
On Sparse Canonical Correlation Analysis

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Abstract

The classical Canonical Correlation Analysis (CCA) identifies the correlations between two sets of multivariate variables based on their covariance, which has been widely applied in diverse fields such as computer vision, natural language processing, and speech analysis. Despite its popularity, CCA can encounter challenges in explaining correlations between two variable sets within high-dimensional data contexts. Thus, this paper studies Sparse Canonical Correlation Analysis (SCCA) that enhances the interpretability of CCA. We first show that SCCA generalizes three well-known sparse optimization problems, sparse PCA, sparse SVD, and sparse regression, which are all classified as NP-hard problems. This result motivates us to develop strong formulations and efficient algorithms. Our main contributions include (i) the introduction of a combinatorial formulation that captures the essence of SCCA and allows the development of approximation algorithms; (ii) the establishment of the complexity results for two low-rank special cases of SCCA; and (iii) the derivation of an equivalent mixed-integer semidefinite programming model that facilitates a specialized branch-and-cut algorithm with analytical cuts. The effectiveness of our proposed formulations and algorithms is validated through numerical experiments.

1 Introduction

The Canonical Correlation Analysis (CCA), proposed by H. Hotelling [23], aims to identify the correlations between two sets of multivariate variables based on their covariance. Since then, CCA has become a powerful statistical technique used for multivariate data analysis, with its applications across diverse fields such as computer vision [24], natural language processing [38], and speech analysis [21]. Despite its popularity, CCA can encounter challenges in explaining correlations between two variable sets within high-dimensional data contexts, such as genomic datasets [36]. In contrast, Sparse Canonical Correlation Analysis (SCCA), which seeks sparse linear combinations of these variable sets, offers substantially enhanced interpretability [41, 42, 44].

Formally, this paper studies the SCCA problem:

$$v^* := \max_{\mathbf{x} \in \mathbb{R}^n, \mathbf{y} \in \mathbb{R}^m} \{ \mathbf{x}^\top \mathbf{A} \mathbf{y} : \mathbf{x}^\top \mathbf{B} \mathbf{x} \leq 1, \mathbf{y}^\top \mathbf{C} \mathbf{y} \leq 1, \|\mathbf{x}\|_0 \leq s_1, \|\mathbf{y}\|_0 \leq s_2 \}, \quad (\text{SCCA})$$

where $s_1 \leq n$, $s_2 \leq m$ are positive integers and $\begin{pmatrix} \mathbf{B} & \mathbf{A} \\ \mathbf{A}^\top & \mathbf{C} \end{pmatrix}$ denotes a covariance matrix of $(n+m)$ random variables. Specifically, \mathbf{B} and \mathbf{C} are the covariance matrices of the n and m random variables, respectively, and $\mathbf{A} \in \mathbb{R}^{n \times m}$ is the cross-covariance matrix between n and m random variables.

Hence, $\begin{pmatrix} \mathbf{B} & \mathbf{A} \\ \mathbf{A}^\top & \mathbf{C} \end{pmatrix}$, \mathbf{B} , \mathbf{C} are positive semidefinite matrices of size $(n+m)$, n , and m , respectively.

Here, matrices \mathbf{B} , \mathbf{C} can be singular, i.e., some random variables may be dependent on others. In fact, the covariance matrices \mathbf{B} , \mathbf{C} are often low-rank, especially within the high-dimension low-sample size data context (see, e.g., the gene expression data in [41]).

The **SCCA** problem generalizes three widely-studied sparsity-constrained optimization problems as special cases, which are sparse PCA [2, 13, 27], sparse SVD [28, 41], and sparse regression [22, 3]. To be specific, when $n = m$, $s_1 = s_2$, \mathbf{B}, \mathbf{C} are identity matrices, and \mathbf{A} is a positive semidefinite matrix, **SCCA** reduces to the classic sparse PCA problem; when \mathbf{B}, \mathbf{C} are identity matrices, **SCCA** becomes the sparse SVD problem; and when \mathbf{A} is rank-one, Section 3 shows that **SCCA** is equivalent to two sparse linear regression subproblems.

1.1 Main contributions

SCCA is generally NP-hard, given that its special cases, sparse PCA, sparse SVD, and sparse regression are all classified as NP-hard problems. We are motivated to develop efficient formulations and algorithms for **SCCA** through a mixed-integer optimization lens. The main contributions, along with the structure of the remainder of this paper, are the following:

- (i) In Section 2, we present an exact semidefinite programming (SDP) reformulation and derive a closed-form optimal value of classic CCA problem. We also develop an equivalent combinatorial formulation of **SCCA**, which allows the development of approximation algorithms;
- (ii) When the covariance matrix $\begin{pmatrix} \mathbf{B} & \mathbf{A} \\ \mathbf{A}^\top & \mathbf{C} \end{pmatrix}$ is low-rank, Section 3 studies the complexity of two special cases of **SCCA**. This motivates us to develop a polynomial-time exact algorithm of complexity $\mathcal{O}(n^3 + m^3)$ for solving **SCCA** to global optimality when the sparsity levels (i.e., s_1 and s_2) meet or exceed the ranks of \mathbf{B} and \mathbf{C} ;
- (iii) Section 4 derives an equivalent mixed-integer SDP (MISDP) reformulation for **SCCA**. When applying the Benders decomposition approach, instead of solving the large-scale SDPs, we design a customized branch-and-cut algorithm with closed-form cuts, which can successfully solve **SCCA** to optimality; and
- (iv) Section 5 numerically test the proposed formulations and algorithms. It is noted that our polynomial-time exact algorithm can solve real-world instances with $n = 19,672$ and $m = 2,149$ variables in seconds, provided that both s_1 and s_2 are at least the ranks of \mathbf{B} and \mathbf{C} .

Our analyses and results can be extended to **SCCA** with multiple pairs of basis vectors (\mathbf{x}, \mathbf{y}) , allowing for a more flexible and comprehensive exploration of correlations among data sets. The detailed formulations of multiple **SCCA**, along with the computational results, are provided in Appendix F.

1.2 Relevant literature

SCCA. To the best of our knowledge, the work [36] was the first paper that introduced the concept of **SCCA** to select only small subsets of variables to better explain the relationship between many genetic loci and gene expression phenotypes. A handful subset of features enhances interpretability, a desirable property, especially in complex data analysis, which has been successfully demonstrated in Sparse PCA [25]. To obtain sparse canonical loadings (\mathbf{x}, \mathbf{y}) , [39] first applied elastic net penalty to the classical CCA via an iterative regression procedure. In a seminal work on **SCCA** [41], the authors proposed a rigorous formulation by enforcing the ℓ_1 constraints on variables (\mathbf{x}, \mathbf{y}) and developed a penalized matrix decomposition method to solve the penalized CCA problem. Then, extensive research has focused on various penalty norm functions to obtain sparse canonical loadings (see, e.g., [20, 26, 39, 42, 10]). In particular, [10] penalized multiple canonical loadings by ℓ_1 norm and computed the sparse solution by the linearized Bregman method. It should be noted that under the assumption that the leading canonical loadings are sparse, [7, 17, 18] established theoretical guarantees of iterative approaches for estimating sparse solutions. Another research direction in **SCCA** introduced penalty functions based on group structural information of input data and developed group **SCCA** methods [29, 30]. For a comprehensive overview of CCA and **SCCA** methods, we refer readers to the survey by [44] and the references therein. These approaches, however, do not strictly enforce the exact sparsity requirement but only approximate the sparsity requirement (i.e., the ℓ_0 norm) by a convex function. Another relevant work [40] introduced binary variables to recast **SCCA** as a mixed-integer nonconvex program under the assumption of positive definite matrices \mathbf{B}, \mathbf{C} , based on which they designed a branch-and-bound algorithm. Different from the literature, our work does not require positive definiteness assumption of matrices \mathbf{B}, \mathbf{C} , and we are able to

obtain mixed-integer conic and semidefinite programming reformulations, allowing for better exact and approximation algorithms.

Connections to and differences with sparse PCA and sparse SVD. Analogous to **SCCA**, both sparse PCA [13, 25] and sparse SVD [28] select small subsets of variables to improve the interpretability of dimensionality reduction methods: PCA and SVD. Considerable investigation has been conducted on solving sparse PCA and sparse SVD from three angles: convex relaxations [12–14], approximation algorithms [6, 9, 28], and exact algorithms [2, 27, 28]. As mentioned before, in sparse PCA and sparse SVD, the covariance matrices \mathbf{B}, \mathbf{C} are identity. Such a setting dramatically simplifies the subset selection problems of sparse PCA and sparse SVD compared to that of **SCCA**, as in these problems, it suffices to focus on the selection of a submatrix of the matrix \mathbf{A} . Specifically, it is shown in [11, 27, 35] that sparse PCA reduces to selecting a principal submatrix of \mathbf{A} to maximize the largest eigenvalue(s) and sparse SVD reduces to selecting a possibly non-symmetric submatrix of \mathbf{A} to maximize the largest singular value(s) [28]. Quite differently, the combinatorial reformulation (1) of **SCCA** aims to simultaneously select a sized- $(s_1 \times s_1)$ principal submatrix of \mathbf{B} , a sized- $(s_2 \times s_2)$ principal submatrix of \mathbf{C} , and a sized- $(s_1 \times s_2)$ submatrix of \mathbf{A} . These fundamental differences in the underlying formulations of sparse PCA and sparse SVD preclude the direct application of their existing algorithms to the **SCCA**.

Notations: The following notation is used throughout the paper. We use bold lower-case letters (e.g., \mathbf{x}) and bold upper-case letters (e.g., \mathbf{X}) to denote vectors and matrices, respectively, and we use corresponding non-bold letters (e.g., x_i) to denote their components. We let $\mathcal{S}^n, \mathcal{S}_+^n, \mathcal{S}_{++}^n$ denote the set of all the $n \times n$ symmetric real matrices, the set of all the $n \times n$ symmetric positive semidefinite matrices, and the set of all the $n \times n$ symmetric positive definite matrices, respectively. We let \mathbf{I} denote the identity matrix and let $\mathbf{0}$ denote the vector or matrix with all-zero entries. We let \mathbb{R}_+^n denote the set of all n -dimensional nonnegative vectors. We let $[n] = \{1, 2, \dots, n\}$, $[s, n] = \{s, s+1, \dots, n\}$. Given a matrix $\mathbf{A} \in \mathbb{R}^{n \times m}$ and two subsets $S \subseteq [n], T \subseteq [m]$, we let \mathbf{A}^\dagger denote the pseudo inverse of matrix \mathbf{A} , let $\mathbf{A}_{S,T}$ denote a submatrix of \mathbf{A} with rows and columns indexed by sets S, T , respectively, and let $(\mathbf{A}_{S,T})^\dagger$ denote the pseudo inverse of submatrix $\mathbf{A}_{S,T}$. For a set S and an integer k , we define the set $S + k = \{i + k | i \in S\}$. Given a vector $\mathbf{a} \in \mathbb{R}^n$ and a subset $S \subseteq [n]$, we let \mathbf{a}_S denote a subvector of \mathbf{a} in the subset S . We define $[\lambda]_+ = \max\{\lambda, 0\}$. We let $\sigma_{\max}(\cdot)$ denote the largest singular value function and let $\lambda_{\max}(\cdot)$ denote the largest eigenvalue value function.

2 A combinatorial reformulation of **SCCA**

This section introduces an equivalent combinatorial optimization reformulation of **SCCA**. This reformulation serves as the foundation for developing two effective approximation algorithms.

2.1 An exact semidefinite programming representation of CCA

To begin with, let us focus on the classic CCA problem, which refers to **SCCA** without zero-norm constraints, as defined below:

$$\max_{\mathbf{x} \in \mathbb{R}^n, \mathbf{y} \in \mathbb{R}^m} \{ \mathbf{x}^\top \mathbf{A} \mathbf{y} : \mathbf{x}^\top \mathbf{B} \mathbf{x} \leq 1, \mathbf{y}^\top \mathbf{C} \mathbf{y} \leq 1 \}. \quad (\text{CCA})$$

This formulation of **CCA** can be regarded as a quadratically constrained quadratic program concerning the variables $\begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix} \in \mathbb{R}^{n+m}$. We next define three-block matrices of size $(n+m)$ below that aid in the presentation of our results.

$$\tilde{\mathbf{A}} = \begin{pmatrix} \mathbf{0} & \mathbf{A}/2 \\ \mathbf{A}^\top/2 & \mathbf{0} \end{pmatrix}, \quad \tilde{\mathbf{B}} = \begin{pmatrix} \mathbf{B} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}, \quad \tilde{\mathbf{C}} = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{C} \end{pmatrix}.$$

By introducing a size- $(n+m)$ matrix variable $\mathbf{X} = \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix} \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix}^\top$ and removing the rank-one constraint on \mathbf{X} , we can obtain an SDP relaxation of (CCA), as described below

$$\max_{\mathbf{X} \in \mathcal{S}_+^{m+n}} \{ \text{tr}(\tilde{\mathbf{A}} \mathbf{X}) : \text{tr}(\tilde{\mathbf{B}} \mathbf{X}) \leq 1, \text{tr}(\tilde{\mathbf{C}} \mathbf{X}) \leq 1 \}. \quad (\text{SDP Relaxation})$$

Next, let us present a key lemma regarding properties of block matrices being positive semidefinite, fundamental for reformulating the **SCCA**.

