol{x},\boldsymbol{y})$$
$$\text{with } \phi_{ik}^{(1)}, \phi_{ij}^{(2)} \in \Sigma[\boldsymbol{x},\boldsymbol{y},\mathcal{A}^{\omega-1}(C_i)]. \tag{31}$$

Here, $\{C_1,\dots,C_\ell\}$ is a qualified collection. $\{K_1,\dots,K_\ell\}$ and $\{J_1,\dots,J_\ell\}$ are each disjoint partitions of $\{1,\dots,m\}$ and $\{1,\dots,s\}$. ω is a positive integer. Note that $\deg(L) = 2\omega$. In the proposition and its proof below, we denote an element in the support of polynomials in $\mathbb{R}[\boldsymbol{x},\boldsymbol{y}]$ as $(\boldsymbol{\alpha}_{\boldsymbol{x}}, \boldsymbol{\alpha}_{\boldsymbol{y}})$, and it corresponds to the power of the monomial $\boldsymbol{x}^{\boldsymbol{\alpha}_{\boldsymbol{x}}}\boldsymbol{y}^{\boldsymbol{\alpha}_{\boldsymbol{y}}}$.

Proposition 4. *If $L(\boldsymbol{x},\boldsymbol{y})$ of (31) is an SOS polynomial such that $L(\boldsymbol{x},\boldsymbol{y}) \in \Sigma[\boldsymbol{x},\boldsymbol{y},\mathcal{G}]$ for $\mathcal{G} \subseteq \mathbb{Z}_+^{n+m}$, then, we have $|(\boldsymbol{\alpha}_{\boldsymbol{x}}, \mathbf{0})| \le \omega - 1$ for any $(\boldsymbol{\alpha}_{\boldsymbol{x}}, \mathbf{0}) \in \mathcal{G}$.*

Proof. Let $\mathcal{F}$ be the support of L, and let $\mathcal{F}^e$ be the even subset of $\mathcal{F}$. Define $\mathcal{F}_{=0}^e := \{(\boldsymbol{\beta}_{\boldsymbol{x}}, \boldsymbol{\beta}_{\boldsymbol{y}}) \in \mathcal{F}^e : \boldsymbol{\beta}_{\boldsymbol{y}} = \mathbf{0}\}$ and $\mathcal{F}_{\ne 0}^e := \mathcal{F}^e \setminus \mathcal{F}_{=0}^e$. The element $(\boldsymbol{\beta}_{\boldsymbol{x}}, \mathbf{0}) \in \mathcal{F}$ satisfies $|(\boldsymbol{\beta}_{\boldsymbol{x}}, \mathbf{0})| \le 2\omega - 1$ and thus, for any $\boldsymbol{\beta} \in \mathcal{F}_{=0}^e$, we have $|\boldsymbol{\beta}| \le 2\omega - 2$ for the same reason as in Proposition 3. From $\mathcal{F}^e = \mathcal{F}_{=0}^e \cup \mathcal{F}_{\ne 0}^e$ and Theorem 2, we have $\mathcal{G} \subseteq \frac{1}{2}\mathrm{co}(\mathcal{F}_{=0}^e \cup \mathcal{F}_{\ne 0}^e)$. Let $(\boldsymbol{\alpha}_{\boldsymbol{x}}, \mathbf{0}) \in \mathcal{G} \subseteq \frac{1}{2}\mathrm{co}(\mathcal{F}_{=0}^e \cup \mathcal{F}_{\ne 0}^e)$. Then, $(\boldsymbol{\alpha}_{\boldsymbol{x}}, \mathbf{0})$ can be represented as a convex combination of only the elements in $\mathcal{F}_{=0}^e$. The rest of the proof is analogous to the proof of Proposition 3. ∎

The remaining discussion is similar to the one of the previous subsection. Proposition 4 suggests that the representation of $L - \eta$ for (30) can be rewritten as $L - \eta = \sum_{i=1}^{\ell}(f_{i1}^2 + \cdots + f_{ir_i}^2)$ for some $f_{i1}, \ldots, f_{ir_i} \in \mathbb{R}[\boldsymbol{x}, \mathcal{A}^{\omega}(C_i) \setminus \mathcal{H}^{\omega}(C_i)]$. Here, $\mathcal{H}^{\omega}(C) := \{\boldsymbol{\alpha} = (\boldsymbol{\alpha_x}, \boldsymbol{\alpha_y}) \in \mathbb{Z}_+^n \times \mathbb{Z}_+^m : |\boldsymbol{\alpha}| = \omega \text{ and } \alpha_i = 0 \text{ if } i \notin C \cap \{1, \ldots, n\}\}$ for $C \subseteq \{1, \ldots, n+m\}$.

