

Convex relaxation for the generalized maximum-entropy sampling problem

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Abstract

The generalized maximum-entropy sampling problem (GMESP) is to select an order- s principal submatrix from an order- n covariance matrix, to maximize the product of its t greatest eigenvalues, $0 < t \leq s < n$. It is a problem that specializes to two fundamental problems in statistical design theory: (i) maximum-entropy sampling problem (MESP); (ii) binary D-optimality (D-Opt). In the general case, it is motivated by a selection problem in the context of PCA (principal component analysis).

We introduce the first convex-optimization based relaxation for GMESP, study its behavior, compare it to an earlier spectral bound, and demonstrate its use in a branch-and-bound scheme. We find that such an approach is practical when $s - t$ is very small.

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1 Introduction

Let C be a symmetric positive-semidefinite matrix with rows/columns indexed from $N := \{1, 2, \dots, n\}$, with $n > 1$ and $\text{rank}(C) := r$. For integers t and s , such that $0 < t \leq r$ and $t \leq s < n$, we define the *generalized maximum-entropy sampling problem* (see [25, 16])

$$(\text{GMESP}) \quad z(C, s, t) := \max \left\{ \sum_{\ell=1}^t \log(\lambda_{\ell}(C[S(x), S(x)])) : \mathbf{e}^{\top} x = s, x \in \{0, 1\}^n \right\},$$

where $S(x)$ denotes the support of $x \in \{0, 1\}^n$, $C[S, S]$ denotes the principal submatrix indexed by S , and $\lambda_{\ell}(X)$ denotes the ℓ -th greatest eigenvalue of a symmetric matrix X .

Twenty-five years ago, **GMESP** was introduced as a common generalization of MESP and binary D-Opt (see [25], but not widely disseminated until [16]). MESP, a central problem in statistics and information theory, corresponds to the problem of selecting a subvector of size s from a Gaussian n -vector, so as to maximize the “differential entropy” (see [23]) of the chosen subvector; see [9]. MESP is the special case of **GMESP** for which $t := s$. The relationship with binary D-Opt is more involved. Given an $n \times r$ matrix \mathcal{A} of full column

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rank, binary D-Opt corresponds to the special case of **GMESP** for which $C := \mathcal{A}\mathcal{A}^\top$, and $t := r$. D-Opt is equivalent to the problem of selecting a set of s design points from a given set of n potential design points (the rows of \mathcal{A}), so as to minimize the volume of a confidence ellipsoid for the least-squares parameter estimates in the resulting linear model (assuming additive Gaussian noise); see [21], for example.

For the general case of **GMESP**, we can see it as motivated by a selection problem in the context of PCA (principal component analysis); see, for example, [12] and the references therein, for the important topic of PCA. Specifically, **GMESP** amounts to selecting a subvector of size s from a Gaussian n -vector, so that geometric mean of the variances associated with the t largest principal components is maximized. Linking this back to MESP, we can see that problem as selecting a subvector of size s from a Gaussian n -vector, so that the geometric mean of the variances associated with *all* principal components is maximized. We use the geometric mean of the variances, so as to encourage a selection where all t of them are large and similar in value;² we note that maximizing the geometric mean is equivalent to maximizing the log of the product.

Expanding on our motivation for **GMESP**, we assume that we are in a setting where we have n observable Gaussian random variables, with a possibly low-rank covariance matrix. We assume that observations are costly, and so we want to select $s \ll n$ for observation. Even the s selected random variables may have a low-rank covariance matrix. Posterior to the selection, we would then carry out PCA on the associated order- s covariance matrix, with the aim of identifying the most informative $t < s$ latent/hidden random variables, where we define *most informative* as corresponding to maximizing the geometric mean of the variances of the t dominant principal components.

We also define the *constrained generalized maximum-entropy sampling problem*

(CGMESP)

$$z(C, s, t, A, b) := \max \left\{ \sum_{\ell=1}^t \log(\lambda_\ell(C[S(x), S(x)]) : \mathbf{e}^\top x = s, Ax \leq b, x \in \{0, 1\}^n \right\},$$

which is useful in practical applications where there are budget constraints, logistical constraints, etc., on which sets of size s are feasible. Correspondingly, we also refer to CMESP (the constrained version of MESP) and CD-Opt (the constrained version of D-Opt).