Lemma 1 ([16]) *For any symmetric matrix $\begin{pmatrix} \mathbf{B} & \mathbf{A} \\ \mathbf{A}^\top & \mathbf{C} \end{pmatrix} \in \mathcal{S}^{n+m}$, the followings are equivalent:*

- (i) *The block matrix is positive semidefinite;*
- (ii) *$\mathbf{B} \in \mathcal{S}_+^n$, $(\mathbf{I} - \mathbf{B}\mathbf{B}^\dagger)\mathbf{A} = \mathbf{0}$, $\mathbf{C} - \mathbf{A}^\top \mathbf{B}^\dagger \mathbf{A} \in \mathcal{S}_+^m$; and*
- (iii) *$\mathbf{C} \in \mathcal{S}_+^m$, $(\mathbf{I} - \mathbf{C}\mathbf{C}^\dagger)\mathbf{A}^\top = \mathbf{0}$, $\mathbf{B} - \mathbf{A}\mathbf{C}^\dagger \mathbf{A}^\top \in \mathcal{S}_+^n$.*

Inspired by **Lemma 1**, we hereby establish the equivalence between **CCA** and its **SDP Relaxation**. Remarkably, both of these problems achieve the same optimal value, namely $\sigma_{\max}(\sqrt{\mathbf{B}^\dagger \mathbf{A} \sqrt{\mathbf{C}^\dagger}})$.

Proposition 1 *For the **CCA** problem, we have the following results.*

- (i) *Both **CCA** and its **SDP Relaxation** have an optimal value $\sigma_{\max}(\sqrt{\mathbf{B}^\dagger \mathbf{A} \sqrt{\mathbf{C}^\dagger}})$;*
- (ii) *A pair of optimal solutions $(\mathbf{x}^*, \mathbf{y}^*)$ to **CCA** satisfies*

$$\mathbf{x}^* = \sqrt{\mathbf{B}^\dagger} \mathbf{q}, \quad \mathbf{y}^* = \sqrt{\mathbf{C}^\dagger} \mathbf{p},$$

where $\mathbf{q} \in \mathbb{R}^n$, $\mathbf{p} \in \mathbb{R}^m$ denote a pair of leading singular vectors of matrix $\sqrt{\mathbf{B}^\dagger \mathbf{A} \sqrt{\mathbf{C}^\dagger}}$; and

- (iii) *An optimal solution \mathbf{X}^* to the **SDP Relaxation** is*

$$\mathbf{X}^* = \begin{pmatrix} \mathbf{x}^* \\ \mathbf{y}^* \end{pmatrix} \begin{pmatrix} \mathbf{x}^* \\ \mathbf{y}^* \end{pmatrix}^\top.$$

Proof. See Appendix A.1. □

Proposition 1 motivates the following observation on the optimal values of **CCA** and **SCCA**.

Observation 1 *The optimal value of **CCA** is upper bounded by 1, so is the optimal value of **SCCA**.*

It is noteworthy that the results presented in **Proposition 1** are established through a distinct methodology. This methodology leverages the positive semidefinite condition of block matrices, as shown in **Lemma 1**, and incorporates duality theory. This approach differs from most prior research [31, 37, 44], which proved Part (i) of **Proposition 1** by relying on the singular value decomposition and assuming that matrices \mathbf{B} and \mathbf{C} are positive definite (i.e., full rank). To the best of our knowledge, [10] showed parts (i) and (ii) of **Proposition 1** for a special low-rank **CCA** problem, where the authors assumed that the covariance matrices are defined as $\mathbf{A} = \mathbf{U}\mathbf{V}^\top$, $\mathbf{B} = \mathbf{U}\mathbf{U}^\top$, and $\mathbf{C} = \mathbf{V}\mathbf{V}^\top$. Remarkably, **Proposition 1** extends this result to a more general scenario where \mathbf{B} and \mathbf{C} are not constrained to be strictly positive definite and \mathbf{A} is not constrained to directly depend on \mathbf{B} , \mathbf{C} , allowing for rank deficiencies and flexible data structure.

2.2 An equivalent formulation of **SCCA**

In this subsection, we transform **SCCA** into a combinatorial optimization problem, according to the insights provided by **Proposition 1**.

Theorem 1 ***SCCA** is equivalent to the following combinatorial optimization:*

$$v^* = \max_{S_1 \subseteq [m], |S_1| \leq s_1, S_2 \subseteq [n], |S_2| \leq s_2} \left\{ \sigma_{\max} \left(\sqrt{(\mathbf{B}_{S_1, S_1})^\dagger} \mathbf{A}_{S_1, S_2} \sqrt{(\mathbf{C}_{S_2, S_2})^\dagger} \right) \right\}. \quad (1)$$

Proof. See Appendix A.2. □

The combinatorial formulation (1) presents significant computational difficulties when attempting to solve **SCCA**. The primary obstacles are two-fold: first, simultaneously selecting submatrices from the matrices \mathbf{A} , \mathbf{B} , \mathbf{C} requires a sophisticated optimization across multiple dimensions. Second,

the selection criterion is particularly complex, as it involves optimizing the largest singular value of the product of the selected submatrix of \mathbf{A} and the square root of pseudo-inverse submatrices of \mathbf{B} and \mathbf{C} . These complexities necessitate effective optimization solution procedures to address the high-dimensional and non-convex nature of the problem.

Motivated by [Theorem 1](#), we customize the greedy and local search algorithms for [SCCA](#) (1) that has been widely used in the literature to solve special cases of [SCCA](#), such as sparse PCA and sparse SVD in literature (see, e.g., [27, 28]). The detailed implementations can be found in [Appendix B](#).

3 Low-rank [SCCA](#)

In practice, it is common that the sample covariance matrix $\begin{pmatrix} \mathbf{B} & \mathbf{A} \\ \mathbf{A}^\top & \mathbf{C} \end{pmatrix}$ exhibits low-rank characteristics. This phenomenon is especially prominent when dealing with high-dimensional, low-sample size data, e.g., the real gene expression data in [41]. In this section, we study two special cases of low-rank [SCCA](#) and their computational complexities. Specifically, we develop a polynomial-time exact algorithm of complexity $\mathcal{O}(n^3 + m^3)$ for solving [SCCA](#) to global optimality when sparsity levels (i.e., s_1 and s_2) exceed or equal the ranks of \mathbf{B} and \mathbf{C} . Besides, we recast [SCCA](#) into mixed-integer convex quadratic programming when matrix \mathbf{A} is rank-one.

3.1 Special Case I: [SCCA](#) with low-rank covariance matrices

In this section, we show that the computational complexity of [SCCA](#) is contingent upon the ranks of the covariance matrices \mathbf{B} and \mathbf{C} . To be more precise, when the sparsity level s_1 (or s_2) is equal to or greater than the rank r (or \hat{r}) of the covariance matrix \mathbf{B} (or \mathbf{C}), the imposition of a zero-norm constraint over \mathbf{x} (or \mathbf{y}) in [SCCA](#) becomes redundant. Consequently, lower ranks in the covariance matrices correspond to better computational complexity in solving [SCCA](#).

Theorem 2 Suppose $r = \text{rank}(\mathbf{B})$ and $\hat{r} = \text{rank}(\mathbf{C})$, then [SCCA](#) takes a complexity of $\mathcal{O}(n^{r-1}m^{\hat{r}-1} + n^{\hat{r}-1} + m^{r-1})$. The following results hold:

(i) When $s_1 \geq r$ and $s_2 \geq \hat{r}$, the [SCCA](#) problem is equivalent to [CCA](#), i.e.,

$$v^* = \max_{\mathbf{x} \in \mathbb{R}^n, \mathbf{y} \in \mathbb{R}^m} \{ \mathbf{x}^\top \mathbf{A} \mathbf{y} : \mathbf{x}^\top \mathbf{B} \mathbf{x} \leq 1, \mathbf{y}^\top \mathbf{C} \mathbf{y} \leq 1 \}; \quad (2)$$

(ii) When $s_1 \geq r$ and $s_2 < \hat{r}$, the [SCCA](#) problem can be reduced to

$$v^* = \max_{\mathbf{x} \in \mathbb{R}^n, \mathbf{y} \in \mathbb{R}^m} \{ \mathbf{x}^\top \mathbf{A} \mathbf{y} : \mathbf{x}^\top \mathbf{B} \mathbf{x} \leq 1, \mathbf{y}^\top \mathbf{C} \mathbf{y} \leq 1, \|\mathbf{y}\|_0 \leq s_2 \}; \quad (3)$$

(iii) When $s_1 < r$ and $s_2 \geq \hat{r}$, the [SCCA](#) problem can be reduced to

$$v^* = \max_{\mathbf{x} \in \mathbb{R}^n, \mathbf{y} \in \mathbb{R}^m} \{ \mathbf{x}^\top \mathbf{A} \mathbf{y} : \mathbf{x}^\top \mathbf{B} \mathbf{x} \leq 1, \mathbf{y}^\top \mathbf{C} \mathbf{y} \leq 1, \|\mathbf{x}\|_0 \leq s_1 \}. \quad (4)$$

Proof. See [Appendix A.3](#). □

The results in [Theorem 2](#) build on the covariance structure of the data matrix. Specifically, if \mathbf{B} and \mathbf{C} are of rank r and \hat{r} , respectively, there are only r and \hat{r} linearly independent vectors in the subspaces corresponding to \mathbf{B} and \mathbf{C} . Thus, the cosine of the principal angle can always be represented by these r and \hat{r} vectors. As a result, the canonical directions of CCA consist of only r and \hat{r} nonzero elements. We further make the following remarks about [Theorem 2](#):

- (i) [Theorem 2](#) implies the complexity of solving [SCCA](#), as summarized in the corollary below.
- (ii) Inspired by Part (i) of [Theorem 2](#), we also develop a polynomial-time exact algorithm yielding an optimal solution to [SCCA](#) (1) when $s_1 \geq r$ and $s_2 \geq \hat{r}$. The detailed implementation can be found in [Algorithm 1](#), which successfully solves some large instances with up to $n = 19,672$ and $m = 2,149$ variables in seconds in our numerical experiments; and
- (iii) The proof of [Theorem 2](#) implies that [CCA](#) always admits an optimal sparse solution $(\mathbf{x}^*, \mathbf{y}^*)$ satisfying $\|\mathbf{x}^*\|_0 \leq r$ and $\|\mathbf{y}^*\|_0 \leq \hat{r}$. We show in [Proposition 1](#) that the [SDP Relaxation](#) of [CCA](#) is exact. Therefore, as a side product, we provide the first-known sufficient condition about (i.e., $s_1 \geq r$ and $s_2 \geq \hat{r}$) when the convex [SDP Relaxation](#) matches [SCCA](#).

Corollary 1 Suppose $r = \text{rank}(\mathbf{B})$ and $\hat{r} = \text{rank}(\mathbf{C})$. There exists an algorithm that can find an optimal solution to **SCCA** in $\mathcal{O}(n^{r-1}m^{\hat{r}-1})$ time complexity.

Proposition 2 Suppose $r = \text{rank}(\mathbf{B})$ and $\hat{r} = \text{rank}(\mathbf{C})$. Then Algorithm 1 returns an optimal solution to **SCCA** (1) in $\mathcal{O}(n^3 + m^3)$ time complexity when $s_1 \geq r$ and $s_2 \geq \hat{r}$.

Proof. Following the proof of **Theorem 2**, we can show that the output solution of Algorithm 1 is optimal to **SCCA** (1). In addition, the Step 2 of Algorithm 1 needs computing the eigendecomposition of matrix $\mathbf{B} \in \mathcal{S}_+^n$, which takes a time of $\mathcal{O}(n^3)$. Given a matrix $\mathbf{Q} \in \mathbb{R}^{n \times (n-r)}$, it also takes a time of $\mathcal{O}(n^3)$ to find its $(n-r)$ linearly independent rows at Step 3 through the QR decomposition [19]. Hence, Algorithm 1 takes a complexity of $\mathcal{O}(n^3 + m^3)$. \square

Algorithm 1 An exact algorithm for **SCCA** (1) when $s_1 \geq r$ and $s_2 \geq \hat{r}$

- 1: **Input:** Matrices $\mathbf{A} \in \mathbb{R}^{m \times n}$, $\mathbf{B} \in \mathcal{S}_+^m$, $\mathbf{C} \in \mathcal{S}_+^m$ and integers $s_1 \in [r, n]$, $s_2 \in [\hat{r}, m]$
- 2: Compute the eigenvectors $\mathbf{Q} \in \mathbb{R}^{n \times (n-r)}$ of \mathbf{B} that correspond to its $(n-r)$ zero eigenvalues,
- 3: Find $(n-r)$ linearly independent rows in \mathbf{Q} , and collect their indices into a subset $T_1^* \subseteq [n]$
- 4: Perform the same procedure on matrix \mathbf{C} to obtain the subset $T_2^* \subseteq [m]$
- 5: Define the subsets $S_1^* = [n] \setminus T_1^*$ and $S_2^* = [m] \setminus T_2^*$, and compute

$$v^* = \sigma_{\max} \left(\sqrt{(\mathbf{B}_{S_1^*, S_1^*})^\dagger} \mathbf{A}_{S_1^*, S_2^*} \sqrt{(\mathbf{C}_{S_2^*, S_2^*})^\dagger} \right)$$

- 6: **Output:** An optimal solution (S_1^*, S_2^*) and optimal value v^*
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3.2 Special Case II: **SCCA** with a rank-one cross-covariance matrix

In this subsection, we study the other interesting low-rank special case of **SCCA** where the cross-covariance matrix \mathbf{A} is rank-one. For this special case, we prove its NP-hardness with reduction to the sparse regression problem. We further demonstrate that rank-one **SCCA** can be simplified to solving two Mixed-Integer Convex Quadratic Programs (MICQPs), which can be more scalable than directly solving **SCCA**. Our numerical findings confirm this improved scalability.