$(\mathbf{R}_s)$ is a special case of (30), if we match the variable $(\boldsymbol{z}, \boldsymbol{w}) \in \mathbb{R}^{(q-1)(p-1)} \times \mathbb{R}^{qp}$ of $(\mathbf{R}_s)$ to the variable $(\boldsymbol{x}, \boldsymbol{y}) \in \mathbb{R}^n \times \mathbb{R}^m$ of (30). $(\mathbf{R}_s)$ has Δ_s° defined in Subsection 3.3.2 as the qualified collection; the maximum components are $C_{ji}^{(1)}$ of size $q+1$ if $q \le p$, otherwise, $\widetilde{C}_{ji}^{(1)}$ of size $p+1$. Note that each element of $C_{ji}^{(1)}$ or $\widetilde{C}_{ji}^{(1)}$ corresponds to z_{ji}. Let $(\mathbf{R}_s^{\omega})$ be the SDP relaxations for $(\mathbf{R}_s)$ induced from Δ_s°. Then, the maximum size of the matrix variables in $(\mathbf{R}_s^{\omega})$ is

$$\begin{pmatrix} \min\{p+1, q+1\} + \omega - 1 \\ \omega - 1 \end{pmatrix}$$

since $\mathcal{A}^{\omega}(C) \backslash \mathcal{H}^{\omega}(C) = \mathcal{A}^{\omega-1}(C)$ for $C = C_{ji}^{(1)}$ or $C = \widetilde{C}_{ji}^{(1)}$. It is evaluated as $O((\min\{p,q\})^{\omega-1})$. We denote such a size-reduced SDP relaxation for $(\mathbf{R}_s)$ as $(\hat{\mathbf{R}}_s^{\omega})$, and its dual as $(\hat{\mathbf{R}}_{s,*}^{\omega})$.

For the primal-dual pair of $(\hat{\mathbf{R}}_s^{\omega})$ and $(\hat{\mathbf{R}}_{s,*}^{\omega})$, the result is similar to Proposition 2. Namely, let $\zeta(\hat{\mathbf{R}}_s^{\omega})$ and $\zeta(\hat{\mathbf{R}}_{s,*}^{\omega})$ be the optimal values of $(\hat{\mathbf{R}}_s^{\omega})$ and $(\hat{\mathbf{R}}_{s,*}^{\omega})$, respectively. Let ζ be the global optimal value ζ of $(\mathbf{R}_s)$. Then, $\lim_{\omega\to\infty} \zeta(\hat{\mathbf{R}}_s^{\omega}) = \lim_{\omega\to\infty} \zeta(\hat{\mathbf{R}}_{s,*}^{\omega}) = \zeta$. Unlike the case of a quadratic cost function, the linear part solution $\boldsymbol{z}_{lin}^{\omega} \in \mathbb{R}^{(q-1)(p-1)+qp}$ of $(\mathbf{R}_{s,*}^{\omega})$ may not be feasible in $(\mathbf{R}_s)$ since it has the quadratic constraints $w_{ji}^2 - v_{ji}(\boldsymbol{z}) \ge 0$. However, a feasible solution can be constructed from $\boldsymbol{z}_{lin}^{\omega}$ in the following manner. Depending on the positions of $\boldsymbol{z}$ and $\boldsymbol{w}$, we divide $\boldsymbol{z}_{lin}^{\omega}$ into two component vectors $\boldsymbol{z}^{\omega} \in \mathbb{R}^{(q-1)(p-1)}$ and $\boldsymbol{w}^{\omega} \in \mathbb{R}^{qp}$ such that $\boldsymbol{z}_{lin}^{\omega} = (\boldsymbol{z}^{\omega}, \boldsymbol{w}^{\omega}) \in \mathbb{R}^{(q-1)(p-1)} \times \mathbb{R}^{qp}$. For $\tilde{\boldsymbol{w}}^{\omega} = (\tilde{w}_{ji}^{\omega} : j \in J, i \in I)$ with $\tilde{w}_{ji}^{\omega} = v_{ji}(\boldsymbol{z}^{\omega})^{1/2}$, define $\boldsymbol{z}_{fea}^{\omega} := (\boldsymbol{z}^{\omega}, \tilde{\boldsymbol{w}}^{\omega})$. Then, $\boldsymbol{z}_{fea}^{\omega}$ is a feasible solution of $(\mathbf{R}_s)$. Let $f(\boldsymbol{z}_{fea}^{\omega})$ denote the cost function value of $(\mathbf{R}_s)$ at $\boldsymbol{z}_{fea}^{\omega}$. Accordingly, we have

$$\zeta(\hat{\mathbf{R}}_s^{\omega}) = \zeta(\hat{\mathbf{R}}_{s,*}^{\omega}) \le \zeta \le f(\boldsymbol{z}_{fea}^{\omega}) \quad \text{for any positive integer } \omega \ge 2.$$