The main approach for solving **GMESP** and **CGMESP** to optimality is B&B (branch-and-bound); see [16]. Lower bounds are calculated by local search (especially for **GMESP**), rounding, etc. Upper bounds are calculated in a variety of ways. The only upper-bounding method in the literature uses spectral information; see [25, 16].

Some very good upper-bounding methods for CMESP and CD-Opt are based on convex relaxations; see [4, 1, 2, 20, 19, 8, 21]. For CMESP, a “down branch” is realized by deleting a symmetric row/column pair from C . An “up branch” corresponds to calculating a Schur complement. For CD-Opt, a “down branch” amounts to eliminating a row from \mathcal{A} , and an “up branch” corresponds to adding a rank-1 symmetric matrix before applying a determinant operator to an order- r symmetric matrix that is linear in x (see [18] and [21] for details).

For the general case of **CGMESP** and the spectral bounding technique, we refer to [16] for a discussion of an “up branch”, which is actually quite complicated and probably not very efficient. We will present a convex relaxation for **CGMESP** that is amenable to the use of a simple “up branch”. Our new “generalized factorization bound” for **CGMESP** generalizes

² In this spirit, the product of sample variances is used in Bartlett’s test of homogeneity of variances; see [24, Section 10.21, pp. 296].

(i) the “factorization bound” for CMESP (see [8]), and (ii) the “natural bound” for binary CD-Opt (see [21]). We wish to emphasize that it does *not* generalize the “factorization bound” for binary CD-Opt.

Organization and Contributions. In §2, we introduce the generalized factorization bound as the Lagrangian dual of a non-convex relaxation and establish its basic properties and its relation with the spectral bound from [16]. In §3, we apply Lagrangian duality again, reaching a more tractable formulation for calculating the generalized factorization bound. In §4, we present results from computational experiments with a B&B algorithm based on the generalized factorization bound, where we demonstrate favorable computational performance when $s - t$ is small. In §5, we describe some directions for further study.

Notation. We let \mathbb{S}_+^n (resp., \mathbb{S}_{++}^n) denote the set of positive semidefinite (resp., definite) symmetric matrices of order n . We let $\text{Diag}(x)$ denote the $n \times n$ diagonal matrix with diagonal elements given by the components of $x \in \mathbb{R}^n$, and $\text{diag}(X)$ denote the n -dimensional vector with elements given by the diagonal elements of $X \in \mathbb{R}^{n \times n}$. We denote an all-ones vector by \mathbf{e} and the i -th standard unit vector by \mathbf{e}_i . For matrices A and B with the compatible shapes, $A \bullet B := \text{tr}(A^\top B)$ is the matrix dot-product. For a matrix A , we denote row i by A_i and column j by $A_{.j}$.

2 Generalized factorization bound

Suppose that the rank of C is $r \geq t$. We factorize $C = FF^\top$, with $F \in \mathbb{R}^{n \times k}$, for some k satisfying $r \leq k \leq n$. This could be a Cholesky-type factorization, as in [20] and [19], where F is lower triangular and $k := r$, it could be derived from a spectral decomposition $C = \sum_{i=1}^r \lambda_i v_i v_i^\top$, by selecting $\sqrt{\lambda_i} v_i$ as the column i of F , $i = 1, \dots, k := r$, or it could be derived from the matrix square root of C , where $F := C^{1/2}$, and $k := n$.

For $x \in [0, 1]^n$, we define $f(x) := \sum_{\ell=1}^t \log(\lambda_\ell(F(x)))$, where $F(x) := \sum_{i \in N} F_i^\top F_i x_i = F^\top \text{Diag}(x) F$, and

$$(\text{GFact}) \quad z_{\text{GFact}}(C, s, t, A, b; F) := \max \{ f(x) : \mathbf{e}^\top x = s, Ax \leq b, 0 \leq x \leq \mathbf{e} \}.$$

Next, we see that [GFact](#) gives an upper bound for [CGMESP](#).