We observe that **SCCA** can be separable over variables \mathbf{x} and \mathbf{y} for the rank-one \mathbf{A} . In fact, suppose that $\mathbf{A} = \mathbf{a}\mathbf{b}^\top$, then **SCCA** is equivalent to

$$v^* = \max_{\mathbf{x} \in \mathbb{R}^n, \mathbf{y} \in \mathbb{R}^m} \{ \mathbf{x}^\top \mathbf{a} \mathbf{b}^\top \mathbf{y} : \mathbf{x}^\top \mathbf{B} \mathbf{x} \leq 1, \mathbf{y}^\top \mathbf{C} \mathbf{y} \leq 1, \|\mathbf{x}\|_0 \leq s_1, \|\mathbf{y}\|_0 \leq s_2 \} \quad (5)$$

which can be equivalently the product of the optimal values of the following two subproblems:

$$\begin{aligned} v_x &= \max_{\mathbf{x} \in \mathbb{R}^n} \{ \mathbf{a}^\top \mathbf{x} : \mathbf{x}^\top \mathbf{B} \mathbf{x} \leq 1, \|\mathbf{x}\|_0 \leq s_1 \}, \\ v_y &= \max_{\mathbf{y} \in \mathbb{R}^m} \{ \mathbf{b}^\top \mathbf{y} : \mathbf{y}^\top \mathbf{C} \mathbf{y} \leq 1, \|\mathbf{y}\|_0 \leq s_2 \}. \end{aligned} \quad (6)$$

That is, the identity $v^* = v_x v_y$ holds. Next, we show that each subproblem in (6) can be reduced to the classic sparse regression problem [1, 33] and is thus NP-hard as shown below.

Theorem 3 When matrix $\mathbf{A} = \mathbf{a}^\top \mathbf{b}$ is rank-one, each maximization problem in (6) is NP-hard.

Proof. See Appendix A.4. \square

Theorem 3 links the maximization problem (6) and the well-known sparse regression problem, implying that even solving the rank-one **SCCA** problem (5) is NP-hard. However, it also motivates us to adapt existing mixed-integer optimization techniques from sparse regression (see, e.g., [1, 4, 43]) to tackle each subproblem in (6). By introducing binary variables to model the zero-norm constraint, we derive equivalent MICQP formulations for subproblems (6) in Appendix C. There are two types of formulations depending on whether matrices \mathbf{B} and \mathbf{C} are positive definite, which build on the Big-M and perspective techniques, respectively.

4 Reformulating **SCCA** as a mixed-integer semidefinite program (MISDP)

While the combinatorial formulation (1) is elegant in its structure, it poses significant challenges when attempting to solve it to optimality using branch-and-bound based methods. To fill this gap, in this section, we derive an equivalent MISDP formulation for **SCCA**, amenable for developing exact methods.

First, it is noted that an optimal solution $(\mathbf{x}^*, \mathbf{y}^*)$ to **SCCA** is always bounded that satisfies $\|\mathbf{x}^*\|_2^2 \leq M_1$ and $\|\mathbf{y}^*\|_2^2 \leq M_2$, where we specify the construction of the coefficients M_1 and M_2 in Appendix C.1. Such bounds are essential to the derivation of the MISDP. It is convenient to introduce the following notation about $\{M_{ii}\}_{i \in [n+m]}$:

$$M_{ii} = M_1, \forall i \in [n], \quad M_{ii} = M_2, \forall i \in [n+1, n+m].$$

Theorem 4 *The **SCCA** is equivalent to the following MISDP:*

$$v^* = \max_{\mathbf{X} \in \mathcal{S}_+^{n+m}, \mathbf{z} \in \mathcal{Z}} \{ \text{tr}(\tilde{\mathbf{A}}\mathbf{X}) : \text{tr}(\tilde{\mathbf{B}}\mathbf{X}) \leq 1, \text{tr}(\tilde{\mathbf{C}}\mathbf{X}) \leq 1, X_{ii} \leq M_{ii}z_i, \forall i \in [n+m] \}. \quad (7)$$

where the feasible set is defined as $\mathcal{Z} = \{ \mathbf{z} \in \{0, 1\}^{n+m} : \sum_{i \in [n]} z_i \leq s_1, \sum_{i \in [n+1, n+m]} z_i \leq s_2 \}$.

Proof. See Appendix A.5. \square

Note that the proposed MISDP formulation (7) is of size $(n+m) \times (n+m)$ since our matrix variable \mathbf{X} replaces $\begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix} \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix}^\top$ in **SCCA**.

We have formulated **SCCA** as a mixed-integer convex optimization problem in Theorem 4. Unfortunately, no commercial solvers can efficiently solve MISDP problems. We derive an equivalent mixed-integer linear program of **SCCA** with exponentially many linear constraints and an efficient separation oracle based on the approach introduced by [15], which allows us to develop a tailored branch-and-cut algorithm. First, by separating the binary variables \mathbf{z} , we rewrite the MISDP (7) as

$$v^* = \max_{\mathbf{z} \in \mathcal{Z}, v} \{ v : v \leq f(\mathbf{z}) \}, \quad (8)$$

where the function $f(\mathbf{z})$ is defined as

$$f(\mathbf{z}) = \max_{\mathbf{X} \in \mathcal{S}_+^{n+m}} \left\{ \text{tr}(\tilde{\mathbf{A}}\mathbf{X}) : \text{tr}(\tilde{\mathbf{B}}\mathbf{X}) \leq 1, \text{tr}(\tilde{\mathbf{C}}\mathbf{X}) \leq 1, X_{ii} \leq M_{ii}z_i, \forall i \in [n+m] \right\}. \quad (9)$$

For any feasible solution $\hat{\mathbf{z}} \in \mathcal{Z}$ of the problem (8), by leveraging the concavity of function $f(\cdot)$, the linear inequality

$$v \leq f(\hat{\mathbf{z}}) + \partial f(\hat{\mathbf{z}})^\top (\mathbf{z} - \hat{\mathbf{z}})$$

cuts off the solution $\hat{\mathbf{z}}$ unless it happened to be optimal in (8), which paves the way for a delayed cut-generation procedure within a branch-and-bound framework. As the linear inequality of the above type needs to be added dynamically given different solutions $\hat{\mathbf{z}}$ at each iteration, it calls for an efficient evaluation of function $f(\hat{\mathbf{z}})$ and its subgradient. To speed up the computation, we derive the closed-form expression for both of them. The detailed derivations can be found in Appendix D.

Strategies to improve computational speed in practice: First, we provide a variable-fixing method that can identify some binary variables of the MISDP (7) being one at optimality. Removing these pre-selected variables from the feasible set reduces the problem size of **SCCA**. Second, we enhance the branch-and-cut algorithm with a high-quality warm start solution obtained from the local search algorithm. Third, by relaxing the binary variables in the MISDP (7) to be continuous or computing **CCA**, we can obtain an upper bound of **SCCA**, and the gap between this bound and the local search output gives an initial gap at the root node. Finally, at each iteration, the branching node is selected based on its potential to decrease the current upper bound instead of random branching.

5 Numerical results

This section tests the numerical performance of our formulations and algorithms on synthetic and real data. All the experiments are conducted in Python 3.6 with calls to Gurobi 9.5.2 and MOSEK 10.0.29 on a PC with 10-core CPU, 16-core GPU, and 16GB of memory. The codes and data used in our experiments are available at <https://github.com/yongchunli-13/SCCA.git>.

5.1 Experimental setup

Synthetic data generation: Before we present the empirical results, we first describe the properties of the synthetic data which shall be used throughout this section. By following [32], given parameters (n, m, s_1, s_2) , we first synthetically generate positive definite matrices $\mathbf{B}^* \in \mathcal{S}_{++}^n$ and $\mathbf{C}^* \in \mathcal{S}_{++}^m$ by $\mathbf{B}^* = \hat{\mathbf{B}}\hat{\mathbf{B}}^\top + \mathbf{I}$ and $\mathbf{C}^* = \hat{\mathbf{C}}\hat{\mathbf{C}}^\top + \mathbf{I}$, respectively, where $\hat{\mathbf{B}}$ and $\hat{\mathbf{C}}$ consist of elements generated from a normal distribution $\mathcal{N}(0, 1)$. Then, we let $\mathbf{A}^* \in \mathbb{R}^{n \times m} = \lambda \mathbf{B}^* \mathbf{u} \mathbf{v}^\top \mathbf{C}^*$, where we generate λ uniformly from $(0, 1)$, and vectors \mathbf{u}, \mathbf{v} are generated from a normal distribution $\mathcal{N}(0, 1)$ that satisfy $\|\mathbf{u}\|_0 = s_1$, $\|\mathbf{v}\|_0 = s_2$, $\mathbf{u}^\top \mathbf{B}^* \mathbf{u} = 1$ and $\mathbf{v}^\top \mathbf{C}^* \mathbf{v} = 1$. Next, we sample $N = 5,000$ data samples from a normal distribution $\mathcal{N}\left(\mathbf{0}, \begin{pmatrix} \mathbf{B}^* & \mathbf{A}^* \\ (\mathbf{A}^*)^\top & \mathbf{C}^* \end{pmatrix}\right)$ and compute their sample covariance matrix to obtain the testing data $\begin{pmatrix} \mathbf{B} & \mathbf{A} \\ \mathbf{A}^\top & \mathbf{C} \end{pmatrix}$.

Real data: To obtain a comprehensive understanding of the overall performance of our algorithms, we further conduct experiments on six UCI datasets [5] with sizes ranging from 34 to 385 variables. The dataset is split into the first n variables and the remaining m variables to construct the sample covariance matrices $\mathbf{A}, \mathbf{B}, \mathbf{C}$. Besides, we examine the performance of the proposed algorithms on the real breast cancer dataset [8] that contain $n = 19,672$ and $m = 2,149$ variables. The information on each dataset is summarized in Appendix E.

Throughout, the computational time is in seconds, the time limit is one hour, and the dashed line “-” denotes the unsolved case within the time limit. Note that we let **LB** denote the lower bound obtained from the approximation algorithm, and we let **UB** denote the upper bound obtained from convex relaxations of **SCCA**. Besides, we define **gap(%)** = $100 \times (\text{UB} - v^*)/v^*$ to be the optimality gap, and we replace v^* with the best lower bound when v^* is not available. We define **MIPGap(%)** to be the gap of exact algorithms at termination. Notably, the complexity analysis of the **SCCA** problems in Section 3 indicates that its solution process depends on the ranks of the data matrices. Therefore, we present the numerical results under both full-rank and low-rank cases for a comprehensive evaluation.

5.2 Illustration of the impact sparsity levels on SCCA

In this subsection, we apply the local search algorithm to evaluating the performance of **SCCA** against different sparsity levels s_1 and s_2 . Specifically, for a given dataset, we compute the ratio of correlations between **SCCA** and **CCA** for various s_1, s_2 parameters. We test the real UCI data and synthetic data, and the results are displayed in Figure 1 and Figure 2. This visualization provides insights for the maximum sparsity **SCCA** can achieve while maintaining the correlation of full data. For the real UCI data, **SCCA** almost recovers the correlation of **CCA** when $s_1 \approx n/2$ and $s_2 \approx m/2$.

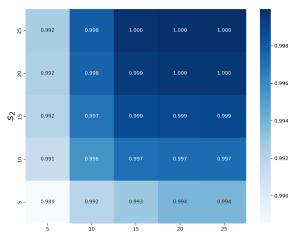


Figure 1: On UCI data with $n, m = 28, 29$

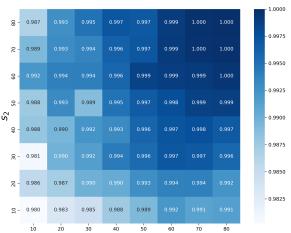


Figure 2: On synthetic data with $n, m = 80, 80$

5.3 Solving SCCA with full-rank matrices

The numerical results on synthetic and real data are presented in Table 1 and Table 2, respectively, which include multiple instances with various parameters (n, m, s_1, s_2) . First, we observe that the greedy and local search algorithms are scalable, and their outputs match the optimal values for most solved testing cases. That is, they achieve zero optimality gaps on these cases. In the “Convex relaxation” column, we compute an upper bound by solving either the continuous relaxation of MISDP (7) or **CCA**, and we use **CCA** for $n \geq 40$ and $m \geq 40$ cases for efficiency. It is seen that the upper bound maintains an optimality gap at most 2.78%. Then, we apply the branch-and-cut algorithm to solve **SCCA** to optimality, which can handle the case up to a size of $n = m = 120$ in

Table 1. The unsolved case in [Table 1](#) may be because the initial gap is weak at the root node, implying that the branch-and-cut algorithm explores a considerable amount of nodes before termination (see, e.g., $n = m = 80$ and $s_1 = s_2 = 10$). Hence, the branch-and-cut algorithm may struggle with large-scale instances with weak initial gaps.

