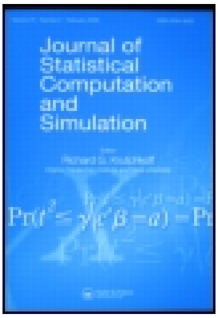

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A convex quadratic semi-definite programming approach to the partial additive constant problem in multidimensional scaling

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Bénasséni [*Partial additive constant*, J. Statist. Comput. Simul. 49 (1994), pp. 179–193] studied the partial additive constant problem in multidimensional scaling. This problem is quite challenging to solve, and Bénasséni proposed a numerical procedure for two special cases: the cross-set partial perturbation and the within-set partial perturbation. This paper casts the problem as a modern quadratic semi-definite programming (QSDP) problem, which is not only capable of dealing with general cases, but also enjoys a number of good properties. One of the good properties is that the proposed approach can find the minimal constant under very weak conditions. Another is that there exists a ready-to-use numerical package such as the QSDP solver in Toh [*An inexact path-following algorithm for convex quadratic SDP*, Math. Program. 112 (2008), pp. 221–254], allowing a great deal of flexibility in choosing the index set to which the partial constant should be added. Our numerical results show a significant improvement over that reported in Bénasséni (1994).

Keywords: partial additive constant; multidimensional scaling; positive semi-definite programming; Farkas' lemma; Lagrange multiplier

AMS Subject Classification: 90C22; 90C25; 90C90

1. Introduction

Suppose we have n objects with pairwise dissimilarities d_{ij} between objects i and j (often representing the psychological distance between i and j). The main purpose (in the narrow sense) of multidimensional scaling [1, Section 1] is to map these objects into n points $\{x_1, \dots, x_n\}$ in a low-dimensional metric space such that the metric distance between x_i and x_j matches the dissimilarity d_{ij} as closely as possible. There are a large number of ways to achieve this purpose. For a complete review on this topic, see Cox and Cox [2] and Borg and Groenen [3].

If the metric space is Euclidean (as assumed in this paper) and the match is exact (i.e. $\|x_i - x_j\| = d_{ij}$ for all $i \neq j$), then the dissimilarity matrix $D := (d_{ij})$ is said to have an exact Euclidean representation. A well-known result [4, pp. 254–259], which can be traced back to Schoenberg [5] and Young and Householder [6], is that D has an exact Euclidean representation

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if and only if the matrix

$$B := -\frac{1}{2}H(D \circ D)H \quad \text{with } H := I - \frac{1}{n}ee^{\mathrm{T}} \tag{1}$$

is positive semi-definite, where I is the identity matrix and e is the vector of all ones in $\Re^n$. ':=' means 'define' and $A \circ B$ is the Hadamard product between two matrices A and B of the same size (i.e. $(A \circ B)_{ij} = A_{ij}B_{ij}$). The exact match problem has its roots deep in the Euclidean distance geometry [7].

Due to various reasons such as non-metric measurement in d_{ij}, B is often not positive semi-definite. Fortunately, for this case, a simple adjustment can be made on D so that the resulting B matrix is positive semi-definite. The idea is to add a positive constant c to every d_{ij}^2 (i.e. added to the squared distance). To put it in detail, define the matrix $D(c)$ by

$$(D(c))_{ij} := \sqrt{d_{ij}^2 + c(1 - \delta^{ij})}, \quad \forall\, i,j,$$

where $c \geq 0$ and δ^{ij} is the Kronecker symbol. Let

$$B(c) := -\frac{1}{2}H(D(c) \circ D(c))H = B + \frac{c}{2}H. \tag{2}$$

Then, there exists a positive c such that $B(c)$ is positive semi-definite. The minimal value for such c is $(-2\lambda_n(B))$, where $\lambda_n(B)$ is the smallest eigenvalue of B. This is the famous additive constant problem first formulated by Guttman [8, p. 78]; [9, p. 477]. A constructive proof of this result can be found in [10].

Another type of additive constant problem results from the simple adjustment being made on d_{ij} (instead of on d_{ij}^2). Let

$$(D(\alpha))_{ij} := d_{ij} + \alpha(1 - \delta^{ij}), \quad \forall\, i,j$$

and define

$$B(\alpha) := -\frac{1}{2}H(D(\alpha) \circ D(\alpha))H. \tag{3}$$

The question as to what is the minimal value of α such that $B(\alpha)$ is positive semi-definite proved quite a challenging problem. Messick and Abelson [11] first formulated this adjustment and considered the effect of the values of α in Equation (3) on the resulting eigenvalues and eigenvectors of $B(\alpha)$. Cooper [12] suggested a 'solution' that allows for an additional 'discrepancy' term being added to d_{ij}. This question was finally settled by Cailliez [13]. In fact, the minimal value of α is the largest eigenvalue of a certain matrix. We will not go into any of these details, as we will only focus on the first adjustment scheme.

Both types of the additive constant problems have been reviewed in [1, Section 2.1.2]; [2, Section 2.2.8]; [14]. In both $B(c)$ of Equation (2) and $B(\alpha)$ of Equation (3), the constant is added to every element for (i,j) with $i \neq j$. Bénasséni [15], however, argued that there are cases where a constant should only be added to a group of pairs (i,j), whose dissimilarities d_{ij} are often over- or under-estimated. Let $\mathcal{B}$ denote the set of such indices and define the adjustment matrix

Δ by

$$\Delta_{ij} := \begin{cases} 1 & \text{if } (i,j) \in \mathcal{B}, \\ 0 & \text{otherwise,} \end{cases} \quad \text{and} \quad A := -\frac{1}{2} H \Delta H. \tag{4}$$

The resulting B matrix is given by

$$B(c) := -\frac{1}{2} H(D \circ D + c\Delta)H = B + cA. \tag{5}$$

The structure of Δ depends on the choice of $\mathcal{B}$. The constant c can be negative if d_{ij}^2 is over-estimated or positive if it is under-estimated for $(i,j) \in \mathcal{B}$. The purpose now is to seek the minimal absolute value of c such that $B(c)$ in Equation (5) is positive semi-definite. This is the partial additive constant problem studied in [15], and it can be formulated as a problem in the form of modern semi-definite programming (SDP):

$$\min |c| \quad \text{s.t. } B + cA \succeq 0, \tag{6}$$

where $X \succeq 0$ means X is symmetric and positive semi-definite.

Unlike the additive constant problem, the partial constant problem (6) is no longer analytically solvable. Bénasséni [15] proposed a numerical method, which, despite under rather restrictive assumptions (e.g. some are not easy to be verified), only applies to the cross-set and within-set examples described in Examples 2.2 and 2.3 (this has been pointed out in [2, p. 48]). This method is based on the belief that the eigenvectors of B are good approximations to that of $B(c)$. Given the upper semi-continuity of eigenvectors [16, Lemma 3], this belief might be true if $|c|$ is small and only if one can find a pair of such close eigenvectors, which is equivalent to solving a non-convex optimization problem. Bénasséni then used the eigenvectors of B to calculate n intervals, each containing at least one eigenvalue of $B(c)$. Under the assumptions that these intervals are separate from each other and B has just one negative eigenvalue, one can find conditions on c to make $B(c)$ positive semi-definite. If B has m negative eigenvalues, then $B(c)$ can be made positive semi-definite using m successive modifications with different choices of $\mathcal{B}$ and a new constant c at each modification.