► Theorem 1.

$$z(C, s, t, A, b) \leq z_{\text{GFact}}(C, s, t, A, b; F).$$

Proof It suffices to show that for any feasible solution x of [CGMESP](#) with finite objective value, we have $\sum_{\ell=1}^t \log(\lambda_\ell(C[S(x), S(x)])) = f(x)$. Let $S := S(x)$. Then, for $S \subset N$ with $|S| = s$ and $\text{rank}(C[S, S]) \geq t$, we have $F(x) = \sum_{i \in S} F_i^\top F_i = F[S, \cdot]^\top F[S, \cdot] \in \mathbb{S}_+^k$. Also, we have $C[S, S] = F[S, \cdot] F[S, \cdot]^\top \in \mathbb{S}_+^s$. Now, we observe that the nonzero eigenvalues of $F[S, \cdot]^\top F[S, \cdot]$ and $F[S, \cdot] F[S, \cdot]^\top$ are identical and the rank of these matrices is at least t . So, the t largest eigenvalues of these matrices are positive and identical. The result follows. ◀

From the proof, we see that replacing $0 \leq x \leq \mathbf{e}$ with $x \in \{0, 1\}^n$ in [GFact](#), we get an exact mixed-integer nonlinear optimization (MINLO) formulation for [CGMESP](#). But [GFact](#) is not generally a convex program, so we cannot make direct use of such a formulation and [Theorem 1](#). We will overcome this difficulty using Lagrangian duality, obtaining an upper bound for z_{GFact} . We first re-cast [GFact](#) as

$$\max \left\{ \sum_{\ell=1}^t \log(\lambda_\ell(W)) : F(x) = W, \mathbf{e}^\top x = s; Ax \leq b; 0 \leq x \leq \mathbf{e} \right\},$$

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and consider the Lagrangian function

$$\mathcal{L}(W, x, \Theta, v, \nu, \pi, \tau) := \sum_{\ell=1}^t \log(\lambda_{\ell}(W)) + \Theta \bullet (F(x) - W) + v^{\top}x + \nu^{\top}(\mathbf{e} - x) + \pi^{\top}(b - Ax) + \tau(s - \mathbf{e}^{\top}x),$$

with $\text{dom } \mathcal{L} = \mathbb{S}_+^{k,t} \times \mathbb{R}^n \times \mathbb{S}^k \times \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}$, where $\mathbb{S}_+^{k,t}$ denotes the convex set of $k \times k$ positive semidefinite matrices with rank at least t .

The corresponding dual function is

$$\mathcal{L}^*(\Theta, v, \nu, \pi, \tau) := \sup_{W \in \mathbb{S}_+^{k,t}, x} \mathcal{L}(W, x, \Theta, v, \nu, \pi, \tau),$$

and the corresponding Lagrangian dual problem is

$$z_{\text{DGFact}}(C, s, t, A, b; F) := \inf \{ \mathcal{L}^*(\Theta, v, \nu, \pi, \tau) : v \geq 0, \nu \geq 0, \pi \geq 0 \}.$$

We call $z_{\text{DGFact}} := z_{\text{DGFact}}(C, s, t, A, b; F)$ the generalized factorization bound. We note that

$$\begin{aligned} & \sup_{W \in \mathbb{S}_+^{k,t}, x} \left\{ \sum_{\ell=1}^t \log(\lambda_{\ell}(W)) + \Theta \bullet (F(x) - W) + v^{\top}x + \nu^{\top}(\mathbf{e} - x) + \pi^{\top}(b - Ax) + \tau(s - \mathbf{e}^{\top}x) \right\} \\ (1) \quad &= \sup_{W \in \mathbb{S}_+^{k,t}} \left\{ \sum_{\ell=1}^t \log(\lambda_{\ell}(W)) - \Theta \bullet W \right\} \\ (2) \quad &+ \sup_x \{ \Theta \bullet F(x) + v^{\top}x - \nu^{\top}x - \pi^{\top}Ax - \tau \mathbf{e}^{\top}x + \nu^{\top} \mathbf{e} + \pi^{\top}b + \tau s \}. \end{aligned}$$

In Theorems 2 and 3 we analytically characterize the suprema in (1) and (2). The proof of Theorem 2 can be found in the full version [22]. The result in Theorem 3 follows from the fact that a linear function is bounded above only when it is identically zero.