Table 1: Evaluation of algorithms on synthetic data

n	m	s_1 s_2		Greedy		Local search		Convex relaxation			Branch-and-cut		
				LB	time	LB	time	UB	gap(%)	time	v^*	MIPGap(%)	time
20	20	5	5	0.244	0.01	0.244	0.02	0.256	1.23	1	0.244	0.00	9
20	20	10	10	0.275	0.02	0.275	0.04	0.278	1.23	1	0.275	0.00	4
40	40	5	5	0.695	0.03	0.695	0.05	0.701	0.83	1	0.695	0.00	1
40	40	10	10	0.705	0.06	0.705	0.12	0.708	0.45	1	0.705	0.00	7
60	60	5	5	0.885	0.04	0.885	0.09	0.887	0.28	1	0.885	0.00	1
60	60	10	10	0.884	0.09	0.884	0.19	0.887	0.28	1	0.884	0.00	8
80	80	5	5	0.633	0.06	0.633	0.12	0.650	2.78	1	0.633	0.00	1705
80	80	10	10	0.631	0.13	0.631	0.26	0.644	2.02	1	0.643	1.85	-
100	100	5	5	0.942	0.09	0.942	0.16	0.944	0.23	1	0.942	0.00	4
100	100	10	10	0.940	0.17	0.940	0.34	0.942	0.23	1	0.940	0.00	15
120	120	5	5	0.845	0.11	0.845	0.27	0.853	0.97	1	0.845	0.00	924
120	120	10	10	0.848	0.21	0.848	0.43	0.856	0.85	1	0.855	0.80	-

Table 2: Evaluation of algorithms on six UCI datasets

n	m	s_1 s_2		Greedy		Local search		Convex relaxation			Branch-and-cut		
				LB	time	LB	time	\hat{v}	gap(%)	time	v^*	MIPGap(%)	time
17	17	5	5	0.970	0.01	0.971	0.04	0.984	1.35	1	0.980	0.00	1
17	17	10	10	0.981	0.02	0.983	0.14	0.984	0.09	1	0.983	0.00	1
28	29	5	5	0.761	0.02	0.761	0.05	0.769	1.11	1	0.761	0.00	6
28	29	10	10	0.766	0.04	0.766	0.07	0.769	0.45	1	0.766	0.00	22
32	32	5	5	0.991	0.02	0.991	0.04	0.993	0.17	1	0.991	0.00	1
32	32	10	10	0.992	0.04	0.992	0.12	0.993	0.05	1	0.992	0.00	1
38	39	5	5	1	0.02	0.02	0.06	0.16	0.00	0.01	1	0.00	2
38	39	10	10	1	0.04	0.05	0.07	0.47	0.00	0.01	1	0.00	2
64	64	5	5	0.998	0.05	0.998	0.39	0.999	0.07	1	0.998	0.00	1
64	64	10	10	0.999	0.09	0.999	0.59	0.999	0.02	1	0.999	0.00	2
192	193	5	5	1	0.21	1	0.46	1	0.00	1	1	0.00	36
192	193	10	10	1	0.36	1	0.68	1	0.00	1	1	0.00	37

5.4 Solving SCCA with low-rank matrices

Despite the high dimensions of the breast cancer dataset [\[8\]](#), the resulting sample covariance matrices B and C have a rank of 89, i.e., $r = \hat{r} = 89$. When $s_1 \geq r$ and $s_2 \geq \hat{r}$, we apply Algorithm [1](#) to solving [SCCA](#) that returns optimal solutions and values in one second, as shown in [Table 3](#). If $s_1 < r$ and $s_2 < \hat{r}$, Algorithm [1](#) cannot be applied and the proposed branch-and-cut algorithm is hard to scale to this dataset. Hence, we only consider using approximation algorithms to solve [SCCA](#) for small s_1 and s_2 cases in [Table 4](#). To be specific, we randomly sample n and m variables from the breast cancer data to construct testing cases. As displayed in [Table 4](#), the greedy and local search algorithms run fast, and the local search algorithm slightly outperforms the greedy output.

Table 3: Solving SCCA by Algorithm [1](#) on breast cancer data when $s_1 \geq r$ and $s_2 \geq \hat{r}$

Table 4: Approximation algorithms on breast cancer data when $s_1 \leq r$ and $s_2 \leq \hat{r}$

n	m	s_1 s_2		Algorithm 1		
				v^*	MIPGap(%)	time
100	100	100	100	1	0.00	1
19,672	2,149	150	150	1	0.00	1
		200	200	1	0.00	1
		250	250	1	0.00	1

n	m	s_1 s_2		Greedy		Local search	
				LB	time	LB	time
100	100	10	10	0.983	0.17	0.985	0.63
500	500	10	10	0.991	1	0.993	6
800	800	10	10	0.993	5	0.993	37
1000	1000	20	20	1	12	1	146

The SCCA [\(5\)](#) problem with a rank-one matrix A can be more tractable, as we can equivalently decompose it into two MICQPs (see Appendix [C](#)). By approximating A with a rank-one matrix

including leading singular value and vectors, **Table 5** presents the numerical results for solving rank-one SCCA (5). The continuous relaxation of the MICQPs also provides an upper bound and is denoted by the **Perspective relaxation** in **Table 5**. We see that the perspective relaxation is computationally efficient and yields small optimality gaps. Besides, we can directly solve two MICQPs below via Gurobi to find the optimal value of rank-one SCCA (5), i.e., $v^* = v_x v_y$, where the performance can be found in the last column of **Table 5**. We can address the rank-one SCCA (5) problem up to size 200×200 within one hour, improving the problem-solving capacity compared to the size- 120×120 full-rank SCCA (5) in **Table 1**. However, it should be pointed out that the **SCCA** may not be mixed-integer convex quadratic representable in general.

Table 5: Solving SCCA on synthetic data with a rank-one matrix A

n	m	s_1	s_2	Greedy		Local Search		Perspective relaxation		SCCA (5)			
				LB	time	LB	time	UB	gap(%)	time	v^*	MIPGap(%)	time
50	50	5	5	0.753	0.04	0.753	0.07	0.757	0.57	1	0.753	0.00	1
50	50	10	10	0.753	0.07	0.753	0.15	0.757	0.46	1	0.753	0.00	9
100	100	5	5	0.975	0.09	0.975	0.16	0.977	0.21	1	0.975	0.00	2
100	100	10	10	0.966	0.17	0.966	0.33	0.969	0.35	1	0.966	0.00	25
150	150	5	5	0.850	0.15	0.850	0.26	0.859	1.08	1	0.850	0.00	9
150	150	10	10	0.857	0.27	0.857	0.53	0.867	1.13	1	0.857	0.00	167
200	200	5	5	0.810	0.23	0.810	0.37	0.828	2.19	2	0.810	0.00	55
200	200	10	10	0.816	0.39	0.816	0.74	0.833	2.11	2	0.816	0.00	1692

5.5 Experimental comparison of SCCA algorithms

This section compares the proposed local search algorithm with the SCCA methods of [10, 37, 41] in correlation (Corr) value, the zero norm of \mathbf{x} (denoted by $S.\mathbf{x}$), the zero norm of \mathbf{y} (denoted by $S.\mathbf{y}$), and running time. The computational results on synthetic, UCI, and breast cancer data are presented in **Table 6**, where we highlight the best correlation and sparsity results in bold. Unlike the local search algorithm, these existing methods do not strictly enforce the exact sparsity requirement, i.e., the zero-norm constraints on variables \mathbf{x}, \mathbf{y} . Consequently, the local search algorithm achieves the best sparsity for nearly all testing cases. More importantly, the local search algorithm yields a larger correlation value than these existing methods in 16 out of 22 testing cases. Finally, the running time of the local search algorithm dominates that of [10, 37].

Table 6: Comparison of **SCCA** algorithms in Correlation, sparsity, and time

n	m	s_1	s_2	Local search			[41]			[37]			[10]						
				Corr	$S.\mathbf{x}$	$S.\mathbf{y}$	time	Corr	$S.\mathbf{x}$	$S.\mathbf{y}$	time	Corr	$S.\mathbf{x}$	$S.\mathbf{y}$	time	Corr	$S.\mathbf{x}$	$S.\mathbf{y}$	time
20	20	5	5	0.244	5	5	0.04	0.200	9	11	0.01	0.239	13	14	2	0.256	18	16	15
20	20	10	10	0.275	10	10	0.06	0.212	7	8	0.01	0.259	19	14	2	0.278	18	18	12
40	40	5	5	0.695	5	5	0.08	0.594	23	30	0.03	0.659	26	19	2	0.696	17	18	13
40	40	10	10	0.705	10	10	0.17	0.597	17	15	0.01	0.660	19	22	2	0.704	16	20	15
60	60	5	5	0.885	5	5	0.13	0.794	37	45	0.01	0.865	27	25	3	0.880	10	8	23
60	60	10	10	0.884	10	10	0.27	0.777	33	36	0.01	0.847	31	31	3	0.879	12	15	23
80	80	5	5	0.633	5	5	0.17	0.534	55	43	0.03	0.606	36	32	3	0.634	33	23	34
80	80	10	10	0.631	10	10	0.37	0.528	53	38	0.02	0.603	29	41	3	0.632	36	41	32
100	100	5	5	0.942	5	5	0.22	0.813	58	63	0.02	0.902	46	33	4	0.941	5	5	38
100	100	10	10	0.940	10	10	0.49	0.768	54	55	0.02	0.884	47	37	4	0.938	10	10	37
120	120	5	5	0.845	5	5	0.42	0.681	83	74	0.02	0.804	37	43	4	0.833	10	8	47
120	120	10	10	0.848	10	10	0.59	0.720	71	76	0.02	0.821	39	36	4	0.840	13	12	47
17	17	5	5	0.971	5	5	0.04	0.794	6	9	0.01	0.742	10	8	2	0.970	14	16	15
28	29	5	5	0.761	5	5	0.05	0.704	23	29	0.01	0.667	3	7	2	0.744	24	19	15
32	32	5	5	0.991	5	5	0.04	0.730	31	23	0.01	0.904	15	10	2	0.906	18	15	43
38	39	5	5	1	5	5	0.15	0.994	8	9	0.43	0.997	38	23	3	1	24	32	29
64	64	5	5	0.998	5	5	0.38	0.897	64	64	0.01	0.990	7	6	2	0.997	33	31	19
192	193	5	5	1	5	5	0.45	0.103	82	50	0.21	0.856	13	12	10	1	11	6	45
100	100	10	10	0.985	10	10	0.63	0.936	18	41	0.01	0.686	42	43	4	0.952	75	76	36
500	500	10	10	0.993	10	10	6	0.977	78	200	0.78	0.871	173	371	31	0.935	74	44	50
800	800	10	10	0.993	10	10	37	0.974	133	316	1.94	0.879	280	526	50	0.990	84	63	57
1000	1000	10	10	0.995	10	10	11	0.980	166	401	7.30	0.848	401	558	58	0.985	80	59	60

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Appendices

A Proofs of technical results

A.1 Proof of Proposition 1

Proof. The proof includes three parts.

Part (i). To prove the equivalence between **CCA** and its **SDP Relaxation**, let us introduce the Lagrangian multipliers $\theta_1 \geq 0, \theta_2 \geq 0$ corresponding to two constraints in **SDP Relaxation**, which leads to the following Lagrangian dual problem

$$\min_{\theta_1 \geq 0, \theta_2 \geq 0} \left\{ \theta_1 + \theta_2 : \theta_1 \tilde{\mathbf{B}} + \theta_2 \tilde{\mathbf{C}} \succeq \tilde{\mathbf{A}} \right\} = \min_{\theta_1 \geq 0, \theta_2 \geq 0} \left\{ \theta_1 + \theta_2 : \begin{pmatrix} \theta_1 \mathbf{B} & \frac{\mathbf{A}}{-2} \\ \frac{\mathbf{A}^\top}{-2} & \theta_2 \mathbf{C} \end{pmatrix} \succeq 0 \right\} \quad (10)$$

where the equation results from the definition of block matrices $\tilde{\mathbf{A}}, \tilde{\mathbf{B}}$, and $\tilde{\mathbf{C}}$. Given the nonzero matrices $\mathbf{A} \neq \mathbf{0}, \mathbf{B} \neq \mathbf{0}, \mathbf{C} \neq \mathbf{0}$ and positive semidefinite matrices $\mathbf{B} \succeq 0, \mathbf{C} \succeq 0$, following **Lemma 1**, we must have $\theta_2 \mathbf{C} - \mathbf{A}^\top (\theta_1 \mathbf{B})^\dagger \mathbf{A} / 4 \succeq 0$ and $\theta_1 \mathbf{B} - \mathbf{A} (\theta_2 \mathbf{C})^\dagger \mathbf{A}^\top / 4 \succeq 0$, implying that either $\theta_1 = 0$ or $\theta_2 = 0$ is infeasible to the minimization problem above. That is, $\theta_1 > 0$ and $\theta_2 > 0$ must hold.

According to **Lemma 1**, the block matrix $\begin{pmatrix} \mathbf{B} & \mathbf{A} \\ \mathbf{A}^\top & \mathbf{C} \end{pmatrix}$ is positive semidefinite, implying that $(\mathbf{I} - \mathbf{C}\mathbf{C}^\dagger)\mathbf{A}^\top = \mathbf{0}, (\mathbf{I} - \mathbf{B}\mathbf{B}^\dagger)\mathbf{A} = \mathbf{0}$. Then, it is easy to show

$$(\mathbf{I} - \theta_2 \mathbf{C} (\theta_2 \mathbf{C})^\dagger) \frac{\mathbf{A}^\top}{2} = \mathbf{0}, \forall \theta_2 > 0.$$

Given $\theta_1, \theta_2 > 0$ and using **Lemma 1**, the result above allows us to further simplify the right-hand side minimization problem in (10) to

$$\begin{aligned} & \min_{\theta_1 \geq 0, \theta_2 \geq 0} \left\{ \theta_1 + \theta_2 : 4\theta_1 \theta_2 \mathbf{B} \succeq \mathbf{A} \mathbf{C}^\dagger \mathbf{A}^\top \right\} \\ &= \min_{\theta_1 \geq 0, \theta_2 \geq 0} \left\{ \theta_1 + \theta_2 : 4\theta_1 \theta_2 \geq \sigma_{\max}^2 \left(\sqrt{\mathbf{B}^\dagger} \mathbf{A} \sqrt{\mathbf{C}^\dagger} \right) \right\} = \sigma_{\max} \left(\sqrt{\mathbf{B}^\dagger} \mathbf{A} \sqrt{\mathbf{C}^\dagger} \right), \end{aligned}$$

where the first equation is because

$$\begin{aligned} 4\theta_1 \theta_2 \mathbf{B} \succeq \mathbf{A} \mathbf{C}^\dagger \mathbf{A}^\top &\iff 4\theta_1 \theta_2 \mathbf{I} \succeq \sqrt{\mathbf{\Lambda}^{-1}} \mathbf{Q}^\top \mathbf{A} \mathbf{C}^\dagger \mathbf{A}^\top \mathbf{Q} \sqrt{\mathbf{\Lambda}^{-1}} \\ &\iff 4\theta_1 \theta_2 \geq \lambda_{\max} \left(\sqrt{\mathbf{\Lambda}^{-1}} \mathbf{Q}^\top \mathbf{A} \mathbf{C}^\dagger \mathbf{A}^\top \mathbf{Q} \sqrt{\mathbf{\Lambda}^{-1}} \right) \\ &\iff 4\theta_1 \theta_2 \geq \lambda_{\max} \left(\sqrt{\mathbf{C}^\dagger} \mathbf{A}^\top \mathbf{B}^\dagger \mathbf{A} \sqrt{\mathbf{C}^\dagger} \right) \iff 4\theta_1 \theta_2 \geq \sigma_{\max}^2 \left(\sqrt{\mathbf{B}^\dagger} \mathbf{A} \sqrt{\mathbf{C}^\dagger} \right), \end{aligned}$$

where we let $\mathbf{B} = \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^\top$ denote the eigendecomposition of matrix \mathbf{B} with $\mathbf{\Lambda}$ containing all the positive eigenvalues.