Note that in general, a similar relation to the above one does not hold for the cost function value $f(\boldsymbol{z}_{lin}^{\omega})$ of $(\mathbf{R}_s)$ at the linear part solution $\boldsymbol{z}_{lin}^{\omega}$. This is because $\boldsymbol{z}_{lin}^{\omega}$ may not be feasible in $(\mathbf{R}_s)$.

4.3 Comparison with SDP Relaxations of Kim et al. in [12]

As stated in Section 1, our method was inspired by the work of Kim et al. in [12]. Consider a POP of the form $(\mathbf{P})$ whose CSP matrix is not sparse. Using a nonsingular linear transformation $\boldsymbol{T} \in \mathbb{R}^{n\times n}$ of variables, Kim et al.'s method tries to transform the POP into

$$\text{Minimize} \quad f^{\circ}(\boldsymbol{y}) \quad \text{subject to} \quad g_k^{\circ}(\boldsymbol{y}) \ge 0, \ k = 1, \ldots, m \tag{32}$$

whose CSP matrix is as sparse as possible. Here, $f^{\circ}(\boldsymbol{y}) = f(\boldsymbol{T}\boldsymbol{y})$ and $g_k^{\circ}(\boldsymbol{y}) = g_k(\boldsymbol{T}\boldsymbol{y})$ with $\boldsymbol{x} = \boldsymbol{T}\boldsymbol{y}$. In this method, finding such variable transformation $\boldsymbol{T}$ is formulated as combinatorial problems, and heuristic algorithms are used to solve the problems. After the transformation, SparsePOP [29] is employed to solve the SDP relaxations for the transformed POP (32).

The practical performance of this method was evaluated in [12], and the numerical results were reported about the sizes of the SDP relaxations for several POPs. We can find the results about the CCTPs with a quadratic concave cost function f_{ij} of (15). These results correspond to our SDP relaxations $(\hat{\mathbf{R}}_q^\omega)$. We compare their results with our SDP relaxations.

Table 1: Maximum sizes of the matrix variables in SDPs with $\omega = 2$.

p	5	5	5	5	6	7	8	9
q	5	10	15	20	6	7	8	9
$(\hat{\mathbf{R}}_q^\omega)$	7	7	7	7	8	9	10	11
[12]	10	14	17	16	17	15	22	25

Table 1 compares the sizes of the SDPs. The "p" and "q" indicate the number of suppliers and demanders in the formulation of the CCTP $(\mathbf{Q})$. The third row lists the maximum sizes of the variable of our SDP relaxations $(\hat{\mathbf{R}}_q^\omega)$ with $\omega = 2$. The fourth one lists those of [12] (Table 6 of Subsection 4.2 of that paper). Note that from (29), the maximum size of variable of $(\hat{\mathbf{R}}_q^\omega)$ is $p + 2$ when $p \leq q$ and $\omega = 2$. From the table, we see that the sizes of $(\hat{\mathbf{R}}_q^\omega)$ are smaller than those of [12] for the test cases reported in the paper.

Remark 2. The paper [12] of Kim et al. reports that numerical difficulties sometimes occurred in solving the SDP relaxations for the transformed CCTPs by their method even if the size of CCTPs is small. It appears that one of the reasons is in numerical errors caused by the application of linear transformation $\boldsymbol{T}$ to CCTPs. Such numerical errors are not caused in our variable transformation approach.

5 Numerical Experiments

Subsection 5.1 is about the component sizes in qualified collections obtained by Cholesky factorization of the CSP matrices for the transformed CCTPs $(\mathbf{R}_q)$ and $(\mathbf{R}_s)$. Subsection 5.2 is about the performance evaluation of the SDP relaxations $(\hat{\mathbf{R}}_q^\omega)$ and $(\hat{\mathbf{R}}_s^\omega)$. All the experiments were done on a 2.4 GHz AMD Opteron CPU and 8.0 GB memory.