► **Theorem 2.** (see [19, Lemma 1]) For $\Theta \in \mathbb{S}^k$, we have

$$(3) \quad \sup_{W \in \mathbb{S}_+^{k,t}} \left(\sum_{\ell=1}^t \log(\lambda_{\ell}(W)) - W \bullet \Theta \right) = \begin{cases} -t - \sum_{\ell=k-t+1}^k \log(\lambda_{\ell}(\Theta)), & \text{if } \Theta \succ 0; \\ +\infty, & \text{otherwise.} \end{cases}$$

► **Theorem 3.** For $(\Theta, v, \nu, \pi, \tau) \in \mathbb{S}^k \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}$, we have

$$\begin{aligned} & \sup_x \{ \Theta \bullet F(x) + v^{\top}x - \nu^{\top}x - \pi^{\top}Ax - \tau \mathbf{e}^{\top}x + \nu^{\top} \mathbf{e} + \pi^{\top}b + \tau s \} \\ &= \begin{cases} \nu^{\top} \mathbf{e} + \pi^{\top}b + \tau s, & \text{if } \text{diag}(F\Theta F^{\top}) + v - \nu - A^{\top}\pi - \tau \mathbf{e} = 0; \\ +\infty, & \text{otherwise.} \end{cases} \end{aligned}$$

Considering Theorems 2 and 3, we see that the Lagrangian dual of **GFact** is equivalent to

$$\begin{aligned} (DGFact) \quad z_{\text{DGFact}}(C, s, t, A, b; F) &= \min - \sum_{\ell=k-t+1}^k \log(\lambda_{\ell}(\Theta)) + \nu^{\top} \mathbf{e} + \pi^{\top}b + \tau s - t \\ &\text{subject to:} \\ &\text{diag}(F\Theta F^{\top}) + v - \nu - A^{\top}\pi - \tau \mathbf{e} = 0, \\ &\Theta \succ 0, v \geq 0, \nu \geq 0, \pi \geq 0. \end{aligned}$$

From Lagrangian duality, we conclude that **DGFact** is a convex program. Nevertheless, we note that **GFact** is not generally a convex program, so we will not generally have strong duality between **GFact** and **DGFact**.

Next, we establish two properties for the generalized factorization bound that were similarly established for the factorization bound for MESP in [8]. Specifically, we show that the generalized factorization bound for **CGMESP** is invariant under multiplication of C by a scale factor γ , up to the additive constant $-t \log \gamma$, and is also independent of the factorization of C . The proofs of the results are similar to the ones presented in [8] for MESP.

► **Theorem 4.** For all $\gamma > 0$ and factorizations $C = FF^\top$, we have

$$z_{\text{DGFact}}(C, s, t, A, b; F) = z_{\text{DGFact}}(\gamma C, s, t, A, b; \sqrt{\gamma}F) - t \log \gamma.$$

► **Theorem 5.** $z_{\text{DGFact}}(C, s, t, A, b; F)$ does not depend on the chosen F .

[16] presents a *spectral bound* for **GMESP**, $\sum_{\ell=1}^t \log \lambda_\ell(C)$. Next, we present a relation between the generalized factorization bound and the spectral bound for **GMESP**.