As a result, the dual problem of **SDP Relaxation** admits an optimal value of $\sigma_{\max} \left(\sqrt{\mathbf{B}^\dagger} \mathbf{A} \sqrt{\mathbf{C}^\dagger} \right)$, which gives an upper bound of the **CCA** and its **SDP Relaxation**. Next, we construct their optimal solutions, which exactly attain this upper bound. Thus, this upper bound is achievable and equals their optimal values.

Part (ii). For the **CCA**, let us consider a part of optimal solutions $(\mathbf{x}^*, \mathbf{y}^*)$ below

$$\mathbf{x}^* = \sqrt{\mathbf{B}^\dagger} \mathbf{q}, \quad \mathbf{y}^* = \sqrt{\mathbf{C}^\dagger} \mathbf{p},$$

with $\mathbf{q} \in \mathbb{R}^n, \mathbf{p} \in \mathbb{R}^m$ denoting a pair of leading singular vectors of matrix $\sqrt{\mathbf{B}^\dagger} \mathbf{A} \sqrt{\mathbf{C}^\dagger}$.

First, $(\mathbf{x}^*, \mathbf{y}^*)$ is feasible to the **CCA** as

$$(\mathbf{x}^*)^\top \mathbf{B} \mathbf{x}^* = \mathbf{q}^\top \sqrt{\mathbf{B}^\dagger} \mathbf{B} \sqrt{\mathbf{B}^\dagger} \mathbf{q} \leq \mathbf{q}^\top \mathbf{q} = 1, \quad (\mathbf{y}^*)^\top \mathbf{C} \mathbf{y}^* = \mathbf{p}^\top \sqrt{\mathbf{C}^\dagger} \mathbf{C} \sqrt{\mathbf{C}^\dagger} \mathbf{p} \leq \mathbf{p}^\top \mathbf{p} = 1,$$

where the inequalities stem from the facts that $\mathbf{I} \succeq \sqrt{\mathbf{B}^\dagger} \mathbf{B} \sqrt{\mathbf{B}^\dagger}$ and $\mathbf{I} \succeq \sqrt{\mathbf{C}^\dagger} \mathbf{C} \sqrt{\mathbf{C}^\dagger}$.

On the other hand, according to the definitions of \mathbf{q}, \mathbf{p} , we can show that $(\mathbf{x}^*, \mathbf{y}^*)$ is optimal to the **CCA**, i.e.,

$$(\mathbf{x}^*)^\top \mathbf{A} \mathbf{y}^* = \mathbf{q}^\top \sqrt{\mathbf{B}^\dagger} \mathbf{A} \sqrt{\mathbf{C}^\dagger} \mathbf{p} = \sigma_{\max} \left(\sqrt{\mathbf{B}^\dagger} \mathbf{A} \sqrt{\mathbf{C}^\dagger} \right).$$

Part (iii). In a similar vein, we can show that $\mathbf{X}^* = \begin{pmatrix} \mathbf{x}^* \\ \mathbf{y}^* \end{pmatrix} \begin{pmatrix} \mathbf{x}^* \\ \mathbf{y}^* \end{pmatrix}^\top$ is optimal to **SDP Relaxation** with the optimal value $\sigma_{\max} \left(\sqrt{\mathbf{B}^\dagger} \mathbf{A} \sqrt{\mathbf{C}^\dagger} \right)$. \square

A.2 Proof of Theorem 1

Proof. By introducing the subsets (S_1, S_2) to denote the supports of variables (\mathbf{x}, \mathbf{y}) in **SCCA**, then we can remove the zero-norm constraints on (\mathbf{x}, \mathbf{y}) and reformulate **SCCA** as

$$v^* = \max_{\substack{S_1 \subseteq [m], |S_1| \leq s_1, \\ S_2 \subseteq [n], |S_2| \leq s_2}} \max_{\substack{\mathbf{x} \in \mathbb{R}^{|S_1|}, \\ \mathbf{y} \in \mathbb{R}^{|S_2|}}} \{ \mathbf{x}^\top \mathbf{A}_{S_1, S_2} \mathbf{y} : \mathbf{x}^\top \mathbf{B}_{S_1, S_1} \mathbf{x} \leq 1, \mathbf{y}^\top \mathbf{C}_{S_2, S_2} \mathbf{y} \leq 1 \}. \quad (11)$$

Following from the Part (i) in [Proposition 1](#), we can show that for any subsets $S_1 \subseteq [n], S_2 \subseteq [m]$, the following identity holds.

$$\begin{aligned} & \max_{\mathbf{x} \in \mathbb{R}^{|S_1|}, \mathbf{y} \in \mathbb{R}^{|S_2|}} \{ \mathbf{x}^\top \mathbf{A}_{S_1, S_2} \mathbf{y} : \mathbf{x}^\top \mathbf{B}_{S_1, S_1} \mathbf{x} \leq 1, \mathbf{y}^\top \mathbf{C}_{S_2, S_2} \mathbf{y} \leq 1 \} \\ &= \sigma_{\max} \left(\sqrt{(\mathbf{B}_{S_1, S_1})^\dagger} \mathbf{A}_{S_1, S_2} \sqrt{(\mathbf{C}_{S_2, S_2})^\dagger} \right). \end{aligned}$$

Plugging the result above into the inner maximization problem in (11), we complete the proof. \square

A.3 Proof of Theorem 2

Proof. The proof is split into three parts.

Part (i). It suffices to prove that **CCA** admits an optimal solution $(\mathbf{x}^*, \mathbf{y}^*)$ satisfying $\|\mathbf{x}^*\|_0 \leq r$ and $\|\mathbf{y}^*\|_0 \leq \hat{r}$. Then, $(\mathbf{x}^*, \mathbf{y}^*)$ is also feasible and optimal to **SCCA**, which implies the equivalence between **SCCA** and **CCA**.

First, according to Part (ii) in [Proposition 1](#), we can obtain a closed-form optimal solution $(\hat{\mathbf{x}}, \hat{\mathbf{y}})$ for the **CCA**. By adjusting $(\hat{\mathbf{x}}, \hat{\mathbf{y}})$, we will construct a new optimal sparse solution $(\mathbf{x}^*, \mathbf{y}^*)$ satisfying $\|\mathbf{x}^*\|_0 \leq r$ and $\|\mathbf{y}^*\|_0 \leq \hat{r}$.

For matrix $\mathbf{B} \in \mathcal{S}_+^n$, we let $\{\mathbf{q}_i\}_{i \in [n-r]} \in \mathbb{R}^n$ denote the eigenvectors corresponding to $(n-r)$ zero eigenvalues of \mathbf{B} . Thus, $\{\mathbf{q}_i\}_{i \in [n-r]}$ are orthonormal. There exists a size- $(n-r)$ subset $S \subseteq [n]$ such that the subvectors $\{(\mathbf{q}_i)_S\}_{i \in [n-r]}$ are linearly independent, where $(\mathbf{q}_i)_S$ denotes the subvector of \mathbf{q}_i indexed by S for each $i \in [n-r]$. As a result, there exist a vector $(\gamma_1, \dots, \gamma_{n-r})^\top$ such that

$$\hat{\mathbf{x}}_S = \sum_{i \in [n]} \gamma_i (\mathbf{q}_i)_S. \quad (12)$$

Let us now construct solution \mathbf{x}^*

$$\mathbf{x}^* = \hat{\mathbf{x}} - \sum_{i \in [n-r]} \gamma_i \mathbf{q}_i,$$

where $x_i^* = 0$ for all $i \in S$ based on the equation (12) and $|S| = n-r$, implying $\|\mathbf{x}^*\|_0 \leq r$. In addition, we show that the new solution \mathbf{x}^* is still optimal to **CCA**. First, \mathbf{x}^* is feasible since

$$(\mathbf{x}^*)^\top \mathbf{B} (\mathbf{x}^*) = \hat{\mathbf{x}}^\top \mathbf{B} \hat{\mathbf{x}} \leq 1,$$

where the equation is due to $\mathbf{B} \mathbf{q}_i = \mathbf{0}$ for all $i \in [n-r]$.

Given the positive semidefinite block matrix $\begin{pmatrix} \mathbf{B} & \mathbf{A} \\ \mathbf{A}^\top & \mathbf{C} \end{pmatrix}$, using Part (ii) of [Lemma 1](#), the identity $(\mathbf{I} - \mathbf{B} \mathbf{B}^\dagger) \mathbf{A} = \mathbf{0}$ is equivalent to $\sum_{i \in [n-r]} \mathbf{q}_i \mathbf{q}_i^\top \mathbf{A} = \mathbf{0}$. Then, for each $i \in [n-r]$, multiplying

\mathbf{q}_i^\top on both sides of this equation leads to

$$\mathbf{q}_i^\top \left(\sum_{j \in [n-r]} \mathbf{q}_j \mathbf{q}_j^\top \mathbf{A} \right) \mathbf{A} = \mathbf{q}_i^\top \mathbf{0} \implies \mathbf{q}_i^\top \mathbf{A} = \mathbf{0},$$

where the result follows from $\mathbf{q}_i^\top \mathbf{q}_j = 0$ for any $i \neq j$. Then, we can show the optimality of the new solution \mathbf{x}^* :

$$(\mathbf{x}^*)^\top \mathbf{A} \hat{\mathbf{y}} = \hat{\mathbf{x}}^\top \mathbf{A} \hat{\mathbf{y}} + \sum_{i \in [n-r]} \beta_i \mathbf{q}_i^\top \mathbf{A} \hat{\mathbf{y}} = \hat{\mathbf{x}}^\top \mathbf{A} \hat{\mathbf{y}}.$$

Similarly, we can also construct an optimal sparse solution \mathbf{y}^* by leveraging $\hat{\mathbf{y}}$ and eigenvectors of zero eigenvalues of \mathbf{C} such that $\|\mathbf{y}^*\|_0 \leq s_2$.

Therefore, there exists an optimal solution $(\mathbf{x}^*, \mathbf{y}^*)$ to the **CCA** whose zero norms are bounded from above by r, \hat{r} , respectively. Adding the constraints $\|\mathbf{x}\|_0 \leq r, \|\mathbf{y}\|_0 \leq \hat{r}$ to the **CCA** does not affect the optimality, which gives an equivalent formulation (2) of **CCA**.

Part (ii). Suppose that $(\tilde{\mathbf{x}}, \tilde{\mathbf{y}})$ denotes an optimal solution to problem (3). When $s_1 \geq r$, following the proof of Part (I), $\tilde{\mathbf{x}}$, we can construct another optimal solution \mathbf{x}^* whose zero norm is bounded by r and $(\mathbf{x}^*, \tilde{\mathbf{y}})$ is feasible and optimal to **SCCA**.

Part (iii). Similarly, we can reduce **SCCA** to problem (4). We thus complete the proof. \square

A.4 Proof of Theorem 3

Proof. Let us first consider the maximization problem over \mathbf{x} in (6), i.e.,

$$v_x = \max_{\mathbf{x} \in \mathbb{R}^n} \{ \mathbf{a}^\top \mathbf{x} : \mathbf{x}^\top \mathbf{B} \mathbf{x} \leq 1, \|\mathbf{x}\|_0 \leq s_1 \}. \quad (13)$$

Then, we derive a combinatorial optimization reformulation of problem (13) based on the result below.

Claim 1 For any subset $S \subseteq [n]$, $\max_{\mathbf{x} \in \mathbb{R}^{|S|}} \{ \mathbf{a}_S^\top \mathbf{x} : \mathbf{x}^\top \mathbf{B}_{S,S} \mathbf{x} \leq 1 \} = \sqrt{\mathbf{a}_S^\top (\mathbf{B}_{S,S})^\dagger \mathbf{a}_S}$.

Proof. Given $\mathbf{A} = \mathbf{ab}^\top$, since the matrix $\begin{pmatrix} \mathbf{B} & \mathbf{ab}^\top \\ \mathbf{b}^\top \mathbf{a} & \mathbf{C} \end{pmatrix}$ is positive semidefinite, using **Lemma 1**, the identity $(\mathbf{I} - \mathbf{B}_{S,S} \mathbf{B}_{S,S}^\dagger) \mathbf{a}_S \mathbf{b}^\top = \mathbf{0}$ must hold for any subset S . As a result, we have $\mathbf{a}_S - \mathbf{B}_{S,S} \mathbf{B}_{S,S}^\dagger \mathbf{a}_S = \mathbf{0}$ as vector \mathbf{b} is nonzero.