5.1 Component Sizes in Qualified Collections by Cholesky Factorization of CSP Matrices

We showed that $(\mathbf{R}_q)$ has qualified collections Δ of (16) and $\widetilde{\Delta}$ of (18). These Δ and $\widetilde{\Delta}$ consist of components of size $q + 1$ and size $p + 1$, respectively. Also, $(\mathbf{R}_s)$ has qualified collections Δ of (25) and $\widetilde{\Delta}$ of (26). The maximum component sizes in these Δ and $\widetilde{\Delta}$ are $q+1$

and $p+1$, respectively. Since $(\mathbf{R}_q)$ and $(\mathbf{R}_s)$ can have qualified collections other than those which we obtained, there might be qualified collections whose component sizes are much smaller. The numerical method presented in [28] can often find qualified collections with small components. We thus performed the numerical method and checked the component sizes of the qualified collections obtained by it.

In the method of [28], as stated in the last of Section 3.1, the ordering of the row and column indices of CSP matrix has an effect on the component sizes of the qualified collections. In the experiments, we used two ordering methods implemented in MATLAB: minimum degree ordering and reverse Cuthill-McKee ordering. The numerical results are summarized in Table 2. All test cases satisfy $p \le q$, and thus, the maximum sizes of components in $\widetilde{\Delta}$ of (18) are listed in the third row of "ours" and $\widetilde{\Delta}$ of (26) in the sixth row of "ours". The fourth and fifth rows list the maximum sizes of components in the qualified collections obtained by the method of [28] with the use of the two ordering methods for $(\mathbf{R}_q)$. The seventh and eighth rows correspond to those for $(\mathbf{R}_s)$.

From the table, we can see that the maximum component sizes of our qualified collections are smaller than or equal to those obtained by [28]. These results imply that the component sizes of our qualified collections are relatively smaller among those of the others.

Table 2: Maximum sizes of components in qualified collections.

	p	5	5	10	10	15	15	20	20	25	25
	q	200	600	100	300	60	200	50	150	40	120
	ours	6	6	11	11	16	16	21	21	26	26
$(\mathbf{R}_q)$	minimum degree	6	6	18	18	30	34	40	40	56	67
	reverse Cuthill-McKee	8	8	18	18	28	28	38	38	48	48
	ours	6	6	11	11	16	16	21	21	26	26
$(\mathbf{R}_s)$	minimum degree	6	6	18	18	29	29	38	39	48	48
	reverse Cuthill-McKee	8	8	18	18	28	28	38	38	48	48

5.2 Practical Performance of Proposed Relaxation Methods

We conducted numerical experiments to evaluate the performance of SDP relaxations $(\hat{\mathbf{R}}_q^\omega)$ for $(\mathbf{R}_q)$ and $(\hat{\mathbf{R}}_s^\omega)$ for $(\mathbf{R}_s)$. Two types of experiment were conducted: the first ones examined the accuracy of the approximate solutions for $(\mathbf{R}_q)$ and $(\mathbf{R}_s)$, and the second ones evaluated how large of a problem can be handled in a reasonable amount of computational time.

For the construction of $(\hat{\mathbf{R}}_q^\omega)$ and $(\hat{\mathbf{R}}_s^\omega)$ with convergence property, we need to reformulate $(\mathbf{R}_q)$ and $(\mathbf{R}_s)$ into the form of (7) by adding many redundant box constraints. Therefore, the obtained SDP relaxations for the reformulated problems have many constraints which are derived from the box constraints. To restrict the number of such constraints, we used the SDP relaxations constructed for the original form of $(\mathbf{R}_q)$ and $(\mathbf{R}_s)$ as $(\hat{\mathbf{R}}_q^\omega)$ and $(\hat{\mathbf{R}}_s^\omega)$ in the experiments.

We modified SparsePOP [29] so it could implement our relaxation methods, and used random test problems for the evaluation. The test problems were as follows. The right-hand coefficients a_i, b_j of CCTPs ($\mathbf{Q}$) were randomly generated integers such that the total value $\sum_{i\in I} a_i = \sum_{j\in J} b_j$ belonged to $[\max\{p,q\}, \max\{10p, 10q\}]$. The settings were taken from [12]. In the case in which f_{ij} was a quadratic concave function of (15), the coefficients μ_{ij} and the constants ν_{ij} were integers randomly chosen from $\mu_{ij} \in [-5,-1],\ \nu_{ij} \in [200, 800]$. The settings were from [12]. In the case in which f_{ij} was a square root concave function of (20), the coefficients μ_{ij} were integers randomly chosen from $\mu_{ij} \in [3, 8]$. The settings were the same as in [1].

All SDPs in the experiments of Tables 3, 4 and 6 were solved by SeDuMi [26]. SeDuMi employs primal-dual type interior point algorithms. The elapsed time for the computation is listed in "time" of the Tables 3 and 6. In the experiments whose results are summarized in Table 5, we used SDPA-GMP [22, 30]. SDPA-GMP employs a multiple precision library and can carry out similar algorithms as SeDuMi does, but with arbitrary arithmetic precision. Hence, it can provide more accurate numerical solutions of SDPs than SeDuMi can, whose arithmetic is double-precision floating point and precision is approximately 16 significant digits.