► **Theorem 6.** Let $C \in \mathbb{S}_+^n$, with $r := \text{rank}(C)$, $0 < t \leq r$, and $t \leq s < n$. Then, for all factorizations $C = FF^\top$, we have

$$z_{\text{DGFact}}(C, s, t, \cdot, \cdot; F) - \sum_{\ell=1}^t \log \lambda_\ell(C) \leq t \log \left(\frac{s}{t} \right).$$

Proof Let $C = \sum_{\ell=1}^r \lambda_\ell(C) u_\ell u_\ell^\top$ be a spectral decomposition of C . By Theorem 5, it suffices to take F to be the symmetric matrix $\sum_{\ell=1}^r \sqrt{\lambda_\ell(C)} u_\ell u_\ell^\top$.

We consider the solution for **DGFact** given by: $\hat{\Theta} := \frac{t}{s} \left(C^\dagger + \frac{1}{\lambda_r(C)} (I - CC^\dagger) \right)$, where $C^\dagger := \sum_{\ell=1}^r \frac{1}{\lambda_\ell(C)} u_\ell u_\ell^\top$ is the Moore-Penrose pseudoinverse of C , $\hat{v} := \frac{t}{s} \mathbf{e} - \text{diag}(F\hat{\Theta}F^\top)$, $\hat{\nu} := 0$, $\hat{\pi} := 0$, and $\hat{\tau} := \frac{t}{s}$. We can verify that the r least eigenvalues of $\hat{\Theta}$ are $\frac{t}{s} \cdot \frac{1}{\lambda_1(C)}$, $\frac{t}{s} \cdot \frac{1}{\lambda_2(C)}$, \dots , $\frac{t}{s} \cdot \frac{1}{\lambda_r(C)}$ and the $n - r$ greatest eigenvalues are all equal to $\frac{t}{s} \cdot \frac{1}{\lambda_r(C)}$. Therefore, $\hat{\Theta}$ is positive definite.

The equality constraint of **DGFact** is clearly satisfied at this solution. Additionally, we can verify that $F\hat{\Theta}F^\top = \frac{t}{s} \sum_{\ell=1}^r u_\ell u_\ell^\top$. As $\sum_{\ell=1}^r u_\ell u_\ell^\top \preceq I$, we conclude that $\text{diag}(F\hat{\Theta}F^\top) \leq \frac{t}{s} \mathbf{e}$. Therefore, $\hat{v} \geq 0$, and the solution constructed is a feasible solution to **DGFact**. Finally, we can see that the objective value of this solution is equal to the spectral bound added to $t \log(s/t)$. The result then follows. ◀

► **Remark 7.** Considering Theorem 6, for $t = s - k$, with constant integer $k \geq 0$, $\lim_{s \rightarrow \infty} t \log(s/t) = k$. Therefore, in this limiting regime, the generalized factorization bound is no more than an additive constant worse than the spectral bound.

Considering Theorem 6, we will see that key quantities are discrete concave in t , in such a way that we get a concave upper bound that only depends on t and s for the difference of two discrete concave upper bounds (which depend on C as well).

► **Theorem 8.**

- (a) $t \log \left(\frac{s}{t} \right)$ is (strictly) concave in t on \mathbb{R}_{++} ;
- (b) $\sum_{\ell=1}^t \log \lambda_\ell(C)$ is discrete concave in t on $\{1, 2, \dots, r\}$;
- (c) $z_{\text{DGFact}}(C, s, t, A, b; F)$ is discrete concave in t on $\{1, 2, \dots, k\}$.

Proof For (a), we see that the second derivative of the function is $-1/t$, which is negative on \mathbb{R}_{++} . For (b), it is easy to check that discrete concavity is equivalent to $\lambda_t(C) \geq \lambda_{t+1}(C)$, for all integers t satisfying $1 \leq t < r$, which we obviously have. For (c), first we observe that we can view $z_{\text{DGFact}}(C, s, t, A, b; F)$ as the pointwise minimum of $-\sum_{\ell=k-t+1}^k \log(\lambda_\ell(\Theta)) + \nu^\top \mathbf{e} + \pi^\top b + \tau s - t$ over the points in the convex feasible region of **DGFact**. So it suffices to demonstrate that the function $-\sum_{\ell=k-t+1}^k \log(\lambda_\ell(\Theta)) + \nu^\top \mathbf{e} + \pi^\top b + \tau s - t$ is discrete concave in t . It is easy to check that this is equivalent to $\lambda_{k-t+1}(C) \geq \lambda_{k-t+2}(C)$, for all integers t satisfying $1 < t \leq k$, which we obviously have. ◀

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Theorem 8, part (c) is very interesting, in connection with the motivating application to PCA. Using convexity, we can compute upper bounds on the value of changing the number t of dominant principal components considered, without having to actually solve further instances of **DGFact** (of course, solve those would give better upper bounds).