Next, the Lagrangian dual of the problem $\max_{\mathbf{x} \in \mathbb{R}^{|S|}} \{ \mathbf{a}_S^\top \mathbf{x} : \mathbf{x}^\top \mathbf{B}_{S,S} \mathbf{x} \leq 1 \}$ can be written as

$$\begin{aligned} \max_{\mathbf{x} \in \mathbb{R}^{|S|}} \{ \mathbf{a}_S^\top \mathbf{x} : \mathbf{x}^\top \mathbf{B}_{S,S} \mathbf{x} \leq 1 \} &= \min_{\mu \geq 0} \max_{\mathbf{x} \in \mathbb{R}^{|S|}} \mathbf{a}_S^\top \mathbf{x} + \mu - \mu \mathbf{x}^\top \mathbf{B}_{S,S} \mathbf{x} \\ &= \min_{\mu \geq 0} \mu + \frac{\mathbf{a}_S^\top \mathbf{B}_{S,S}^\dagger \mathbf{a}_S}{4\mu} = \sqrt{\mathbf{a}_S^\top (\mathbf{B}_{S,S})^\dagger \mathbf{a}_S}, \end{aligned}$$

where the second equation builds on the identity $\mathbf{a}_S - \mathbf{B}_{S,S} \mathbf{B}_{S,S}^\dagger \mathbf{a}_S = \mathbf{0}$ and optimal solution $\mathbf{x}^* = \frac{\mathbf{B}_{S,S}^\dagger \mathbf{a}_S}{\sqrt{\mathbf{a}_S^\top (\mathbf{B}_{S,S})^\dagger \mathbf{a}_S}}$. \diamond

Suppose that an optimal solution to problem (13) admits the support S^* . According to Claim 1, we have

$$v_x = \max_{S \subseteq [n], |S| \leq s} \sqrt{\mathbf{a}_S^\top (\mathbf{B}_{S,S})^\dagger \mathbf{a}_S} = \sqrt{\mathbf{a}_{S^*}^\top (\mathbf{B}_{S^*,S^*})^\dagger \mathbf{a}_{S^*}}.$$

On the other hand, the Lagrangian dual of problem (13) can be written as

$$\begin{aligned} v_x &\leq \min_{\lambda \in \mathbb{R}_+} \max_{\mathbf{x} \in \mathbb{R}^n} \{ \mathbf{a}^\top \mathbf{x} + \lambda - \lambda \mathbf{x}^\top \mathbf{B} \mathbf{x} : \|\mathbf{x}\|_0 \leq s_1 \} \\ &= \min_{\lambda \in \mathbb{R}_+} \max_{S \subseteq [n], |S| \leq s} \lambda + \frac{\mathbf{a}_S^\top (\mathbf{B}_{S,S})^\dagger \mathbf{a}_S}{4\lambda} \\ &\leq \max_{S \subseteq [n], |S| \leq s} \lambda^* + \frac{\mathbf{a}_{S^*}^\top (\mathbf{B}_{S^*,S^*})^\dagger \mathbf{a}_{S^*}}{4\lambda^*} = \sqrt{\mathbf{a}_{S^*}^\top (\mathbf{B}_{S^*,S^*})^\dagger \mathbf{a}_{S^*}} \leq v_x, \end{aligned}$$

where the first equation is due to [Claim 1](#), the second inequality is by plugging the feasible solution $\lambda^* = \frac{\sqrt{\mathbf{a}_{S^*}^\top (\mathbf{B}_{S^*, S^*})^\dagger \mathbf{a}_{S^*}}}{2}$ into minimization problem, and the last equation is from the optimality of subset S^* . Since both left-hand and right-hand sides above equal v_x , the strong duality of problem [\(13\)](#) holds, and all the inequalities above must attain the equalities. That is, problem [\(13\)](#) is equivalent to

$$v_x = \min_{\lambda \in \mathbb{R}_+} \max_{\mathbf{x} \in \mathbb{R}^n} \{ \mathbf{a}^\top \mathbf{x} + \lambda - \lambda \mathbf{x}^\top \mathbf{B} \mathbf{x} : \|\mathbf{x}\|_0 \leq s_1 \}.$$

Since the outer minimization is a one-dimensional convex program that can be solved efficiently, as a result, for any given $\lambda > 0$, the inner maximization is equivalent to solving

$$\max_{\mathbf{x} \in \mathbb{R}^n} \{ \mathbf{a}^\top \mathbf{x} - \lambda \mathbf{x}^\top \mathbf{B} \mathbf{x} : \|\mathbf{x}\|_0 \leq s_1 \}. \quad (14)$$

Next, let us consider the NP-hard sparse regression problem (see, e.g., [\[34\]](#)), which admits

$$\min_{\beta \in \mathbb{R}^n} \{ \|\mathbf{v} - \mathbf{U} \mathbf{x}\|_2^2 : \|\mathbf{x}\|_0 \leq s \} \iff \max_{\mathbf{x} \in \mathbb{R}^n} \{ 2\mathbf{v}^\top \mathbf{U} \mathbf{x} - \mathbf{x}^\top \mathbf{U}^\top \mathbf{U} \beta : \|\mathbf{x}\|_0 \leq s \}, \quad (15)$$

where data matrix \mathbf{U} consists of observations of n variables and vector \mathbf{v} denotes the corresponding response variables.

Suppose that in the problem [\(14\)](#), let us define $\lambda \mathbf{B} = \mathbf{U}^\top \mathbf{U}$ and $\mathbf{a} = 2\mathbf{U}^\top \mathbf{v}$. Then using the singular value decomposition of matrix \mathbf{U} , we see that the following equation still holds.

$$\mathbf{a}_S - \mathbf{B}_{S,S} \mathbf{B}_{S,S}^\dagger \mathbf{a}_S = \mathbf{0}, \forall S \subseteq [n].$$

Thus, for any given $\lambda > 0$, the maximization problem [\(14\)](#) is equivalent to the sparse regression problem [\(15\)](#). This shows that problem [\(13\)](#) is NP-hard.

Similarly, the maximization problem over \mathbf{y} in [\(6\)](#) can also be reduced to the sparse regression problem. \square

A.5 Proof of [Theorem 4](#)

Proof. For the SCCA [\(11\)](#), according to [Proposition 1](#), the inner maximization problem admits an exact semidefinite programming formulation. Using the variables $\mathbf{z} \in \mathcal{Z}$ to describe the set constraints in SCCA [\(11\)](#), we can reformulate it as

$$\begin{aligned} v^* = \max_{\mathbf{z} \in \mathcal{Z}} \max_{\mathbf{X} \in \mathcal{S}_+^{n+m}} & \{ \text{tr}(\tilde{\mathbf{A}} \mathbf{X}) : \text{tr}(\tilde{\mathbf{B}} \mathbf{X}) \leq 1, \text{tr}(\tilde{\mathbf{C}} \mathbf{X}) \leq 1, \\ & X_{ii}(1 - z_i) = 0, \forall i \in [m+n] \}. \end{aligned} \quad (16)$$

[Proposition 3](#) shows that there is an optimal solution $(\mathbf{x}^*, \mathbf{y}^*)$ to [SCCA](#) that satisfies $\|\mathbf{x}^*\|_2^2 \leq M_1$ and $\|\mathbf{y}^*\|_2^2 \leq M_2$. Based on this, we can construct an optimal solution $(\mathbf{z}^*, \mathbf{X}^*)$ for SCCA [\(16\)](#) by letting

$$\mathbf{X}^* = \begin{pmatrix} \mathbf{x}^* \\ \mathbf{y}^* \end{pmatrix} \begin{pmatrix} \mathbf{x}^* \\ \mathbf{y}^* \end{pmatrix}^\top, z_i = \begin{cases} 1 & \text{if } x_i^* \neq 0 \\ 0 & \text{if } x_i^* = 0 \end{cases}, \forall i \in [n], z_{i+n} = \begin{cases} 1 & \text{if } y_i^* \neq 0 \\ 0 & \text{if } y_i^* = 0 \end{cases}, \forall i \in [m],$$

where the optimal solution \mathbf{X}^* satisfies the following inequalities

$$X_{ii}^* = (x_i^*)^2 \leq M_1 z_i, \forall i \in [n], X_{(i+n)(i+n)}^* = (y_i^*)^2 \leq M_2 z_{i+n}, \forall i \in [m].$$

This allows us to recast the SCCA [\(16\)](#) into an MISDP formulation [\(7\)](#). \square

B Implementations of greedy and local search algorithms

This section presents the detailed implementations of greedy and local search algorithms based on the combinatorial formulation [\(1\)](#) of [SCCA](#).

C Mixed-integer convex quadratic programming reformulations

This section shows that each subproblem in [\(6\)](#) can be equivalently formulated by a MICQP. Therefore, SCCA [\(5\)](#) is mixed-integer convex quadratic representable when matrix \mathbf{A} is rank-one.

Algorithm 2 Greedy algorithm for SCCA (1)

- 1: **Input:** Matrices $\mathbf{A} \in \mathbb{R}^{m \times n}$, $\mathbf{B} \in \mathcal{S}_+^m$, $\mathbf{C} \in \mathcal{S}_+^m$ and integers $s_1 \in [n]$, $s_2 \in [m]$
- 2: Compute $(i^*, j^*) \in \operatorname{argmax}_{i \in [m], j \in [n]} \sqrt{(\mathbf{B}_{ii})^\dagger} \mathbf{A}_{ij} \sqrt{(\mathbf{C}_{jj})^\dagger}$
- 3: Define subsets $\hat{S}_1 = \{i^*\}$ and $\hat{S}_2 = \{j^*\}$
- 4: **for** $\ell = 2, \dots, \max\{s_1, s_2\}$ **do**
- 5: **if** $\ell \leq \min\{s_1, s_2\}$ **then**
- 6: $i^* \in \operatorname{argmax}_{i \in [n] \setminus \hat{S}_1} \sigma_{\max} \left(\sqrt{(\mathbf{B}_{\hat{S}_1 \cup \{i\}, \hat{S}_1 \cup \{i\}})^\dagger} \mathbf{A}_{\hat{S}_1 \cup \{i\}, \hat{S}_2} \sqrt{(\mathbf{C}_{\hat{S}_2, \hat{S}_2})^\dagger} \right)$
- 7: Update $\hat{S}_1 = \hat{S}_1 \cup \{i^*\}$
- 8: $j^* \in \operatorname{argmax}_{j \in [m] \setminus \hat{S}_2} \sigma_{\max} \left(\sqrt{(\mathbf{B}_{\hat{S}_1, \hat{S}_1})^\dagger} \mathbf{A}_{\hat{S}_1, \hat{S}_2 \cup \{j\}} \sqrt{(\mathbf{C}_{\hat{S}_2 \cup \{j\}, \hat{S}_2 \cup \{j\}})^\dagger} \right)$
- 9: **else if** $s_1 \leq s_2$ **then**
- 10: $j^* \in \operatorname{argmax}_{j \in [m] \setminus \hat{S}_2} \sigma_{\max} \left(\sqrt{(\mathbf{B}_{\hat{S}_1, \hat{S}_1})^\dagger} \mathbf{A}_{\hat{S}_1, \hat{S}_2 \cup \{j\}} \sqrt{(\mathbf{C}_{\hat{S}_2 \cup \{j\}, \hat{S}_2 \cup \{j\}})^\dagger} \right)$
- 11: Update $\hat{S}_2 = \hat{S}_2 \cup \{j^*\}$
- 12: **else**
- 13: $i^* \in \operatorname{argmax}_{i \in [n] \setminus \hat{S}_1} \sigma_{\max} \left(\sqrt{(\mathbf{B}_{\hat{S}_1 \cup \{i\}, \hat{S}_1 \cup \{i\}})^\dagger} \mathbf{A}_{\hat{S}_1 \cup \{i\}, \hat{S}_2} \sqrt{(\mathbf{C}_{\hat{S}_2, \hat{S}_2})^\dagger} \right)$
- 14: Update $\hat{S}_1 = \hat{S}_1 \cup \{i^*\}$
- 15: **end if**
- 16: **end for**
- 17: **Output:** \hat{S}_1, \hat{S}_2

Algorithm 3 Local search algorithm for SSVD (1)

- 1: **Input:** Matrices $\mathbf{A} \in \mathbb{R}^{m \times n}$, $\mathbf{B} \in \mathcal{S}_+^m$, $\mathbf{C} \in \mathcal{S}_+^m$ and integers $s_1 \in [n]$, $s_2 \in [m]$
- 2: Initialize (\hat{S}_1, \hat{S}_2) as the output of greedy Algorithm 2
- 3: **do**
- 4: **for** each pair $(i_1, j_1) \in \hat{S}_1 \times ([n] \setminus \hat{S}_1)$ **do**
- 5: **if** $\sigma_{\max} \left(\sqrt{(\mathbf{B}_{\hat{S}_1 \cup \{j_1\} \setminus \{i_1\}, \hat{S}_1 \cup \{j_1\} \setminus \{i_1\}})^\dagger} \mathbf{A}_{\hat{S}_1 \cup \{j_1\} \setminus \{i_1\}, \hat{S}_2} \sqrt{(\mathbf{C}_{\hat{S}_2, \hat{S}_2})^\dagger} \right) > \sigma_{\max} \left(\sqrt{(\mathbf{B}_{\hat{S}_1, \hat{S}_1})^\dagger} \mathbf{A}_{\hat{S}_1, \hat{S}_2} \sqrt{(\mathbf{C}_{\hat{S}_2, \hat{S}_2})^\dagger} \right)$ **then**
- 6: Update $\hat{S}_1 = \hat{S}_1 \cup \{j_1\} \setminus \{i_1\}$
- 7: **end if**
- 8: **end for**
- 9: **for** each pair $(i_2, j_2) \in \hat{S}_2 \times ([m] \setminus \hat{S}_2)$ **do**
- 10: **if** $\sigma_{\max} \left(\sqrt{(\mathbf{B}_{\hat{S}_1 \cup \{j_2\} \setminus \{i_2\}, \hat{S}_1 \cup \{j_2\} \setminus \{i_2\}})^\dagger} \mathbf{A}_{\hat{S}_1 \cup \{j_2\} \setminus \{i_2\}, \hat{S}_2} \sqrt{(\mathbf{C}_{\hat{S}_2, \hat{S}_2})^\dagger} \right) > \sigma_{\max} \left(\sqrt{(\mathbf{B}_{\hat{S}_1, \hat{S}_1})^\dagger} \mathbf{A}_{\hat{S}_1, \hat{S}_2} \sqrt{(\mathbf{C}_{\hat{S}_2, \hat{S}_2})^\dagger} \right)$ **then**
- 11: Update $\hat{S}_2 = \hat{S}_2 \cup \{j_2\} \setminus \{i_2\}$
- 12: **end if**
- 13: **end for**
- 14: **while** there is still an improvement **do**
- 15: **Output:** \hat{S}_1, \hat{S}_2

C.1 Valid inequalities for SCCA

Before deriving the formulations, we first prove that there exists a bounded optimal solution $(\mathbf{x}^*, \mathbf{y}^*)$ of the **SCCA**. To be specific, we show that there exists an optimal solution $(\mathbf{x}^*, \mathbf{y}^*)$ of the **SCCA** satisfying the constraints $\|\mathbf{x}^*\|_2^2 \leq M_1$ and $\|\mathbf{y}^*\|_2^2 \leq M_2$, where M_1 and M_2 are finite-valued parameters.