The complication of Bénasséni's method prevents it from being widely used, as commented by Camiz [17] and Camiz and Le Calvé [18]. It was also noted by them that the partial additive may be an ideal way to handle problems where only some of the dissimilarity distances are biased. One of the major reasons for the complication, as already noticed in [15], is that problem (6) may not be feasible. For instance, if B has more than one negative eigenvalue, then Equation (6) is infeasible for the case where $\mathcal{B}$ is from the cross-set example 2.2 [15, p. 181]. Efficient methods to deal with the partial additive constant problem remain to be investigated, and this is not an easy task, because any formulation of the partial additive constant problem should by its own nature be in the form of SDP.

The main contribution of this paper is the proposed convex quadratic semi-definite programming (QSDP) model (see Equation (21)) in place of the SDP model (6). We think that our model is more appropriate than the SDP model (6) to deal with the partial additive constant problem, because the QSDP model is always feasible and the Slater condition is always satisfied. Moreover, under very weak conditions such as the existence of Lagrange multipliers for Equation (6), our QSDP model recovers the optimal solution of Equation (6) (Theorem 4.1(iii)). Moreover, feasibility of Equation (6) means the existence of Lagrange multipliers when the matrix A in Equation (6) is positive semi-definite (Corollary 3.5). We also characterize when problem (6) would be infeasible based on a couple of variants of Farkas' lemma in SDP (Section 3.1). When A is positive semi-definite, we are able to give a sufficient condition (easy to verify) for the feasibility (Proposition 3.2). When

A is indefinite, we give a full characterization of the feasibility (Proposition 3.3). Our numerical results obtained from the two examples studied in [15] show a significant improvement over that reported in [15].

Convex QSDP has attracted much attention recently and has proved to be a powerful modelling framework in many applications (see, e.g. [19]). In particular, QSDP has found an important application in modelling the nearest correlation matrix from finance, initiated by Higham [20] (see also [21]). Powerful methods have since been developed in [19,22–26], to just name a few. For a general theory on nonlinear SDPs, which include convex QSDP as a special case, see [27,28]. In our numerical experiment, we used Toh's QSDP solver [25].

This paper is organized as follows. In the next section, we collect some background material for future use. The following section is devoted to problem (6) in order to understand various issues about it. Specifically, Section 3.1 studies the feasibility of Equation (6), and Section 3.2 investigates when a Lagrange multiplier would exist for Equation (6). Our new QSDP model is described in Section 4, where its relationships with Equation (6) are studied. This study leads to an algorithm which enjoys some good properties. Numerical experiments of the new model are included in Section 5. We conclude the paper in Section 6.

2. Preliminaries

In this section, we study the partial additive constant problem from the viewpoint of QSDP under the feasibility assumption. We first note that problem (6) is equivalent to the following problem:

$$\begin{aligned} \min \quad & \frac{1}{2}c^2 \\ \text{s.t.} \quad & B + cA \succeq 0. \end{aligned} \tag{7}$$

The Lagrangian function of Equation (7) is

$$L(c; Z) := \frac{1}{2}c^2 - \langle Z, B + cA \rangle,$$

where $Z \in \mathcal{S}^n$ and $\mathcal{S}^n$ is the space of $n \times n$ symmetric matrices, equipped with the standard trace inner product. Therefore, the Lagrangian dual problem is

$$\max_{Z \succeq 0} \min_{c \in \Re} L(c; Z),$$

which is equivalent to

$$\begin{aligned} \max_{(c,Z)} \quad & -\langle Z, B \rangle - \frac{1}{2}c^2 \\ \text{s.t.} \quad & \langle Z, A \rangle = c, \quad Z \succeq 0. \end{aligned} \tag{8}$$

Equating the objective values in Equations (7) and (8), together with their respective constraints, yields the Karush–Kuhn–Tucker (KKT) condition for Equation (7):

$$\text{(KKT)} \quad \begin{cases} \langle Z, A \rangle = c \\ B + cA \succeq 0, \quad Z \succeq 0, \quad \langle Z, B + cA \rangle = 0. \end{cases} \tag{9}$$

We would like to study when the KKT condition would be satisfied. A pair (c_*, Z^*) satisfying the KKT condition (9) is often referred to as a KKT point of Equation (7) and Z^* is often called the Lagrange multiplier of Equation (7) at c_*. Because problem (7) is convex, the existence of the Lagrange multiplier Z^* at c_* is a sufficient (not a necessary) condition for c_* being the optimal solution of problem (7). The study on Lagrange multipliers will justify our approach proposed later on.

Next, we present three examples which give different structures of A in Equation (4).

Example 2.1 (Additive constant perturbation [8]) In this example,

$$\mathcal{B} = \{1, \ldots, n\} \times \{1, \ldots, n\} \setminus \{(i, i) : i = 1, \ldots, n\},$$

and hence, $\Delta \in \mathcal{S}^n$ is given by $\Delta = ee^{\mathrm{T}} - I$. Consequently,

$$A = -\frac{1}{2} H \Delta H = -\frac{1}{2} H(ee^{\mathrm{T}} - I)H = \frac{1}{2} H.$$

Example 2.2 (Cross-set perturbation [15]) Let $\mathcal{I}, \mathcal{J} \subset \{1, 2, \ldots, n\}$ be two disjoint sets of indices. The dissimilarities within $\mathcal{I}$ and $\mathcal{J}$ are accurately estimated. But the cross-set dissimilarities are uniformly over- or under-estimated. Hence, $\mathcal{B} = \mathcal{I} \times \mathcal{J}$. In this case, Δ is given by

$$\begin{aligned} \Delta_{ij} &= \begin{cases} 1 & \text{if } i \in \mathcal{I},\ j \in \mathcal{J}, \\ 0 & \text{otherwise}, \end{cases} \\ &= e_{\mathcal{I}} e_{\mathcal{J}}^{\mathrm{T}} + e_{\mathcal{J}} e_{\mathcal{I}}^{\mathrm{T}}, \end{aligned}$$

where $e_{\mathcal{I}} \in \Re^n$ is defined by

$$(e_{\mathcal{I}})_i = \begin{cases} 1 & \text{if } i \in \mathcal{I}, \\ 0 & \text{otherwise}, \end{cases}$$

and $e_{\mathcal{J}}$ is defined similarly. A is given by

$$A = -\frac{1}{2} H \Delta H = (|\mathcal{J}| e_{\mathcal{I}} - |\mathcal{I}| e_{\mathcal{J}})(|\mathcal{J}| e_{\mathcal{I}} - |\mathcal{I}| e_{\mathcal{J}})^{\mathrm{T}},$$

where $|\mathcal{I}|$ denotes the cardinality of the set $\mathcal{I}$ and A is a rank-1 matrix.

Example 2.3 (Within-set perturbation [15]) Let $\mathcal{I}$ be a subset of $\{1, \ldots, n\}$. The within-$\mathcal{I}$ squared dissimilarities have been under-valued or over-valued by some amount. In this case, Δ is defined by

$$\Delta = e_{\mathcal{I}} e_{\mathcal{I}}^{\mathrm{T}} - I_{|\mathcal{I}|},$$

where $\mathcal{I}_{|\mathcal{I}|}$ is the diagonal matrix whose diagonal element at (i, i) is 1 for $i \in \mathcal{I}$ and 0 otherwise. Hence,

$$A = -\frac{1}{2} H(e_{\mathcal{I}} e_{\mathcal{I}}^{\mathrm{T}} - I_{|\mathcal{I}|})H.$$

When $I = \{1, \ldots, n\}$, this example becomes Example 2.1.

We note that in both Examples 2.1 and 2.2, A is positive semi-definite. Before proceeding, we collect some known results (some have already been referred to in Section 1) for easy reference. The first result is on the *exact* Euclidean representation (see [1, Theorem 1; 5, 6] for more discussions on this result).