[16] extends the spectral bound to take advantage of the side constraints $Ax \leq b$. In the full version [22], we extend Theorem 8, part (b), to that situation.

In the next theorem, we present for **CGMESP**, a key result to enhance the application of B&B algorithms to discrete optimization problems with convex relaxations. The principle described in the theorem is called *variable fixing*, and has been successfully applied to MESP (see [3, 4]). The similar proof of the theorem for MESP can be found in [9, Theorem 3.3.9].

► **Theorem 9.** *Let*

- LB be the objective-function value of a feasible solution for **CGMESP**,
- $(\hat{\Theta}, \hat{\nu}, \hat{\pi}, \hat{\tau})$ be a feasible solution for **DGFact** with objective-function value $\hat{\zeta}$.

Then, for every optimal solution x^ for **CGMESP**, we have:*

$$\begin{aligned} x_j^* &= 0, \quad \forall j \in N \text{ such that } \hat{\zeta} - LB < \hat{\nu}_j, \\ x_j^* &= 1, \quad \forall j \in N \text{ such that } \hat{\zeta} - LB < \hat{\nu}_j. \end{aligned}$$

3 Duality for DGFact

Although it is possible to directly solve **DGFact** to calculate the generalized factorization bound, it is computationally more attractive to work the Lagrangian dual of **DGFact**. In the following, we construct this dual formulation.

Consider the Lagrangian function corresponding to **DGFact**, after eliminating the slack variable ν ,

$$\begin{aligned} \mathcal{L}(\Theta, \nu, \pi, \tau, x, y, w) &:= -\sum_{\ell=k-t+1}^k \log(\lambda_\ell(\Theta)) + \nu^\top \mathbf{e} + \pi^\top b + \tau s - t \\ &\quad + x^\top (\text{diag}(F\Theta F^\top) - \nu - A^\top \pi - \tau \mathbf{e}) - y^\top \nu - w^\top \pi, \end{aligned}$$

with $\text{dom } \mathcal{L} = \mathbb{S}_{++}^k \times \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^m$.

The corresponding dual function is

$$(4) \quad \mathcal{L}^*(x, y, w) := \inf_{\Theta \in \mathbb{S}_{++}^k, \nu, \pi, \tau} \mathcal{L}(\Theta, \nu, \pi, \tau, x, y, w),$$

and the Lagrangian dual problem of **DGFact** is

$$z_{\text{DDGFact}}(C, s, t, A, b; F) := \max\{\mathcal{L}^*(x, y, z) : x \geq 0, y \geq 0, w \geq 0\}.$$

We note that **DGFact** has a strictly feasible solution (e.g., given by $(\hat{\Theta} := I, \hat{\nu} := 0, \hat{\nu} := \text{diag}(FF^\top) = \text{diag}(C), \hat{\pi} := 0, \hat{\tau} := 0)$). Then, Slater's condition holds for **DGFact** and we are justified to use maximum in the formulation of the Lagrangian dual problem, rather than supremum, as the optimal value of the Lagrangian dual problem is attained.

We have that

$$\begin{aligned} &\inf_{\Theta \in \mathbb{S}_{++}^k, \nu, \pi, \tau} \mathcal{L}(\Theta, \nu, \pi, \tau, x, y, w) = \\ (5) \quad &\inf_{\Theta \in \mathbb{S}_{++}^k} \left\{ -\sum_{\ell=k-t+1}^k \log(\lambda_\ell(\Theta)) + x^\top \text{diag}(F\Theta F^\top) - t \right\} \\ (6) \quad &+ \inf_{\nu, \pi, \tau} \{ \nu^\top (\mathbf{e} - x - y) + \pi^\top (b - Ax - w) + \tau (s - \mathbf{e}^\top x) \}. \end{aligned}$$

Next, we discuss the infima in (5) and (6), for which the following lemma brings a fundamental result.