To evaluate the accuracy of the approximate solutions for ($\mathbf{R}_q$) and ($\mathbf{R}_s$), we adopted the error measures used in [28, 29]. For simplicity of description, we give the form of measures for a POP of the form ($\mathbf{P}$). Let $\zeta(\mathbf{P}^\omega)$ be the optimal value of SDP relaxation ($\mathbf{P}^\omega$) for ($\mathbf{P}$), and let $f(\boldsymbol{x}^\omega)$ be the cost function value of ($\mathbf{P}$) at the approximate solution $\boldsymbol{x}^\omega$ that can be obtained from the optimal solution of ($\mathbf{P}^\omega$). The relative error of the cost function values is computed as

$$\epsilon_{cost}(\boldsymbol{x}^\omega) = \frac{|f(\boldsymbol{x}^\omega) - \zeta(\mathbf{P}^\omega)|}{\max\{1,\ |f(\boldsymbol{x}^\omega)|\}}.$$

If $\boldsymbol{x}^\omega$ is guaranteed to be feasible in ($\mathbf{P}$) and $\epsilon_{cost}(\boldsymbol{x}^\omega)$ is close to 0, we can say that $\boldsymbol{x}^\omega$ is fairly near the global optimal solution of ($\mathbf{P}$). If $\boldsymbol{x}^\omega$ is not guaranteed to be feasible in ($\mathbf{P}$), the feasibility error is evaluated by

$$\epsilon_{fea}(\boldsymbol{x}^\omega) = \min_{k=1,\ldots,m} \{g_k(\boldsymbol{x}^\omega), 0\}.$$

In the case of ($\mathbf{R}_q$), the linear part solution $\boldsymbol{z}^\omega_{lin}$ of ($\hat{\mathbf{R}}^\omega_{q,*}$) is the solution candidate of ($\mathbf{R}_q$). It is always a feasible solution of ($\mathbf{R}_q$). We thus evaluated the accuracy of solution by using $\epsilon_{cost}(\boldsymbol{z}^\omega_{lin})$. In the case of ($\mathbf{R}_s$), two solution candidates are considered: the first candidate is $\boldsymbol{z}^\omega_{fea}$ defined in Subsection 4.2.2 which is always a feasible solution of ($\mathbf{R}_s$), and the second candidate is the linear part solution $\boldsymbol{z}^\omega_{lin}$ of ($\hat{\mathbf{R}}^\omega_{s,*}$) which might not be a feasible solution of ($\mathbf{R}_s$). Hence, we used $\epsilon_{cost}(\boldsymbol{z}^\omega_{fea})$ for the first one and $\epsilon_{cost}(\boldsymbol{z}^\omega_{lin})$ and $\epsilon_{fea}(\boldsymbol{z}^\omega_{lin})$ for the second one.

To evaluate the accuracy of the numerical solution of the SDP, we used the error measures, err1-5, introduced in [21]; these are often called DIMACS errors. We refer the reader to the paper for their precise forms. In our experiments, the feasibility errors, err1, err2, err3 and err4, were almost zero. This means that the numerical solutions satisfied all of the constraints with high accuracy. On the other hand, the duality gap errors, err5 and err6, were relatively high. Here, if the solution is feasible, then, err5 and err6 should coincide under exact arithmetic. We thus report only err5, whose values are listed in "ϵ_{sdp}" of Table 3-6. If ϵ_{sdp} is close to 0, we can say that the numerical solution is fairly close to the optimal one.

Table 3: Accuracy of approximate solutions of $(\hat{\mathbf{R}}_q^\omega)$ and $(\hat{\mathbf{R}}_s^\omega)$ with $\omega = 2$.