LEMMA 2.4 *For any given symmetric matrix, $D \in \mathcal{S}^n$ with*

$$D_{ii} = 0 \quad \text{and} \quad D_{ij} = D_{ji} > 0 \quad \forall\, i \neq j. \tag{10}$$

Then, there exist n points $x_1, x_2, \ldots, x_n$ in $\Re^p$ for some $p > 0$ such that

$$\|x_i - x_j\| = D_{ij} \quad \forall\, i \neq j,$$

if and only if

$$B := -\frac{1}{2}H(D \circ D)H \succeq 0 \quad \text{and} \quad \operatorname{rank}(B) = p.$$

The property defined in Equation (10) is known as the *semi-metric* property [1]. If B is not positive semi-definite in Lemma 2.4, then a constant α can be added to all the squared off-diagonal elements D_{ij}^2 so that the resulting B matrix is positive semi-definite. This is the famous additive constant problem first formulated by Guttman [8, p. 78; 9, p. 78]. We summarize this result as follows.

LEMMA 2.5 *Suppose D and B are given as in Lemma 2.4. We assume that B is not positive semi-definite and we let $\lambda_n(B)$ denote the smallest eigenvalue of B. Define the matrix $D(\alpha) \in \mathcal{S}^n$ by*

$$(D(\alpha))_{ij} := \sqrt{D_{ij}^2 + \alpha(1 - \delta^{ij})}, \quad \forall i, j,$$

where $\alpha \geq 0$ and δ^{ij} is the Kronecker symbol. Define

$$B(\alpha) := -\frac{1}{2}H(D(\alpha) \circ D(\alpha))H = B + \frac{c}{2}H.$$

Then,

$$B(-2\lambda_n(B)) \succeq 0 \quad \text{and} \quad \operatorname{rank}(B(-2\lambda_n(B))) \leq n - 2.$$

The implication of this results is that there exist n points $\{x_1, \ldots, x_n\}$ in $\Re^p$ ($p \leq n - 2$) such that

$$\|x_i - x_j\|^2 = D_{ij}^2 - 2\lambda_n(B) \quad \forall i \neq j.$$

We will also need the following perturbation result of Weyl for the eigenvalues of symmetric matrices (cf. [29, p. 63; 30, p. 367]).

LEMMA 2.6 *Let $\lambda_1 \geq \lambda_2 \geq \cdots \lambda_n$ be the eigenvalues of any $X \in \mathcal{S}^n$ and $\mu_1 \geq \mu_2 \cdots \geq \mu_n$ be the eigenvalues of any $Y \in \mathcal{S}^n$. Then,*

$$|\lambda_i - \mu_i| \leq \|X - Y\| \quad \forall i = 1, \ldots, n.$$

3. Partial additive constant problem

3.1. *Feasibility of problem (7)*

Due to a variety of choices of the index set $\mathcal{B}$, the feasibility of problem (7) becomes a real issue. Bénasséni [15] suggested a trial-and-error strategy to ensure that problem (7) is feasible, though with no guarantee. In this subsection, we would like to characterize when Equation (7) would be feasible.

First of all, we would like to note that when B and A are linearly dependent (unlikely in real applications), then Equation (7) is always feasible. Therefore, we assume that B and A are linearly independent throughout. Applying Farkas' lemma of Ramana [31, Theorem 19] to Equation (7), we immediately have the following.

PROPOSITION 3.1 *The set*

$$\Omega := \{c \in \Re | B + cA \succeq 0\}$$

is feasible if and only if the following semi-definite inequalities in $(U, U_1, W_1) \in \mathcal{S}^n \times \mathcal{S}^n \times \Re^{n\times n}$ *have no solution:*

$$\begin{aligned} \langle U + W_1, B\rangle &= -1 \\ \langle U + W_1, A\rangle &= 0, \\ \langle U_1, B\rangle &= 0, \\ \langle U_1, A\rangle &= 0, \\ U &\succeq 0, \\ \begin{bmatrix} I & W_1^{\mathrm{T}} \\ W_1 & U_1 \end{bmatrix} &\succeq 0. \end{aligned} \tag{11}$$

The above characterization does not rely on the linear independence between B and A. We now consider two cases: the positive semi-definite case (i.e. $A \succeq 0$) and the indefinite case (i.e. neither A nor $(-A)$ is positive semi-definite). For the former case, we can provide a sufficient condition, which is easy to check, for $\Omega \neq \emptyset$ and a simpler characterization of $\Omega \neq \emptyset$ for the latter.

Let $\mathcal{S}^n_+$ denote the cone of all positive semi-definite matrices in $\mathcal{S}^n$. We further let B_+ denote the orthogonal projection of B to $\mathcal{S}^n_+$ and $B_- := B - B_+$. $\mathrm{Null}(X)$ denotes the null space of matrix X.

PROPOSITION 3.2 *Suppose* $A \succeq 0$ *and*

$$\mathrm{Null}(A) \subseteq \mathrm{Null}(B_-). \tag{12}$$

Then, $\Omega \neq \emptyset$.

Proof We only need to prove that Equation (11) is infeasible. Assume, on the contrary, that there exists $(U, U_1, W)\mathcal{S}^n \times \mathcal{S}^n \times \Re^{n\times n}$ satisfying Equation (11). We will eventually prove that each column of U and that of W_1 belong to $\mathrm{Null}(B)$, implying $\langle U + W_1, B\rangle = 0$. This contradicts the first condition in Equation (11) and hence completes the proof.

We note that the last constraint in Equation (11) is equivalent to the Schur complement being positive semi-definite:

$$U_1 \succeq W_1 W_1^{\mathrm{T}}.$$

Because $A \succeq 0$, we have from the fourth condition in Equation (11) that

$$0 = \langle A, U_1\rangle \geq \langle A, W_1 W_1^{\mathrm{T}}\rangle = \|\sqrt{A} W_1\|^2 \geq 0,$$

which implies $\sqrt{A}W_1 = 0$, or equivalently, $AW_1 = 0$. Hence, each column of W_1 belongs to $\mathrm{Null}(A)$ and consequently belongs to $\mathrm{Null}(B_-)$. This yields

$$\langle W_1, B_-\rangle = \mathrm{trace}(B_- W_1) = 0. \tag{13}$$

We also note that

$$\langle A, U_1\rangle = 0, \quad U_1 \succeq 0, \quad \text{and} \quad A \succeq 0.$$

This is the complementarity condition in SDP. It means each column of U_1 belongs to $\mathrm{Null}(A)$ and hence to $\mathrm{Null}(B_-)$, implying $\langle U_1, B_-\rangle = 0$.

The third condition in Equation (11) implies

$$\begin{aligned}
0 = \langle U_1, B\rangle &= \langle U_1, B_+ + B_-\rangle \\
&= \langle U_1, B_+\rangle \\
&\geq \langle W_1 W_1^{\mathrm{T}}, B_+\rangle \\
&= \mathrm{trace}((\sqrt{B_+}W_1)^{\mathrm{T}}(\sqrt{B_+}W_1)) \geq 0,
\end{aligned}$$

yielding $\sqrt{B_+}W_1 = 0$ and hence $B_+W_1 = 0$. This leads to

$$\langle W_1, B_+\rangle = \mathrm{trace}(B_+W_1) = 0. \tag{14}$$

The combination of Equation (13) and Equation (14) gives us

$$\langle W_1, B\rangle = 0. \tag{15}$$

We already proved that $AW_1 = 0$. The second condition in Equation (11) becomes $\langle U, A\rangle = 0$. Note also that $U \succeq 0$ and $A \succeq 0$. By following a similar argument along the lines considered above, we can prove

$$\langle U, B\rangle = 0,$$

which together with Equation (15) implies $\langle U + W_1, B\rangle = 0$, contradicting the first condition in Equation (11). The proof is completed. ■

It is worth noting that for the additive constant Example 2.1, we always have

$$\mathrm{Null}(A) = \mathrm{Null}(H) = \mathrm{span}\{e\} \subset \mathrm{Null}(B) \subseteq \mathrm{Null}(B_-).$$

That is, the additive constant problem is always feasible. If A is indefinite, system (11) becomes much more simplified in the sense that we can choose $W_1 = U_1 = 0$, but U has to be positive definite (i.e. $U \succ 0$).