► **Lemma 10.** (see [20, Lemma 13]) Let $\lambda \in \mathbb{R}_+^k$ with $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_k$ and let $0 < t \leq k$. There exists a unique integer ι , with $0 \leq \iota < t$, such that

$$(7) \quad \lambda_\iota > \frac{1}{t - \iota} \sum_{\ell=\iota+1}^k \lambda_\ell \geq \lambda_{\iota+1},$$

with the convention $\lambda_0 = +\infty$.

Suppose that $\lambda \in \mathbb{R}_+^k$, and assume that $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_k$. Given integer t with $0 < t \leq k$, let ι be the unique integer defined by Lemma 10. We define

$$(8) \quad \phi_t(\lambda) := \sum_{\ell=1}^{\iota} \log(\lambda_\ell) + (t - \iota) \log\left(\frac{1}{t - \iota} \sum_{\ell=\iota+1}^k \lambda_\ell\right).$$

Also, for $X \in \mathbb{S}_+^k$, we define $\Gamma_t(X) := \phi_t(\lambda(X))$.

Considering the definition of Γ_t , we analytically characterize the infimum in (5) in Theorem 11. Its proof can be found in the full version [22].

► **Theorem 11.** (see [20, Lemma 16]) For $x \in \mathbb{R}^n$, we have

$$\begin{aligned} & \inf_{\Theta \in \mathbb{S}_{++}^k} - \sum_{\ell=k-t+1}^k \log(\lambda_\ell(\Theta)) + x^\top \text{diag}(F\Theta F^\top) - t \\ &= \begin{cases} \Gamma_t(F(x)), & \text{if } F(x) \succeq 0 \text{ and } \text{rank}(F(x)) \geq t; \\ -\infty, & \text{otherwise.} \end{cases} \end{aligned}$$

Finally, we analytically characterize the infimum in (6) in Theorem 12. Its proof follows from the fact that a linear function is bounded below only when it is identically zero.

► **Theorem 12.** For $(x, y, w) \in \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^m$, we have

$$\begin{aligned} & \inf_{\nu, \pi, \tau} \nu^\top (\mathbf{e} - x - y) + \pi^\top (b - Ax - w) + \tau (s - \mathbf{e}^\top x) \\ &= \begin{cases} 0, & \text{if } \mathbf{e} - x - y = 0, \quad b - Ax - w = 0, \quad s - \mathbf{e}^\top x = 0; \\ -\infty, & \text{otherwise.} \end{cases} \end{aligned}$$

Considering Theorems 11 and 12, the Lagrangian dual of [DGFact](#) is equivalent to

$$(DDGFact) \quad z_{DDGFact}(C, s, t, A, b; F) = \max \{ \Gamma_t(F(x)) : \mathbf{e}^\top x = s, Ax \leq b, 0 \leq x \leq \mathbf{e} \},$$

From Lagrangian duality, we have that [DDGFact](#) is a convex program. Moreover, because [DGFact](#) has a strictly feasible solution, if [DDGFact](#) has a feasible solution with finite objective value, then we have strong duality between [DDGFact](#) and [DGFact](#).

Finally, for developing a nonlinear-programming algorithm for [DDGFact](#), we consider in the next theorem, an expression for the gradient of its objective function. The proof is similar to the one presented for MESP in [8, Theorem 2.10].