		$(\hat{\mathbf{R}}_q^\omega)$			$(\hat{\mathbf{R}}_s^\omega)$		
p	q	$\epsilon_{cost}(\boldsymbol{z}_{lin}^\omega)$	ϵ_{sdp}	time	$\epsilon_{cost}(\boldsymbol{z}_{fea}^\omega)$	ϵ_{sdp}	time
5	80	2.03e–03	-1.20e–09	3m	9.65e–02	-4.95e–07	11m
5	100	1.97e–03	-2.75e–08	4m	1.23e–01	-9.78e–07	15m
5	120	1.40e–03	-4.48e–09	6m	1.37e–01	-1.40e–06	18m
5	140	1.56e–03	-5.83e–09	8m	1.32e–01	-7.21e–06	20m
5	160	1.96e–03	-1.73e–07	10m	1.43e–01	-1.84e–06	21m

Table 3 summarizes the results of the first experiments with the relaxation order $\omega = 2$ whose purpose is to assess the accuracy of the approximate solutions of $(\hat{\mathbf{R}}_q^\omega)$ and $(\hat{\mathbf{R}}_s^\omega)$. The data in the table is the average of the values returned by the relaxation methods on 10 different test problems for each size. The left side of the table lists the results of $(\hat{\mathbf{R}}_q^\omega)$, and the right side lists those of $(\hat{\mathbf{R}}_s^\omega)$. For the case of $(\hat{\mathbf{R}}_q^\omega)$, since the relative errors of the cost function value $\epsilon_{cost}(\boldsymbol{z}_{lin}^\omega)$ are around 1.0e-03, we can conclude that the approximate solutions $\boldsymbol{z}_{lin}^\omega$ are close to the global optimal solutions of $(\mathbf{R}_q)$. Meanwhile, for the case of $(\hat{\mathbf{R}}_s^\omega)$, the relative errors $\epsilon_{cost}(\boldsymbol{z}_{fea}^\omega)$ are around 1.0e-01. Thus, we see that there is a distance between the approximate solutions $\boldsymbol{z}_{fea}^\omega$ and the global optimal ones of $(\mathbf{R}_s)$.

The numerical results of the first experiments suggest that $(\hat{\mathbf{R}}_s^\omega)$ of relaxation order $\omega = 2$ is not a strong SDP relaxation for the test problems. To increase the strength, we need to increase the relaxation order ω. We here refer to the numerical results in [28]; the linear part solutions of the SDP relaxations for their test problems are fairly close to the global optimal ones if the relaxation order is $\omega = 2$ or 3. Hence, we tried to solve the SDP relaxations $(\hat{\mathbf{R}}_s^\omega)$ with $\omega = 3$. However, numerical difficulties often occurred in the computation, and the accuracy of the numerical solutions was low even if solved. In particular, inaccuracy became pronounced as the problem size grew. Therefore, we employed SDPA-GMP as well as SeDuMi and chose the test problems of $(p, q) = (5, 5), (5, 20)$ to examine the strength of relaxation $(\hat{\mathbf{R}}_s^\omega)$ with $\omega = 3$. In the use of SDPA-GMP, we prepared the input data of the SDPs with a precision of 120 digits, and set the precision of floating point arithmetic in SDPA-GMP as approximately 120 significant digits.

Tables 4 and 5 summarize the results when using SeDuMi and SDPA-GMP. The data in the tables is the average of values returned by the relaxation methods $(\hat{\mathbf{R}}_s^\omega)$ on 5 different test problems for each size. In general, SDPA-GMP takes more computational time over SeDuMi. In fact, SDPA-GMP spent about 4 days to solve $(\hat{\mathbf{R}}_s^\omega)$ of $\omega = 3$ for $(p, q) = (5, 20)$, while SeDuMi took about 30 minutes for the computation.

For the case of $(p, q) = (5, 5)$, the two tables show that the significant improvements were obtained in $\epsilon_{fea}(\boldsymbol{z}_{lin}^\omega)$ and $\epsilon_{cost}(\boldsymbol{z}_{fea}^\omega)$ after increasing the relaxation order from $\omega = 2$

Table 4: $(\hat{\mathbf{R}}_s^\omega)$ for $(\mathbf{R}_s)$ with $\omega = 2, 3$ when using SeDuMi.

		$\epsilon_{cost}(\boldsymbol{z}_{fea}^\omega)$	$\epsilon_{cost}(\boldsymbol{z}_{lin}^\omega)$	$\epsilon_{fea}(\boldsymbol{z}_{lin}^\omega)$	ϵ_{sdp}
$(p, q) = (5, 5)$	$\omega = 2$	1.57e–01	2.24e–09	-1.78e+00	-9.22e–10
	$\omega = 3$	3.44e–02	3.05e–07	-1.64e–02	-1.27e–07
$(p, q) = (5, 20)$	$\omega = 2$	1.16e–01	2.60e–07	-2.08e+00	-1.22e–07
	$\omega = 3$	2.18e–01	1.06e–05	-1.47e+00	-4.98e–06

Table 5: $(\hat{\mathbf{R}}_s^\omega)$ for $(\mathbf{R}_s)$ with $\omega = 2, 3$ when using SDPA-GMP.