PROPOSITION 3.3 *Suppose that A is indefinite. Then, the set Ω is feasible if and only if the following system of semi-definite inequalities in $U \in \mathcal{S}^n$ is infeasible*:

$$\begin{aligned}
\langle U, B\rangle &= -1, \\
\langle U, A\rangle &= 0, \\
U &\succ 0.
\end{aligned} \tag{16}$$

Proof Consider the following system in $y = [y_0, y_1]^{\mathrm{T}} \in \Re^2$:

$$\begin{aligned}
y_0B + y_1A &\succeq 0, \\
y_0B + y_1A &\neq 0, \\
b^{\mathrm{T}}y &\geq 0,
\end{aligned} \tag{17}$$

where $b = [1, 0]^{\mathrm{T}} \in \Re^2$.

We claim that $\Omega \neq \emptyset$ if and only if system (17) is feasible. For the necessary part, suppose $c \in \Omega$. Then, $(y_0 = 1, y_1 = c)$ satisfies system (17) due to the linear independence of B and A. For the sufficiency part, let (y_0, y_1) be a feasible point of system (17). Then, we must have $y_0 > 0$. Otherwise, $y_0 = 0$ would imply $y_1A \succeq 0$. If $y_1 \neq 0$ and $y_1A \succeq 0$ contradicts the indefiniteness of A. If $y_1 = 0$, we would have $y_0B + y_1A = 0$, contradicting the second condition in system (17). It is easy to see that $y_1/y_0 \in \Omega$.

Now the result follows from Farkas' lemma [32, Theorem 8], which says that system (17) is feasible if and only if system (16) is infeasible. ■

3.2. *Existence of Lagrange multipliers for problem (7)*

The following result extends Lemma 2.5 from the additive constant problem to any partial additive constant problem. It also characterizes when there exists a Lagrange multiplier.

THEOREM 3.4 *We assume that problem (7) is feasible and B is not positive semi-definite. Let c_* be its optimal solution. Define*

$$\mathcal{N}_* := \{x \in \Re^n | c_* x^{\mathrm{T}} A x \le 0\} \quad \textit{and} \quad \mathcal{M}_* := \mathrm{Null}(B + c_* A).$$

Then, the following statements hold:

(i) $\mathrm{rank}(B + c_* A) \le n - 2$.
(ii) *There exists a Lagrange multiplier Z^* for problem (7) at c_* if and only if*

$$\mathcal{M}_* \setminus \mathcal{N}_* \ne \emptyset.$$

Proof We first note that $c_* \ne 0$ due to the assumption that B is not positive semi-definite. Let $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_n \ge 0$ be the eigenvalues of $(B + c_* A)$ in a non-increasing order, and let $\{v_1, \ldots, v_n\}$ be the corresponding orthonormal eigenvectors ($\|v_i\| = 1$ and $v_i^T v_j = 0$ for any $i \ne j$). We also note that 0 is an eigenvalue of $B + cA$ for any $c \in \Re^n$ and $e/\sqrt{n}$ is the associated normalized eigenvector. Without loss of generality, we assume

$$\lambda_r = \lambda_{r+1} = \cdots = \lambda_n = 0,$$

for some $1 \le r \le n$.

(i) It suffices to prove $p \le n - 1$ so that $(B + c_* A)$ has repeated zero eigenvalues. Assume, on the contrary, that $r = n$. Hence, $\lambda_n = 0$, $v_n = e/\sqrt{n}$ and $\lambda_{n-1} > 0$. Let $\lambda_1(c) \ge \lambda_2(c) \ge \cdots \ge \lambda_n(c)$ denote the eigenvalues of $B + cA$ for any $c \in \Re^n$. Then, it follows from Lemma 2.6 that

$$|\lambda_i(c) - \lambda_i| \le |c - c^*| \|A\| \quad \forall i = 1, \ldots, n.$$

Let

$$\delta_* := \frac{1}{2} \frac{\lambda_{n-1}}{\|A\|}.$$

It follows that $\delta_* > 0$, because $\lambda_{n-1} > 0$. Then, for any $c = c_* + \delta$ and $|\delta| < \delta_*$, we have

$$\lambda_i(c) \ge \lambda_i - |c - c_*| \|A\| \ge \lambda_i - \delta \|A\| > \lambda_i - \delta_* \|A\| = \lambda_i - \frac{1}{2}\lambda_{n-1} > 0, \\ i = 1, \ldots, n-1.$$

We also note that 0 is always an eigenvalue of $B + cA$. We must have $\lambda_n(c) = 0$. This means that the points of the type $c = c_* + \delta$ with $|\delta| \le \delta_*$ are all feasible to problem (7), contradicting the optimality of c_*. This contradiction implies $\mathrm{rank}(B + c_* A) \le n - 2$.

(ii) (Sufficiency) Since $(B + c_* A)$ is positive semi-definite, we must have that the null space of it is spanned by $\{v_r, v_{r+1}, \ldots, v_n\}$. That is

$$\mathcal{M}_* = \text{span}\{v_p, v_{p+1}, \ldots, v_n\}.$$

Because $\mathcal{M}_* \setminus \mathcal{N}_* \neq \emptyset$, there exists $y \in \Re^n$ such that

$$0 \neq y = \sum_{j=r}^{n} \beta_j v_j \notin \mathcal{N}_* \quad \beta_j \in \Re, \; i = r, \ldots, n.$$

The definition of $\mathcal{N}_*$ implies

$$c_* y^{\mathrm{T}} A y > 0. \tag{18}$$

Moreover, we have

$$0 = y^{\mathrm{T}}(B + c_* A)y = y^{\mathrm{T}} B y + c_* y^{\mathrm{T}} A y,$$

which, by Equation (18), implies

$$y^{\mathrm{T}} B y < 0.$$

Let

$$\beta := -\frac{c_*^2}{y^{\mathrm{T}} B y} > 0 \quad \text{and} \quad Z^* := \beta y y^{\mathrm{T}} \succeq 0.$$

We only need to verify that Z^* satisfies the KKT condition (9). First, it is obvious that

$$Z^* \succeq 0, \quad B + c_* A \succeq 0 \quad \text{and} \quad \langle B + c_* A, Z^* \rangle = \beta y^{\mathrm{T}}(B + c_* A) y = 0. \tag{19}$$

Secondly, it follows from Equation (19) that

$$\langle A, Z^* \rangle = -\langle B, Z^* \rangle / c_* = -\beta y^{\mathrm{T}} B y / c_* = c_*.$$

Therefore, Z^* is a Lagrange multiplier associated with c_*.