Proposition 3 *The **SCCA** admits an optimal solution $(\mathbf{x}^*, \mathbf{y}^*)$ satisfying $\|\mathbf{x}^*\|_2^2 \leq M_1$ and $\|\mathbf{y}^*\|_2^2 \leq M_2$, where $M_1 = 1/\lambda_r(\mathbf{B}) + 1/(\lambda_r(\mathbf{B})s_{\min}(\mathbf{B}))$ and $M_2 = 1/\lambda_{\hat{r}}(\mathbf{C}) + 1/(\lambda_{\hat{r}}(\mathbf{C})s_{\min}(\mathbf{C}))$ with $\lambda_r(\mathbf{B}), \lambda_{\hat{r}}(\mathbf{C})$ being the smallest nonzero eigenvalues of matrices \mathbf{B}, \mathbf{C} and $s_{\min}(\mathbf{R})$ being the smallest nonzero singular value of all the submatrices of the zero eigenvectors of matrix \mathbf{R} .*

Proof. Let $(\mathbf{x}^*, \mathbf{y}^*)$ denote an optimal solution to **SCCA**. We bound $\|\mathbf{x}^*\|_2$ first and the same technique can be also straightforwardly applied to bound $\|\mathbf{y}^*\|_2$.

For matrix $\mathbf{B} \in \mathcal{S}_+^n$ of rank r , we let $\{\mathbf{q}_i\}_{i \in [n]} \in \mathbb{R}^n$ denote the eigenvectors corresponding to n eigenvalues λ of \mathbf{B} such that $\lambda_1 \geq \dots \geq \lambda_r > \lambda_{r+1} = \dots = \lambda_n = 0$. Thus, $\{\mathbf{q}_i\}_{i \in [n]}$ are orthonormal and span the space of \mathbb{R}^n . Hence, there exists $\alpha \in \mathbb{R}^n$ such that $\mathbf{x}^* = \sum_{i \in [n]} \alpha_i \mathbf{q}_i$. Given that $(\mathbf{x}^*)^\top \mathbf{B} \mathbf{x}^* \leq 1$, we have

$$\sum_{i \in [r]} \alpha_i^2 \lambda_i \leq 1.$$

Hence, the values of $\{\alpha_i\}_{i \in [r]}$ are bounded. On the other hand, let us define a subset $S \subseteq [n]$ of size at most s_1 such that $x_i^* \neq 0$ for each $i \in S$ and $x_j^* = 0$ for each $j \in [n] \setminus S$. Then for each $j \in [n] \setminus S$, we arrive at the following linear system:

$$\sum_{j \in [r+1, n]} \alpha_j \hat{\mathbf{q}}_j = - \sum_{i \in [r]} \alpha_i \hat{\mathbf{q}}_i, \quad (17)$$

where $\hat{\mathbf{q}}_i$ denote a subvector of \mathbf{q}_i with indices $[n] \setminus S$ for each $i \in [n]$. For a fixed $\{\alpha_i\}_{i \in [r]}$, since the linear system (17) is nonempty, we let $\bar{\mathbf{Q}}\bar{\alpha} = \bar{\mathbf{q}}$ denote its minimal linear subsystem such that a submatrix $\bar{\mathbf{Q}}$ is non-singular and the index set \hat{S} of $\bar{\alpha}$ is a subset of $[n] \setminus S$. Thus, we can construct an alternative solution $\hat{\alpha}$ such that

$$\hat{\alpha}_i = \begin{cases} \alpha_i, & \text{if } i \in [r], \\ (\bar{\mathbf{Q}}^{-1} \bar{\mathbf{q}})_i, & \text{if } i \in \hat{S}, \\ 0, & \text{otherwise,} \end{cases}$$

and $\hat{\mathbf{x}} = \sum_{i \in [n]} \hat{\alpha}_i \mathbf{q}_i$. According to **Lemma 1**, we have

$$\hat{\mathbf{x}}^\top \mathbf{B} \hat{\mathbf{x}} \leq 1, \hat{\mathbf{x}}^\top \mathbf{A} \mathbf{y}^* = (\mathbf{x}^*)^\top \mathbf{A} \mathbf{y}^*,$$

i.e., $(\hat{\mathbf{x}}, \mathbf{y}^*)$ is also optimal to **SCCA**. Hence,

$$\|\hat{\mathbf{x}}\|_2 \leq \sqrt{\|\bar{\mathbf{Q}}^{-1} \bar{\mathbf{q}}\|_2^2 + \sum_{i \in [r]} \alpha_i^2}$$

Note that $\sum_{i \in [r]} \alpha_i^2 \leq 1/\lambda_r$ and

$$\|\bar{\mathbf{Q}}^{-1} \bar{\mathbf{q}}\|_2^2 \leq \|\bar{\mathbf{Q}}^{-1}\|_2^2 \|\bar{\mathbf{q}}\|_2^2 \leq \frac{1}{s_{\min}(\mathbf{B})} \frac{1}{\lambda_r}$$

where $s_{\min}(\mathbf{B})$ denotes the smallest nonzero singular values of all the submatrices of $[\mathbf{q}_{r+1}, \dots, \mathbf{q}_n]$. In summary, we have

$$\|\hat{\mathbf{x}}\|_2 \leq \sqrt{1/\lambda_r + 1/(\lambda_r s_{\min}(\mathbf{B}))}.$$

This completes the proof. \square

The proof of **Proposition 3** is straightforward in the case when \mathbf{B} and \mathbf{C} are of full rank as in this case the feasible region is a bounded set. In order to prove the result in the case when \mathbf{B} is not full-rank, one has to show that it is possible to construct sparse solutions that are not “too far” away.

In fact, the bounds M_1, M_2 in **Proposition 3** also hold for any given feasible subsets (S_1, S_2) of **SCCA** (1).

Corollary 2 *For any given feasible subsets (S_1, S_2) of **SCCA** 1, there exists a **SCCA** feasible solution (\mathbf{x}, \mathbf{y}) such that the supports of \mathbf{x}, \mathbf{y} are S_1, S_2 , respectively and we have that $\|\mathbf{x}\|_2^2 \leq M_1$ and $\|\mathbf{y}\|_2^2 \leq M_2$, where M_1, M_2 are defined in **Proposition 3**.*

C.2 Equivalent mixed-integer convex quadratic program of rank-one **SCCA**

When matrix \mathbf{A} is rank-one, let us focus on analyzing the subproblem over \mathbf{x} in (6), i.e.,

$$v_x = \max_{\mathbf{x} \in \mathbb{R}^n} \{ \mathbf{a}^\top \mathbf{x} : \mathbf{x}^\top \mathbf{B} \mathbf{x} \leq 1, \|\mathbf{x}\|_0 \leq s_1 \}. \quad (18)$$

Then the second subproblem over \mathbf{y} in (6) simply follows.

According to [Corollary 2](#), introducing the binary variables $\mathbf{z}^1 \in \{0, 1\}^n$ can reformulate the problem (18) as

$$v_x = \max_{\mathbf{x} \in \mathbb{R}^n, \mathbf{z}^1 \in \{0, 1\}^n} \left\{ \mathbf{a}^\top \mathbf{x} : \mathbf{x}^\top \mathbf{B} \mathbf{x} \leq 1, x_i \leq \sqrt{M_1 z_i^1}, \forall i \in [n], \sum_{i \in [n]} z_i^1 \leq s_1 \right\}.$$

When matrix \mathbf{B} is positive definite, there is a positive vector $\mathbf{b} \in \mathbb{R}_{++}^n$ and a positive semidefinite matrix $\hat{\mathbf{B}}$ such that $\mathbf{B} = \hat{\mathbf{B}} + \text{Diag}(\mathbf{b})$. Given this equation, by leveraging the perspective techniques (see, e.g., [\[1, 43\]](#)), we can derive another equivalent MICQP formulation of the problem (18):

$$v_x = \max_{\mathbf{x} \in \mathbb{R}^n, \mathbf{z}^1 \in \{0, 1\}^n, \boldsymbol{\mu} \in \mathbb{R}_+^n} \left\{ \mathbf{a}^\top \mathbf{x} : \mathbf{x}^\top \hat{\mathbf{B}} \mathbf{x} + \sum_{i \in [n]} \mu_i \leq 1, x_i^2 \leq \mu_i z_i^1, \forall i \in [n], \sum_{i \in [n]} z_i^1 \leq s_1 \right\}.$$

which is often stronger than the above formulation.

D A branch-and-cut algorithm with closed-form cuts

By dualizing the inner maximization problem over \mathbf{X} in the MISDP (7), in this subsection, we derive an equivalent mixed-integer linear program for [SCCA](#), which motivates us to develop a branch-and-cut algorithm.

By introducing the Lagrangian multipliers $(\theta_1, \theta_2, \boldsymbol{\lambda})$, the Lagrangian dual of the maximization problem (9) can be written as

$$\begin{aligned} f(\mathbf{z}) &= \min_{\substack{\theta_1 \geq 0, \theta_2 \geq 0, \\ \boldsymbol{\lambda} \in \mathbb{R}_+^{n+m}}} \max_{\mathbf{X} \in \mathcal{S}_+^{n+m}} \text{tr}(\tilde{\mathbf{A}} \mathbf{X}) - \theta_1 \text{tr}(\tilde{\mathbf{B}} \mathbf{X}) - \theta_2 \text{tr}(\tilde{\mathbf{C}} \mathbf{X}) + \theta_1 + \theta_2, \\ &\quad - \sum_{i \in [n+m]} \lambda_i X_{ii} + \sum_{i \in [n+m]} \lambda_i M_{ii} z_i \\ &= \min_{\substack{\theta_1 \geq 0, \theta_2 \geq 0, \\ \boldsymbol{\lambda} \in \mathbb{R}_+^{n+m}}} \left\{ \theta_1 + \theta_2 + \sum_{i \in [n+m]} \lambda_i M_{ii} z_i : \begin{pmatrix} \theta_1 \mathbf{B} & -\mathbf{A}/2 \\ -\mathbf{A}^\top/2 & \theta_2 \mathbf{C} \end{pmatrix} \succeq -\text{Diag}(\boldsymbol{\lambda}) \right\}, \end{aligned} \quad (19)$$

where the strong duality holds due to the function $f(\mathbf{z})$ being concave, bounded, and thus continuous in the set $\hat{\mathcal{Z}}$ and Slater condition holds for any interior point \mathbf{z} in the set $\hat{\mathcal{Z}}$.

Below, we derive the closed-form expression of the function $f(\mathbf{z})$ with the given binary variable $\mathbf{z} \in \mathcal{Z}$. This allows us to reformulate [SCCA](#) (8) as a mixed-integer linear program with exponentially many linear constraints and an efficient separation oracle.

Proposition 4 *The [SCCA](#) (8) is equivalent to*

$$\begin{aligned} v^* &= \max_{\mathbf{z} \in \mathcal{Z}, v} \left\{ v : v \leq \sigma_{\max} \left(\sqrt{(\mathbf{B}_{S_1, S_1})^\dagger} \mathbf{A}_{S_1, S_2} \sqrt{(\mathbf{C}_{S_2, S_2})^\dagger} \right) + \right. \\ &\quad \left. \sum_{i \in S_1 \cup (S_2 + n)} \lambda^* M_{ii} z_i : \forall S_1 \subseteq [n], |S_1| \leq s_1, S_2 \subseteq [m], |S_2| \leq s_2 \right\}, \end{aligned} \quad (20)$$

where for a pair of subsets (S_1, S_2) , the scalar λ^* is defined as the largest positive eigenvalue of matrix $\mathbf{D}_2^\top \mathbf{D}_1^{-1} \mathbf{D}_2 - \mathbf{D}_3$ with

$$\mathbf{D}_1 = \begin{pmatrix} \theta_1^* \mathbf{B}_{S_1, S_1} & -\mathbf{A}_{S_1, S_2}/2 \\ -\mathbf{A}_{S_1, S_2}^\top/2 & \theta_2^* \mathbf{C}_{S_2, S_2} \end{pmatrix}, \quad \mathbf{D}_2 = \begin{pmatrix} \theta_1^* \mathbf{B}_{S_1, [n] \setminus S_1} & -\mathbf{A}_{S_1, [m] \setminus S_2}/2 \\ -\mathbf{A}_{S_2, [n] \setminus S_1}^\top/2 & \theta_2^* \mathbf{C}_{S_2, [m] \setminus S_2} \end{pmatrix},$$

and

$$\mathbf{D}_3 = \begin{pmatrix} \theta_1^* \mathbf{B}_{[n] \setminus S_1, [n] \setminus S_1} & -\mathbf{A}_{[n] \setminus S_1, [m] \setminus S_2}/2 \\ -\mathbf{A}_{[n] \setminus S_1, [m] \setminus S_2}^\top/2 & \theta_2^* \mathbf{C}_{[m] \setminus S_2, [m] \setminus S_2} \end{pmatrix},$$

where $\theta_1^* = \theta_2^* = \sigma_{\max} \left(\sqrt{(\mathbf{B}_{S_1, S_1})^\dagger} \mathbf{A}_{S_1, S_2} \sqrt{(\mathbf{C}_{S_2, S_2})^\dagger} \right) / 2$.