		$\epsilon_{cost}(\boldsymbol{z}_{fea}^\omega)$	$\epsilon_{cost}(\boldsymbol{z}_{lin}^\omega)$	$\epsilon_{fea}(\boldsymbol{z}_{lin}^\omega)$	ϵ_{sdp}
$(p, q) = (5, 5)$	$\omega = 2$	1.54e–01	2.40e–11	-1.78e+00	4.09e–31
	$\omega = 3$	1.50e–02	5.66e–07	-4.39e–03	3.93e–31
$(p, q) = (5, 20)$	$\omega = 2$	7.98e–02	1.24e–11	-1.94e+00	4.01e–31
	$\omega = 3$	2.21e–01	6.67e–03	-1.89e+00	4.58e–31

to $\omega = 3$. In particular, for the 4 out of the 5 test problems, $\epsilon_{cost}(\boldsymbol{z}_{fea}^\omega)$, $\epsilon_{cost}(\boldsymbol{z}_{lin}^\omega)$ and $\epsilon_{fea}(\boldsymbol{z}_{lin}^\omega)$ were less than about 1.0e-06 when we solved $(\hat{\mathbf{R}}_s^\omega)$ of $\omega = 3$ by using SDPA-GMP. Accordingly, we can see that $(\hat{\mathbf{R}}_s^\omega)$ of $\omega = 3$ are tight for these 4 test problems, and give the approximate solutions of the problems with high accuracy.

Meanwhile, for the case of $(p, q) = (5, 20)$, the improvements are slight with the increase of relaxation order, and the errors are large even if $\omega = 3$. Then, we see that $(\hat{\mathbf{R}}_s^\omega)$ of $\omega = 3$ is not a strong SDP relaxation for $(\mathbf{R}_s)$ of size $(p, q) = (5, 20)$. Here, Table 4 suggests that ϵ_{sdp} were not so small when using SeDuMi. Therefore, one may expect that the strength of the SDP relaxation will improve if the SDPs are solved more precisely. However, we can see that the expected results were not attained. Table 5 suggests that SDPA-GMP could solve the SDPs with high accuracy since ϵ_{sdp} are considerably small, while there are no major differences in the errors of Tables 4 and 5. Therefore, even if we solve $(\hat{\mathbf{R}}_s^\omega)$ with $\omega = 3$ for $(\mathbf{R}_s)$ of $(p, q) = (5, 20)$, it is possibly difficult to obtain the approximate solutions of the problems that are close enough to the global optimal ones. In Section 6, we discuss other approaches to improving the accuracy of the approximate solutions.

The computational time for the first experiments listed in Table 3 is less than about 20 minutes. This means our relaxation methods $(\hat{\mathbf{R}}_q^\omega)$ and $(\hat{\mathbf{R}}_s^\omega)$ should work well on larger problems. The aim of the second experiments was to examine it. Table 6 summarizes the results. The data in the table is the average of the results of performing the relaxation methods on 5 different test problems for each size. In the experiments, we used relaxation order $\omega = 2$.

From the table, we can see that even when the problem is a large one, our SDP relaxations can provide approximate solutions with moderately good accuracy. In particular, for the case of $(\hat{\mathbf{R}}_q^\omega)$, $\epsilon_{cost}(\boldsymbol{z}_{lin}^\omega)$ are around 1.0e-02, except for $(p, q) = (5, 400), (5, 600)$. Apart from

Table 6: $(\hat{\mathbf{R}}_q^\omega)$ and $(\hat{\mathbf{R}}_s^\omega)$ with $\omega = 2$ for large size problems.

		$(\hat{\mathbf{R}}_q^\omega)$			$(\hat{\mathbf{R}}_s^\omega)$		
p	q	$\epsilon_{cost}(\boldsymbol{z}_{lin}^\omega)$	ϵ_{sdp}	time	$\epsilon_{cost}(\boldsymbol{z}_{fea}^\omega)$	ϵ_{sdp}	time
5	200	2.73e–03	-1.98e–10	13m	1.72e–01	-4.33e–05	26m
5	400	9.85e–02	-4.55e–09	14m	1.88e–01	-6.93e–05	1h00m
5	600	2.59e–01	-5.34e–09	18m	1.90e–01	-6.05e–05	1h45m
10	100	5.54e–03	-7.15e–11	51m	2.83e–01	-1.77e–05	1h19m
10	150	1.38e–02	-3.18e–10	1h14m	3.00e–01	-5.02e–05	2h44m
10	200	2.86e–02	-5.18e–10	1h55m	3.00e–01	-9.00e–05	3h47m

these test cases, we can conclude that the approximate solutions $\boldsymbol{z}_{lin}^\omega$ are close to the global optimal solutions of $(\mathbf{R}_q)$. For the case of $(\hat{\mathbf{R}}_s^\omega)$, $\epsilon_{cost}(\boldsymbol{z}_{fea}^\omega)$ are around 1.0e-01, and thus, there is a distance between the approximate solutions $\boldsymbol{z}_{fea}^\omega$ and the global optimal ones of $(\mathbf{R}_s)$.