(ii) (Necessity) Suppose problem (7) has a Lagrange multiplier Z^*. We will prove $\mathcal{M}_* \setminus \mathcal{N}_* \neq \emptyset$. Assume, on the contrary, that the set is empty. We must have $\mathcal{M}_* \subseteq \mathcal{N}_*$. By the complementarity condition (the second condition in Equation (9)), Z^* and $(B + c_* A)$ share the same set of eigenvectors. Z^* must take the following form:

$$Z^* = \sum_{j=r}^{n} \beta_j v_j v_j^{\mathrm{T}}, \quad \beta_j \geq 0, \; j \geq r.$$

We also note that $v_i \in \text{Null}(B + c_* A) \subseteq \mathcal{N}_*$ for $i = r, \ldots, n$. Therefore,

$$\langle Z^*, c_* A \rangle = \sum_{j=r}^{n} c_* \beta_j v_j^{\mathrm{T}} A v_j \leq 0.$$

However, it is obvious from the first condition of Equation (9) that

$$c_* \langle A, Z^* \rangle = c_*^2 > 0.$$

This contradiction means that $\mathcal{M}_* \not\subseteq \mathcal{N}_*$ or equivalently $\mathcal{M}_* \setminus \mathcal{N}_* \neq \emptyset$.

∎

If A assumes a further property of positive semi-definiteness, as in the cases of the additive constant problem and the cross-set example 2.2, then it always holds $\mathcal{M}_* \setminus \mathcal{N}_* \neq \emptyset$.

COROLLARY 3.5 *In the case that $A \succeq 0$ in Theorem 3.4, we always have $\mathcal{M}_* \setminus \mathcal{N}_* \neq \emptyset$. That is, there always exists a Lagrange multiplier for problem (7).*

Proof Let us continue the use of notation in Theorem 3.4. Since $A \succeq 0$, the optimal solution $c_* > 0$ and $\mathcal{N}_* = \mathrm{Null}(A)$, the null space of A.

We assume that the claim $\mathcal{M}_* \setminus \mathcal{N}_* \neq \emptyset$ is not true. Then, $\mathcal{M}_* \subseteq \mathcal{N}_*$. One consequence of this assumption is $v_i \in \mathcal{N}_*$ for all $i = r, \ldots, n$. Hence,

$$0 = (B + c_* A)v_i = Bv_i \quad \forall i = r, \ldots, n.$$

Furthermore, for any $c \in \Re$, we have

$$(B + cA)v_i = Bv_i = 0 \quad \forall i = r, \ldots, n. \tag{20}$$

This is equivalent to say that $\{v_r, v_{r+1}, \ldots, v_n\}$ are also eigenvectors of $B + cA$ associated with the eigenvalue *zero*. Similar to the proof of (i) in Theorem 3.4, define

$$\delta_* := \frac{1}{2}\frac{\lambda_{r-1}}{\|A\|}.$$

Note that $\delta_* > 0$, as $\lambda_i > 0$ for $i = 1, \ldots, r-1$. Let $\lambda_1(c) \geq \lambda_2(c) \geq \cdots \geq \lambda_n(c)$ be the eigenvalues of $B + cA$. It follows from Lemma 2.6 that

$$|\lambda_i(c) - \lambda_i| \leq |c - c_*|\|A\| \quad \forall i = 1, \ldots, n.$$

Then, for any $c = c_* + \delta$ with $|\delta| < \delta_*$, we have

$$\lambda_i(c) \geq \lambda_i - |\delta|\|A\| > \lambda_i - \delta_*\|A\| = \lambda_i - \frac{1}{2}\lambda_{r-1} > 0 \quad \forall i = 1, \ldots, r-1.$$

The remaining $(n - r)$ eigenvalues are all zero according to Equation (20). This implies that $B + cA$ is positive semi-definite for all $c = c_* + \delta$ with $|\delta| \leq \delta_*$. For instance, $B + (c_* - \frac{1}{2}\min\{c_*, \delta_*\})A$ is positive semi-definite. This contradicts the optimality of c_* and hence establishes the fact $\mathcal{M}_* \setminus \mathcal{N}_* \neq \emptyset$. The existence of a Lagrange multiplier is the consequence of Theorem 3.4(ii). ■

4. QSDP formulation

The main purpose of this section is to propose a new mathematical optimization model that has the following ideal properties. First, it is always feasible and easy to solve. Secondly, it can reproduce the optimal solution if the original problem (7) is feasible. Lastly, when the original problem is not feasible, it allows easy computations on other choices of $\mathcal{B}$. These properties may sound too demanding. Interestingly, such a model takes the following form of QSDP, which has recently attracted interest from practitioners in both optimization and finance (see Section 1):

$$\begin{aligned} \min_{c \in \Re, W \in \mathcal{S}^n} \quad & f(c, W) := \frac{1}{2}c^2 + \frac{1}{2}\|W - (B + cA) + \rho ee^{\mathrm{T}}\|^2 \\ \text{s.t.} \quad & W \geq B + cA \\ & W \succeq 0, \end{aligned} \tag{21}$$

where $W \geq B + cA$ is in the sense of componentwise and $\rho > 0$ is a penalty parameter.

We have the following comments on the model:

(i) The model is based on the idea of least squares. In order to tackle the possible infeasibility of problem (7), we try to approximate $B + cA$ by a positive semi-definite matrix W in the hope that $B + cA$ will be close to W. We would like our W to approximate $B + cA$ from above (i.e. $W \geq B + cA$). We can view the constant matrix ρee^{T} as a penalty term, which penalizes any deviation of W from $(B + cA)$. ρ is supposed to be large enough.

(ii) The objective function is strongly quadratic in both variables. Let $\nabla^2_{c,W} f(c, W)$ denote the Hessian matrix of $f(c, W)$. Then, it is easy to calculate that

$$(\delta_c, \delta_W) \nabla^2_{c,W} f(c, W) \begin{pmatrix} \delta_c \\ \delta_W \end{pmatrix} = \|\delta_W - \delta_c A\|^2 + \|\delta_c\|^2 > 0, \quad \forall (\delta_c, \delta_W) \neq (0, 0),$$

where $(\delta_c, \delta_W) \in \Re \times \mathcal{S}^n$.

(iii) The model (21) is always feasible and the Slater condition holds (i.e. there exists a positive definite matrix W and $c \in \Re$ such that W is strictly bigger than $B + cA$.) Therefore, the fact in (ii) implies that Equation (21) has a unique optimal solution and that Lagrange multipliers exist [33, Theorem 5.83]. Moreover, the KKT condition holds at the optimal solution. Similar to the derivation of the KKT condition for Equation (7), we can write the KKT condition for Equation (21) as follows:

$$\text{(KKT)} \quad \begin{cases} c - \langle A, W - (B + cA) + \rho ee^{\mathrm{T}} \rangle + \langle A, U \rangle = 0, \\ W - (B + cA) + \rho ee^{\mathrm{T}} - U - Z = 0, \\ W \geq B + cA, \quad U \geq 0, \quad \langle W - (B + cA), U \rangle = 0, \\ W \succeq 0, \quad Z \succeq 0, \quad \langle W, Z \rangle = 0, \end{cases} \tag{22}$$

where $U \in \Re^{n \times n}$ and $Z \in \mathcal{S}^n$ are known as the Lagrange multipliers.

(iv) One may wonder whether the following simpler quadratic SDP is also a suitable formulation:

$$\begin{aligned} \min_{c,W} \quad & \frac{1}{2} c^2 + \frac{1}{2} \|W - (B + cA)\|^2 \\ \text{s.t.} \quad & W \succeq 0. \end{aligned} \tag{23}$$

We note that the objective is also strongly convex in both c and W. However, it is never going to yield the optimal solution on c_* of Equation (7), no matter what the conditions are. Assume that it yields c_*. The corresponding W solution for Equation (23) must be $W_* := B + c_* A$, because any other choice of W would yield a higher objective value for Equation (23). One of the KKT conditions for Equation (23) is

$$c_* - \langle A, W_* - (B + c_* A) \rangle = 0,$$

which leads to $c_* = 0$, contradicting $c_*^2 > 0$.