Proof. First, for any binary variable $\mathbf{z} \in \mathcal{Z}$, suppose $S_1 = \{i : z_i = 1, \forall i \in [n]\}$, $S_2 = \{i - n : z_i = 1, \forall i \in [n+1, n+m]\}$, and $T \subseteq [n+m]$ denotes the support of \mathbf{z} . Then following the proof of [Proposition 1](#), we can construct a rank-one optimal solution $\mathbf{X}^* = \begin{pmatrix} \mathbf{x}^* \\ \mathbf{y}^* \end{pmatrix} \begin{pmatrix} \mathbf{x}^* \\ \mathbf{y}^* \end{pmatrix}^\top$ to the maximization problem below that admits the optimal value $\sigma_{\max} \left(\sqrt{(\mathbf{B}_{S_1, S_1})^\dagger} \mathbf{A}_{S_1, S_2} \sqrt{(\mathbf{C}_{S_2, S_2})^\dagger} \right)$, i.e.,

$$\begin{aligned} & \max_{\mathbf{X} \in \mathcal{S}_+^{n+m}} \{ \text{tr}(\tilde{\mathbf{A}}\mathbf{X}) : \text{tr}(\tilde{\mathbf{B}}\mathbf{X}) \leq 1, \text{tr}(\tilde{\mathbf{C}}\mathbf{X}) \leq 1, X_{ii} = 0, \forall i \in [n+m] \setminus T \} \\ &= \sigma_{\max} \left(\sqrt{(\mathbf{B}_{S_1, S_1})^\dagger} \mathbf{A}_{S_1, S_2} \sqrt{(\mathbf{C}_{S_2, S_2})^\dagger} \right) \geq f(\mathbf{z}), \end{aligned}$$

where the inequality is because the maximization problem above relaxes the valid constraints $X_{ii} \leq M_{ii}$ for all $i \in T$ in maximization problem (9). The result in [Corollary 2](#) suggests that $\mathbf{x}^*, \mathbf{y}^*$ can be bounded and their two norms must not exceed M_1, M_2 , which means that the optimal solution \mathbf{X}^* satisfies the $X_{ii} \leq M_{ii}$ for all $i \in T$. Therefore, \mathbf{X}^* is feasible and optimal to maximization problem (9) and we have that

$$f(\mathbf{z}) = \sigma_{\max} \left(\sqrt{(\mathbf{B}_{S_1, S_1})^\dagger} \mathbf{A}_{S_1, S_2} \sqrt{(\mathbf{C}_{S_2, S_2})^\dagger} \right).$$

According to strong duality, the minimization problem (19) admits an optimal value $\sigma_{\max} \left(\sqrt{(\mathbf{B}_{S_1, S_1})^\dagger} \mathbf{A}_{S_1, S_2} \sqrt{(\mathbf{C}_{S_2, S_2})^\dagger} \right)$. Next, we construct its optimal solution $(\theta_1^*, \theta_2^*, \boldsymbol{\lambda}^*)$.

For any given $\epsilon > 0$, we let $\theta_1^* = f(\mathbf{z})/2$, $\theta_2^* = f(\mathbf{z})/2$, $\hat{\lambda}_i(\epsilon) = \frac{\epsilon}{M_{ii}|T|}$ for all $i \in T$, and $\hat{\lambda}_i(\epsilon) = \lambda^*(\epsilon)$ for all $i \in [n] \setminus T$, where

$$\lambda^*(\epsilon) = \left[\lambda_{\max} \left(\mathbf{D}_2^\top \left(\mathbf{D}_1 + \text{Diag} \left(\hat{\boldsymbol{\lambda}}_T(\epsilon) \right) \right)^{-1} \mathbf{D}_2 - \mathbf{D}_3 \right) \right]_+.$$

It is easy to compute that $\theta_1^* + \theta_2^* + \sum_{i \in [n+m]} \hat{\lambda}_i(\epsilon) M_{ii} z_i = f(\mathbf{z}) + \epsilon$. Thus, for any $\epsilon > 0$, if $(\theta_1^*, \theta_2^*, \hat{\boldsymbol{\lambda}}(\epsilon))$ were feasible, then it is an ϵ -optimal solution to the minimization problem (19). It remains to verify the feasibility of the solution $(\theta_1^*, \theta_2^*, \hat{\boldsymbol{\lambda}}(\epsilon))$, i.e., checking the constraint below

$$\begin{pmatrix} \theta_1^* \mathbf{B} & -\mathbf{A}/2 \\ -\mathbf{A}^\top/2 & \theta_2^* \mathbf{C} \end{pmatrix} + \text{Diag} \left(\hat{\boldsymbol{\lambda}}(\epsilon) \right) \succeq 0.$$

By performing the permutation of the rows and columns of the above matrix, it is sufficient to show that the new block matrix

$$\begin{pmatrix} \mathbf{D}_1 + \text{Diag} \left(\hat{\boldsymbol{\lambda}}_T(\epsilon) \right) & \mathbf{D}_2 \\ \mathbf{D}_2^\top & \mathbf{D}_3 + \lambda^*(\epsilon) \mathbf{I} \end{pmatrix} \succeq 0, \quad (21)$$

is positive semidefinite.

Since $\begin{pmatrix} \mathbf{B}_{S_1, S_1} & -\mathbf{A}_{S_1, S_2}/2 \\ -\mathbf{A}_{S_1, S_2}^\top/2 & \mathbf{C}_{S_2, S_2} \end{pmatrix}$ is a principal submatrix of a positive semidefinite matrix $\begin{pmatrix} \mathbf{B} & -\mathbf{A}/2 \\ -\mathbf{A}^\top/2 & \mathbf{C} \end{pmatrix}$, it is also positive semidefinite. According to [Lemma 1](#) and the fact that $\theta_1^* = \theta_2^* = \sigma_{\max} \left(\sqrt{(\mathbf{B}_{S_1, S_1})^\dagger} \mathbf{A}_{S_1, S_2} \sqrt{(\mathbf{C}_{S_2, S_2})^\dagger} \right) / 2$, the matrix \mathbf{D}_1 is also positive semidefinite. As $\epsilon > 0$, the matrix $\mathbf{D}_1 + \text{Diag} \left(\hat{\boldsymbol{\lambda}}_T(\epsilon) \right)$ must be positive definite, which means that

$$\left(\mathbf{I} - \left(\mathbf{D}_1 + \text{Diag} \left(\hat{\boldsymbol{\lambda}}_T(\epsilon) \right) \right) \left(\mathbf{D}_1 + \text{Diag} \left(\hat{\boldsymbol{\lambda}}_T(\epsilon) \right) \right)^{-1} \right) \mathbf{D}_2 = \mathbf{0}.$$

Besides, according to the definition of $\lambda^*(\epsilon)$, we obtain

$$\mathbf{D}_3 + \lambda^*(\epsilon) \mathbf{I} - \mathbf{D}_2^\top \left(\mathbf{D}_1 + \text{Diag} \left(\hat{\boldsymbol{\lambda}}_T(\epsilon) \right) \right)^{-1} \mathbf{D}_2 \succeq \mathbf{0}.$$

Taking these results together, according to [Lemma 1](#), the constraint in (21) must hold for a given solution $(\theta_1^*, \theta_2^*, \hat{\lambda}(\epsilon))$. Since the objective value corresponding to $(\theta_1^*, \theta_2^*, \hat{\lambda}(\epsilon))$ is at most ϵ larger than the optimal value of problem (19), letting $\epsilon \rightarrow 0$ and using the closedness of the feasible set in problem (19), we can confirm the optimality of $(\theta_1^*, \theta_2^*, \lambda^*)$ with $\lambda_i^* = 0$ for all $i \in T$ and $\lambda_i^* = \lambda^*$ for all $i \in [n] \setminus T$.

Given the closed-form optimal solution to problem (19), the rest of the proof follows from [28, theorem 7]. \square

We note that SCCA (20) can be implemented via a delayed cut-generation procedure. That is, at each feasible branch-and-bound node with a binary solution $\hat{\mathbf{z}}$, let $S_1 = \{i : \hat{z}_i = 1, \forall i \in [n]\}$ and $S_2 = \{i - n : \hat{z}_i = 1, \forall i \in [n+1, n+m]\}$. Then we can compute the corresponding scalar λ^* and generate the following valid inequality based on (20):

$$v \leq \sigma_{\max} \left(\sqrt{(\mathbf{B}_{S_1, S_1})^\dagger} \mathbf{A}_{S_1, S_2} \sqrt{(\mathbf{C}_{S_2, S_2})^\dagger} \right) + \sum_{i \in S_1 \cup (S_2 + n)} \lambda^* M_{ii} z_i.$$

E Data description

Table 7: Description of UCI and breast cancer datasets used

Dataset	# of variables	# of samples	n	m	rank r	rank \hat{r}
<i>dermatology</i>	34	366	17	17	17	17
<i>spambase</i>	57	4601	28	29	28	29
<i>digits</i>	64	1797	32	32	32	32
<i>buzz</i>	77	583250	38	39	38	39
<i>gas</i>	128	2565	64	64	64	64
<i>slice</i>	385	53500	192	193	192	193
<i>breast cancer</i>	21821	89	19,672	2,149	89	89

F Multiple Sparse Canonical Correlation Analysis

The multiple CCA problem can be formulated as follows:

$$\max_{\mathbf{x} \in \mathbb{R}^{n \times k}, \mathbf{y} \in \mathbb{R}^{m \times k}} \{ \text{tr}(\mathbf{x}^\top \mathbf{A} \mathbf{y}) : \mathbf{x}^\top \mathbf{B} \mathbf{x} = \mathbf{I}_k, \mathbf{y}^\top \mathbf{C} \mathbf{y} = \mathbf{I}_k \},$$

where k denotes the number of pairs of basis vectors and \mathbf{I}_k denotes the identity matrix of size k .

As \mathbf{x}, \mathbf{y} can be matrices, we propose adding row sparse constraints to extend [SCCA](#) for multiple vectors, which is defined as:

$$\max_{\mathbf{x} \in \mathbb{R}^{n \times k}, \mathbf{y} \in \mathbb{R}^{m \times k}} \{ \text{tr}(\mathbf{x}^\top \mathbf{A} \mathbf{y}) : \mathbf{x}^\top \mathbf{B} \mathbf{x} = \mathbf{I}_k, \mathbf{y}^\top \mathbf{C} \mathbf{y} = \mathbf{I}_k, \|\mathbf{x}\|_0 \leq s_1, \|\mathbf{y}\|_0 \leq s_2 \},$$

where we let $\|\mathbf{x}\|_0$ and $\|\mathbf{y}\|_0$ denote the number of nonzero rows of \mathbf{x} and \mathbf{y} , respectively.

This multiple SCCA model can (i) compute the multiple weight vectors (\mathbf{x}, \mathbf{y}) simultaneously and (ii) enforce the sparsity and orthogonality strictly. To be specific, the constraints $\mathbf{x}^\top \mathbf{B} \mathbf{x} = \mathbf{I}_k, \mathbf{y}^\top \mathbf{C} \mathbf{y} = \mathbf{I}_k$ ensure the orthogonal left- and right-canonical loading vectors in multiple SCCA. By the definition of row sparsity, the resultant multiple left- and right-basis vectors, i.e., the columns of \mathbf{x} and \mathbf{y} , share the same nonzero rows, respectively.

More importantly, the row-sparsity enables us to readily extend the proposed algorithms to solve multiple SCCA. We have tested them on UCI data, and the computational results are presented in [Table 8](#). As k increases, it takes branch-and-cut a longer time to return an optimal solution.

Table 8: Evaluation of our algorithms for solving multiple SCCA on UCI datasets

n	m	s ₁	s ₂	k	Greedy		Local search		Convex relaxation			Branch-and-cut		
					LB	time	LB	time	UB	gap(%)	time	v*	MIPGap(%)	time
17	17	5	5	2	1.907	0.01	1.935	0.06	1.957	1.14	0.01	1.935	0.00	2
17	17	10	10	3	2.879	0.02	2.884	0.09	2.898	0.45	0.01	2.884	0.00	6
28	29	5	5	2	1.182	0.02	1.233	0.09	1.358	10.19	0.01	1.233	0.00	234
28	29	10	10	3	1.579	0.04	1.586	0.14	1.685	6.23	0.01	1.587	5.33	–
32	32	5	5	2	1.906	0.02	1.906	0.04	1.935	1.55	0.01	1.916	0.00	14
32	32	10	10	3	2.736	0.04	2.741	0.19	2.770	1.05	0.01	2.742	0.00	3093
38	39	5	5	2	2	0.03	2	0.25	2	0.00	0.01	2	0.00	8
38	39	10	10	3	3	0.05	3	0.59	3	0.00	0.01	3	0.00	10
64	64	5	5	2	1.947	0.05	1.991	0.34	1.997	0.29	0.01	1.993	0.15	–
64	64	10	10	3	2.983	0.09	2.989	0.71	2.993	0.14	0.02	2.989	0.14	–
192	193	5	5	2	1.911	0.21	1.991	2.36	1.995	0.22	0.04	1.991	0.21	–
192	193	10	10	3	2.907	0.38	2.951	5.78	2.977	0.90	0.04	2.954	0.78	–

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