6 Concluding Remarks

There remain issues concerning practical implementation. In the experiments, we performed the relaxation methods, and checked the quality of the approximate solutions of the transformed CCTPs. We observed that the quality is sometimes low. One idea for improving quality is to employ local methods which have been developed to compute (local) solutions for nonlinear programming problems. Suppose that we have an approximate solution to the transformed CCTP as a result of performing the relaxation methods. Then, by regarding it as a starting point, we can refine the solution quality by applying local methods to the problem. This approach can be easily implemented by using the option of SparsePOP, and we tried it. In their trials, the active set method, provided by MATLAB optimization toolbox, was employed as the local method. The results made it clear to us that this approach works on problems of moderate size. For instance, the relative error of cost function value $\epsilon_{cost}(\boldsymbol{z}_{fea}^\omega)$ was reduced from 1.23e-01 to 4.09e-02 for the case in which the SDP relaxation $(\hat{\mathbf{R}}_s^\omega)$ with $\omega = 2$ is applied to $(\mathbf{R}_s)$ of $(p, q) = (5, 80)$. This is one of the 10 problems of the experiments reported in Subsection 5.2. On the other hand, we found that the active set method of MATLAB spends a long time and does not work well on larger problems. However, it should be possible to overcome these difficulties by trying different local methods and enhancing the implementation.

Finally, we mention that a similar variable transformation approach can be applied to a generalization of CCTPs. It contains the production-transportation problem [27, 15] and the multiple knapsack problem [24, 5]; the first one is a class of minimum concave cost network flow problems, and the second one is a class of 0/1 integer programming problems and a generalization of knapsack problems.

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Appendix: Proof of Lemma 1

We show 1-2 and 1-3 since 1-1 is trivial. Let a, a_1 and a_2 be nonnegative real numbers, and λ be a real number.

1-2. It follows from the identities in x,

$$\lambda^2 x^2 + \lambda^2 a^2 = \left(\left(\frac{\lambda}{\sqrt{a}} x \right)^2 + \left(\lambda \sqrt{a} \right)^2 \right) x + \left(\left(\frac{\lambda}{\sqrt{a}} x \right)^2 + \left(\lambda \sqrt{a} \right)^2 \right) (a - x),$$

and

$$-\lambda^2 x^2 + \lambda^2 a^2 = \left(\frac{\lambda}{\sqrt{a}} (a - x) \right)^2 x + \left(\left(\frac{\lambda}{\sqrt{a}} x \right)^2 + \left(\lambda \sqrt{a} \right)^2 \right) (a - x).$$

1-3. It follows from the identity in x_1, x_2,

$$\begin{aligned}
\pm\lambda^2 x_1 x_2 + \frac{1}{2}\lambda^2 (a_1^2 + a_2^2) &= \left(\frac{\lambda}{\sqrt{2a_1}} (x_1 \pm x_2) \right)^2 x_1 + \left(\frac{\lambda}{\sqrt{2a_1}} (x_1 \pm x_2) \right)^2 (a_1 - x_1) \\
&\quad - \frac{\lambda^2}{2} x_1^2 + \frac{\lambda^2}{2} a_1^2 - \frac{\lambda^2}{2} x_2^2 + \frac{\lambda^2}{2} a_2^2 \\
&= \left(\left(\frac{\lambda}{\sqrt{2a_1}} (x_1 \pm x_2) \right)^2 + \left(\frac{\lambda}{\sqrt{2a_1}} (a_1 - x_1) \right)^2 \right) x_1 \\
&\quad + \left(\left(\frac{\lambda}{\sqrt{2a_1}} (x_1 \pm x_2) \right)^2 + \left(\frac{\lambda}{\sqrt{2a_1}} x_1 \right)^2 + \left(\lambda \sqrt{\frac{a_1}{2}} \right)^2 \right) (a_1 - x_1) \\
&\quad + \left(\frac{\lambda}{\sqrt{2a_2}} (a_2 - x_2) \right)^2 x_2 \\
&\quad + \left(\left(\frac{\lambda}{\sqrt{2a_2}} x_2 \right)^2 + \left(\lambda \sqrt{\frac{a_2}{2}} \right)^2 \right) (a_2 - x_2).
\end{aligned}$$