THEOREM 4.1 *The following statements about the relationship between* (7) *and* (21) *hold:*

(i) *Let* $(\bar{c}, \overline{W})$ *be the optimal solution of Equation* (21) *and* c_* *be the optimal solution of Equation* (7). *Then, we have*

$$\bar{c}^2 \leq c_*^2. \tag{24}$$

(ii) *Let* $(\bar{c}, \overline{W})$ *be the optimal solution of Equation* (21) *with the property* $B + \bar{c}A \succeq 0$. *Then,* $\bar{c}^2 = c_*^2$. *That is,* $\bar{c}$ *solves problem* (7).

(iii) *Suppose problem* (7) *is feasible and* c_* *is its optimal solution. If we further assume that there exists a Lagrange multiplier* Z^* *for Equation* (7) *at* c_*, *then* $(c_*, B + c_*A)$ *solves problem* (21) *for all* $\rho \geq \max_{1\leq i\leq j\leq n} |Z_{ij}^*|$.

Proof (i) Since $(c_*, W_* := B + c_*A)$ is a feasible point of Equation (21), we must have

$$f(\bar{c}, \overline{W}) \leq f(c_*, W_*).$$

Expansion of both sides leads to

$$\bar{c}^2 \leq c_*^2 + (\|\rho ee^{\mathrm{T}}\|^2 - \|\overline{W} - (B + \bar{c}A) + \rho ee^{\mathrm{T}}\|^2) \leq c_*^2,$$

because the term within the brackets is non-positive due to the constraint $\overline{W} \geq B + \bar{c}A$.

(ii) Since $B + \bar{c}A \succeq 0$, $\bar{c}$ is feasible to Equation (7). Therefore,

$$\bar{c}^2 \geq c_*^2.$$

By the result in (i), we have $\bar{c}^2 = c_*^2$.

(iii) We simply verify that

$$(c := c_*, W := B + c_*A, U := \rho ee^{\mathrm{T}} - Z^*, Z := Z^*)$$

satisfies the KKT condition (22). Note that the conditions in Equation (9) hold at (c_*, Z^*). The first condition in Equation (22) follows from $Ae = 0$ and

$$\langle A, U\rangle = -\langle A, Z^*\rangle = -c_*.$$

The second condition is obvious due to the definition of U. The third condition is also obvious as $W - (B + c_*A) = 0$ and $U_{ij} = \rho - Z_{ij}^* \geq 0$ by the condition on ρ. The last condition is simply the restatement of the third condition in Equation (9) with $W = B + c_*A$ and $c = c_*$. Because problem (21) is convex, the satisfaction of the KKT condition means that $(c_*, B + c_*A)$ solves Equation (21). ∎

The result in (i) states that the solution of problem (21) provides a lower bound for problem (7). The result in (ii) further states that if the solution is also feasible to Equation (7), then this lower bound becomes exact.The reverse relationship is studied by (iii). If problem (7) has a Lagrange multiplier, then problems (7) and (21) produce the same solution on c for reasonably large ρ. In fact, ρ can be made a bit smaller. Let $\mathcal{M}$ denote the set of all Lagrange multipliers of Equation (7) at c_*. Then, ρ can be chosen to satisfy

$$\rho \geq \min_{Z^*\in\mathcal{M}} \max_{1\leq i\leq j\leq n} |Z_{ij}^*|.$$

When A is positive semi-definite, problem (7) has Lagrange multipliers provided that it is feasible (see Corollary 3.5). We, therefore, have the following corollary from Theorem 4.1(iii).

COROLLARY 4.2 *If problem* (7) *is feasible and* $A \succeq 0$, *then both problems* (7) *and* (21) *yield the same optimal solution on* c.

Theorem 4.1 immediately suggests the following computational scheme.

ALGORITHM 4.3

Step 0. *Input: dissimilarity matrix D, perturbed index set $\mathcal{B}$ and penalty parameter $\rho > 0$. Output: $W_{\bar{c}}$ (a positive semi-definite matrix of rank no greater than $(n-2)$).*
Step 1. *Form matrix B by Equation (1) and A by Equation (4). Solve the quadratic SDP (21) for $(\bar{c}, \overline{W})$.*
Step 2. *Let $\mathtt{nrun} = 1$ and*

$$W_{\bar{c}} := B + \bar{c}A.$$

If $W_{\bar{c}} \succeq 0$, we are done. Otherwise, go to Step 3.
Step 3. *While $\lambda_n(W_{\bar{c}}) < 0$ do*
Let $B := W_{\bar{c}}$.
Choose a new $\mathcal{B}$ and form new matrix A by Equation (4)
Solve QSDP (21) for $(\bar{c}, \overline{W})$
Let $W_{\bar{c}} := B + \bar{c}A$
$\mathtt{nrun} := \mathtt{nrun} + 1$.

For a given perturbed index set $\mathcal{B}$, Algorithm 4.3 first solves problem (21). If the resulting matrix $W_{\bar{c}}$ is not positive semi-definite, we choose a new $\mathcal{B}$ and resolve problem (21) (i.e. do the while-loop). We continue this process until the resulting matrix $W_{\bar{c}}$ is positive semi-definite. We use $\mathtt{nrun}$ to denote the number of times that problem (21) has been solved in the process. We can always terminate the while-loop by choosing $\mathcal{B}$ to be the classical additive constant perturbation (in this case, $\bar{c} = -2\lambda_n(B)$). Furthermore, we have the following result for the matrix $W_{\bar{c}}$.

THEOREM 4.4 *Let $W_{\bar{c}}$ be the output matrix in Algorithm 4.3. Then, the following statements hold:*

(i) $\mathrm{rank}(W_{\bar{c}}) \leq n-2$.
(ii) *Suppose Algorithm 4.3 terminates with $\mathtt{nrun} = k (k \geq 1)$. Let the index sets used be $\{\mathcal{B}^1, \ldots, \mathcal{B}^k\}$. The corresponding Δ matrix and A matrix defined in Equation (4) are denoted by $\{\Delta^1, \ldots, \Delta^k\}$ and $(A_1, \ldots, A_k)$, respectively. The c part of the optimal solution of problem (21) at each run is denoted by $c_\ell, \ell = 1, \ldots, k$. Let*

$$W_{\bar{c}} = XX^{\mathrm{T}} = \begin{bmatrix} x_1^{\mathrm{T}} \\ \vdots \\ x_n^{\mathrm{T}} \end{bmatrix} \begin{bmatrix} x_1, \ldots, x_n \end{bmatrix}.$$

We must have

$$\|x_i - x_j\|^2 = d_{ij}^2 + \sum_{\ell=1}^{k} c_\ell \Delta_{ij}^\ell \quad i \neq j.$$

Proof We prove (i) and (ii) together. If Algorithm 4.3 stops at Step 2, then by Theorem 4.1(ii), $\bar{c}$ also solves problem (7). The result

$$\mathrm{rank}(W_{\bar{c}}) = \mathrm{rank}(B + \bar{c}A) \leq n-2$$

follows from Theorem 3.4(i). In this case, $\lambda_n = 0$ and

$$B + \bar{c}A = -\frac{1}{2}H(D \circ D + \bar{c}\Delta)H \succeq 0.$$

It follows from Lemma 2.4 that

$$\|x_i - x_j\|^2 = d_{ij}^2 + \bar{c}\Delta_{ij} \quad \forall i \neq j.$$

Now, we assume that Algorithm 4.3 stops at Step 3 (i.e. $\texttt{nrun} = k$, $k \geq 2$). We only consider the last run. The B matrix in the last run is given by

$$B = -\frac{1}{2}H(D \circ D + c_1\Delta^1 + \cdots + c_{k-1}\Delta^{k-1})H =: -\frac{1}{2}H\tilde{D}H.$$

The QSDP problem solved in the last run is given by Equation (21) with the above-defined B and A being replaced by A_k. Because Algorithm 4.3 terminates at `nrun=k`, c_k must solve problem (7) with the same B and A_k by Theorem 4.1(ii). The above-defined B does not lose any key properties used in Theorem 3.4. Therefore, the proof of Theorem 3.4 still goes through for our new B and A_k. Therefore, $\mathrm{rank}(W_{\bar{c}}) \leq (n-2)$. It also follows from Lemma 2.4 that

$$\begin{aligned} \|x_i - x_j\|^2 &= \tilde{D}_{ij} + c_k\Delta_{ij}^k \\ &= d_{ij}^2 + c_1\Delta_{ij}^1 + \cdots + c_{k-1}\Delta_{ij}^{k-1} + c_k\Delta_{ij}^k \quad \forall i \neq j. \end{aligned}$$

■

5. Numerical examples

In this section, we first report some numerical results on two small examples that have been investigated by Bénasséni [15] to demonstrate the advantage and the potential of our approach. We then apply our algorithm to the example of five socio-economic variables reported by Harman [34] to construct a true distance matrix when some of the raw data are missing.

5.1. *Comparison*

We now list the two examples reported in [15].

Example 5.1 The dissimilarity matrix D is given by

$$D = \begin{bmatrix} 0 & 10 & 14 & 10 & 12 & 9 \\ 10 & 0 & 12 & 13 & 6 & 13 \\ 14 & 12 & 0 & 12 & 7 & 14 \\ 10 & 13 & 12 & 0 & 11 & 9 \\ 12 & 6 & 7 & 11 & 0 & 14 \\ 9 & 13 & 14 & 9 & 14 & 0 \end{bmatrix}.$$

The initial B matrix, $B = -\frac{1}{2}H(D \circ D)H$, has one significant negative eigenvalue -2.031.

Example 5.2 The dissimilarity matrix D is given by

$$D = \begin{bmatrix} 0 & 30 & 35 & 40 & 40 & 30 & 30 & 60 \\ 30 & 0 & 10 & 30 & 40 & 30 & 20 & 50 \\ 35 & 10 & 0 & 40 & 40 & 40 & 30 & 50 \\ 40 & 30 & 40 & 0 & 50 & 35 & 10 & 50 \\ 40 & 40 & 40 & 50 & 0 & 40 & 50 & 60 \\ 30 & 30 & 40 & 35 & 40 & 0 & 10 & 50 \\ 30 & 20 & 30 & 10 & 50 & 10 & 0 & 50 \\ 60 & 50 & 50 & 50 & 60 & 60 & 50 & 0 \end{bmatrix}.$$

The initial B matrix, $B = -\frac{1}{2}H(D \circ D)H$, has two significant negative eigenvalues $(-4.290, -253.681)$.

We run Algorithm 4.3 against each problem for both the cross-set and within-set perturbations illustrated in Examples 2.2 and 2.3, respectively. In our implementation, we set $\rho = 1000$ and use all the default parameter settings for the QSDP solver of [25], except that the tolerance level is set at 10^{-7}.

We let the resulting dissimilarity matrix be $\tilde{D}$, whose B matrix is positive semi-definite. We measure the total distance, denoted by $V(c)$, which has been modified [15, Equation (14)]:

$$V(c) := \sum_{i=1}^{n} \sum_{j=i+1}^{n} |d_{ij}^2 - \tilde{d}_{ij}^2|.$$

In all the tables, we have listed the results obtained from [15] for comparison whenever they are available. If they are not available, we have indicated it by '–'. There are two cases to consider. One is the case when there exists a constant c such that $B + cA \succeq 0$ for the chosen index set $\mathcal{B}$. We call it the feasible case. The other is, of course, the infeasible case.

The Feasible Case. Since B in Example 5.1 has just one negative eigenvalue, it is possible that $B + cA \succeq 0$ is feasible when $\mathcal{B}$ is from the cross-set perturbation defined in Example 2.2. Table 1 reports various choices of $\mathcal{B}$. It can be seen that the solution of problem (21) yields the optimal c_*, which, of course, is in agreement with that reported in [15]. We also found two more feasible cases where $\mathcal{I} = \{3, 5, 6\}$ or $\{2, 5, 6\}$, which are given in the last two rows in Table 1. Similar observations can be made on the results given in Table 2, where the within-set perturbation was used for Example 5.1. Again, for the choices of $\mathcal{B}$, we can find the optimal c_*. The last two rows report the two choices of $\mathcal{B}$ that have negative c_*. Note that for $\mathcal{I} = \{2, 3, 4\}$, Bénasséni [15] only found a feasible value $c = -26.647$ with $V(c) = 79.941$. In contrast, we found $c_* = -5.9285$ with $V(c_*) = 17.9475$, which is much smaller than $V(c)$ and smaller than $V = 60.9386$ obtained by the usual additive constant perturbation.

The matrix B in Example 5.2 has two negative eigenvalues. Therefore, $B + cA \succeq 0$ is never going to be feasible for the cross-set perturbation. However, it is still possible for it to be feasible

Table 1. Results for Example 5.1 on cross-set perturbation with $\mathcal{J} = \{1, \ldots, n\} \setminus \mathcal{I}$.

$\mathcal{I}$	c [15]	$V(c)$	c_*	$V(c_*)$
$\{5\}$	13.647	68.235	3.7722	18.8611
$\{5, 6\}$	8.014	64.112	2.3794	19.0353
$\{1, 5, 6\}$	4.752	42.768	1.8760	16.8837
$\{3, 5, 6\}$	–	–	5.4161	48.7449
$\{2, 5, 6\}$	–	–	18.1093	162.9837

Table 2. Results for Example 5.1 on within-set perturbation with $\mathcal{J} = \{1, \ldots, n\} \setminus \mathcal{I}$.

$\mathcal{I}$	c [15]	$V(c)$	c_*	$V(c_*)$
$\{2, 5\}$	15.424	15.424	5.5120	5.5120
$\{1, 2, 3, 5\}$	6.908	41.448	4.5563	27.3380
$\{3, 4, 5, 6\}$	–	–	7.3514	44.1083
$\{2, 3, 4, 5, 6\}$	5.171	51.710	4.1645	41.6454
$\{1, 2, 3, 4, 5\}$	–	–	4.4515	44.5147
$\{1, 2, 3, 4, 5, 6\}$	4.063	60.939	4.0626	60.9386
$\{2, 3, 4\}$	−26.647	79.941	−5.9825	17.9475
$\{1, 2, 3, 4\}$	–	–	−12.4267	74.5602

Table 3. Results for Example 5.2 on within-set perturbation with $\mathcal{J} = \{1, \ldots, n\} \setminus \mathcal{I}$.

$\mathcal{I}$	c [15]	$V(c)$	c_*	$V(c_*)$
One run of Algorithm 4.3				
$\{2, 3, 4, 5, 6, 7, 8\}$	–	–	510.4736	10720
$\{1, 2, 3, 4, 5, 6, 7\}$	–	–	508.9157	10687
$\{2, 3, 4, 6, 7, 8\}$	–	–	596.3404	89451
$\{2, 3, 4, 5, 6, 7\}$	–	–	518.5548	7778.3
Two runs of Algorithm 4.3				
$\{4, 6, 7\}$	880.065		640.7971	
$\{2, 3\}$	251.187	2891.383	135.6957	2058.0868

for the within-set perturbation. We found such choices of $\mathcal{B}$ in Table 3 given under the column heading 'One run of Algorithm 4.3'. No such $\mathcal{B}$ was reported in [15]. We also note that all values of $V(c_*)$ for these choices are much less than $V = 14206$ obtained by the usual additive constant perturbation.

The infeasible case. Once $\mathcal{B}$ is chosen, it may happen that $B + cA$ is not feasible at all. A trial-and-error scheme, suggested in [15] to tackle this infeasibility, is to try a few different choices of $\mathcal{B}$. When applied to our approach, this scheme becomes the `while-loop` of Algorithm 4.3. It usually works with a careful choice of $\mathcal{B}$. For example, the bottom part of Table 3 reports on two choices of $\mathcal{I}$ for the within-set perturbation. It can be seen that after the first run of Algorithm 4.3 with $\mathcal{I} = \{4, 6, 7\}$, we got $c_* = 640.7971$, which is much less than the value $c = 880.065$ obtained in [15]. After the second run with $\mathcal{I} = \{2, 3\}$, we got $c_* = 135.6957$, which is again much less than the corresponding $c = 251.187$ obtained in [15]. Consequently, our total variation of the squared dissimilarities is equal to $V(c_*) = 2058.0868$, significantly less than $V = 2891.383$ [15], which is, in turn, much less than the value $V = 14206$ obtained by the usual additive constant perturbation. The matrix of the modified dissimilarities that we obtained is

$$\begin{bmatrix} 0 & 30 & 35 & 40 & 40 & 30 & 30 & 60 \\ 30 & 0 & 15.3524 & 30 & 40 & 30 & 20 & 50 \\ 35 & 15.3524 & 0 & 40 & 40 & 40 & 30 & 50 \\ 40 & 30 & 40 & 0 & 50 & 43.1949 & 27.2176 & 50 \\ 40 & 40 & 40 & 50 & 0 & 40 & 50 & 60 \\ 30 & 30 & 40 & 43.1949 & 40 & 0 & 27.2176 & 50 \\ 30 & 20 & 30 & 27.2176 & 50 & 27.2176 & 0 & 50 \\ 60 & 50 & 50 & 50 & 60 & 60 & 50 & 0 \end{bmatrix},$$

whose corresponding eigenvalues of the B matrix are as follows:

$$2406.1994,\ 1502.0622,\ 811.7504,\ 726.1760,\ 448.5209,\ 56.3023,\ 0,\ 0.$$

We note that there are two zero eigenvalues, and this is in agreement with Theorem 4.4(i). We also note that the modified dissimilarities in [15] have corresponding eigenvalues with only one zero eigenvalue.

Because of the ready-to-use optimization package for QSDP (21), our approach allows us to play as many times as we like with the arbitrary choice of $\mathcal{B}$ including the cross-set perturbation, within-set perturbation, combination of the two or any other type of perturbation. For example, it was easy to test the cross-set perturbation on Example 5.2, first with $\mathcal{I} = \{7\}$ and then with $\mathcal{I} = \{2\}$. The resulting total variation of the squared dissimilarities is 5322.2633, which is more than 50% smaller than $V = 11539$ obtained in [15] under the same perturbation scheme.

5.2. *Example of Harman's five socio-economic variables*

We use this example to demonstrate how to construct a distance matrix when the data set is not complete. We refer to [34, p. 14, Table 2.1] for the raw data on five fundamental socio-economic variables. The correlations among the five variables are as follows:

$$C = \begin{bmatrix} 1 & 0.00975 & 0.97245 & 0.43887 & 0.02241 \\ - & 1 & 0.15428 & 0.69141 & 0.86307 \\ - & - & 1 & 0.51472 & 0.12193 \\ - & - & - & 1 & 0.77765 \\ - & - & - & - & 1 \end{bmatrix}.$$

We note that $C \succeq 0$ and $C \geq 0$. It is because of these two properties that the distance matrix associated with C can be constructed by (see [2, Section 1.3.5])

$$D := \sqrt{1 - C}, \tag{25}$$

where the square root is taken componentwise. This distance matrix can be used to conduct multidimensional scaling analysis as described in the books of Cox and Cox [2] and Borg and Groenen [3].

Now, we assume that the last five observations of the first two variables (i.e. total population and median school years in Table 2.1 of [34]) were missing. We can calculate the pairwise correlations from the available data, and the new matrix of correlations is

$$C_{\text{new}} = \begin{bmatrix} 1 & -\mathbf{0.26422} & 0.97245 & 0.43887 & 0.02241 \\ - & 1 & 0.01466 & 0.40508 & 0.75796 \\ - & - & 1 & 0.51472 & 0.12193 \\ - & - & - & 1 & 0.77765 \\ - & - & - & - & 1 \end{bmatrix}.$$

We note that there is a negative correlation between the first two variables (i.e. $C_{\text{new}}(1,2) = -0.26422$) and that the corresponding matrix $D_{\text{new}} = \sqrt{1 - C_{\text{new}}}$ is not a true distance matrix anymore. We now apply our Algorithm 4.3 to D_{new} in order to make it a true distance matrix. Because the first two variables have missing data, we must have

$$C_{\text{new}}(i,j) = C(i,j) \quad \text{for } i,j = 3,4,5.$$

That is, what have been changed are correlations in $C(i,j)$, $i,j = 1,2$. We hence consider a two-step correction of the type of the cross-set perturbation: $\mathcal{I}_1 = \{1\}$ and $\mathcal{I}_2 = \{2\}$. The obtained distance matrix is

$$D_{\text{new}} = \begin{bmatrix} 0 & 1.12438 & 0.21026 & 0.76012 & 0.99712 \\ - & 0 & 0.99264 & 0.77131 & 0.49198 \\ - & - & 0 & 0.69662 & 0.93706 \\ - & - & - & 0 & 0.47154 \\ - & - & - & - & 0 \end{bmatrix}.$$

The total distance altered by D_{new} from D in Equation (25) is

$$V = \sum_{i,j} \frac{(D_{\text{new}}(i,j) - D(i,j))}{2} = 0.6037.$$

We note that this small amount of distance alternation is a price that one has to pay as we are dealing with missing data for some variables.

6. Conclusion

The classical additive constant problem has an analytical solution and remains one of the most often used multidimensional scaling methods in practice. Contrary to this, the partial additive constant problem initially studied by Bénasséni [15] is no longer analytically solvable and is indeed numerically challenging. The main difficulty is with the possible infeasibility issue of mathematical formulations of the problem.

In this paper, we cast the problem as a modern QSDP problem. We studied this new formulation from the viewpoint of optimization and reported some of its favourable properties. Our formulation is always feasible and can find the minimal additive constant provided that a Lagrange multiplier exists. The condition is automatically satisfied if the matrix A is positive semi-definite. Due to the recent advancement in optimization, our QSDP formulation can be easily solved, allowing a great deal of flexibilities while playing with various sets of indices to which a constant can be added. Consequently, one can choose one that has a small total variation of the squared dissimilarities. Numerical results show a significant improvement over that reported in [15].

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