► **Theorem 13.** Let $F(\hat{x}) = \sum_{\ell=1}^k \hat{\lambda}_\ell \hat{u}_\ell \hat{u}_\ell^\top$ be a spectral decomposition of $F(\hat{x})$. Let \hat{i} be the value of ι in Lemma 10, where λ in Lemma 10 is $\hat{\lambda} := \lambda(F(\hat{x}))$. If $\frac{1}{t - \hat{i}} \sum_{\ell=\hat{i}+1}^k \hat{\lambda}_\ell > \hat{\lambda}_{\hat{i}+1}$, then, for $j = 1, 2, \dots, n$,

$$\frac{\partial}{\partial x_j} \Gamma_t(F(\hat{x})) = \sum_{\ell=1}^{\hat{i}} \frac{1}{\hat{\lambda}_\ell} (F_j \cdot \hat{u}_\ell)^2 + \sum_{\ell=\hat{i}+1}^k \frac{t - \hat{i}}{\sum_{i=\hat{i}+1}^k \hat{\lambda}_i} (F_j \cdot \hat{u}_\ell)^2.$$

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As observed in [8], without the technical condition $\frac{1}{t-i} \sum_{\ell=i+1}^k \hat{\lambda}_\ell > \hat{\lambda}_{i+1}$, the formulae above still give a subgradient of Γ_t (see [19]).

As mentioned above, by replacing $0 \leq x \leq \mathbf{e}$ by $x \in \{0, 1\}^n$ in **GFact**, we get an exact but non-convex MINLO formulation for **CGMESP**. On the other hand, replacing $0 \leq x \leq \mathbf{e}$ by $x \in \{0, 1\}^n$ in **DDGFact**, we get a convex formulation for **CGMESP**, which is non-exact generally, except for the important case of $t = s$ when it becomes exact. In Theorem 15, we present properties of the function ϕ defined in (8), which show that the relaxation is non-exact for $t < s$ and exact for $t = s$. In Lemma 14 we prove the relevant facts for their understanding.

► **Lemma 14.** *Let $\lambda \in \mathbb{R}_+^n$ with $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_\delta > \lambda_{\delta+1} = \dots = \lambda_r > \lambda_{r+1} = \dots = \lambda_n = 0$. Then,*

- (a) *For $t = r$, the ι satisfying (7) is precisely δ .*
- (b) *For $r < t \leq n$, the ι satisfying (7) is precisely r .*

Proof For (a), the result follows because

$$\frac{1}{r-\delta} \sum_{\ell=\delta+1}^n \lambda_\ell = \lambda_{\delta+1} \quad \text{and} \quad \lambda_\delta > \lambda_{\delta+1}.$$

For (b), the result follows because

$$\frac{1}{t-r} \sum_{\ell=r+1}^n \lambda_\ell = 0 = \lambda_{r+1} \quad \text{and} \quad \lambda_r > \lambda_{r+1}.$$

◀

► **Theorem 15.** *Let $\lambda \in \mathbb{R}_+^n$ with $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_r > \lambda_{r+1} = \dots = \lambda_n = 0$. Then,*

- (a) $\phi_t(\lambda) > \sum_{\ell=1}^t \log(\lambda_\ell)$, for $0 < t < r$,
- (b) $\phi_t(\lambda) = \sum_{\ell=1}^t \log(\lambda_\ell)$, for $t = r$,
- (c) $\phi_t(\lambda) = -\infty$, for $r < t \leq n$.

where we use $\log(0) = -\infty$.

Proof Part (a) follows from:

$$(t - \iota) \log \left(\frac{1}{t - \iota} \sum_{\ell=\iota+1}^n \lambda_\ell \right) > (t - \iota) \log \left(\frac{1}{t - \iota} \sum_{\ell=\iota+1}^t \lambda_\ell \right) \geq (t - \iota) \left(\frac{\sum_{\ell=\iota+1}^t \log(\lambda_\ell)}{t - \iota} \right).$$

Parts (b) and (c) follow from Lemma 14. ◀

► **Remark 16.** *We can conclude that $z(C, s, t, A, b; F) \leq z_{\text{DDGFact}}(C, s, t, A, b; F)$ from the use of Lagrangian duality. But we note that Theorem 15 gives an alternative and direct proof for this result, besides showing in part (a), that the inequality is strict whenever the rank of any optimal submatrix $C[S, S]$ for **CGMESP** is greater than t .*

Finally, we note that to apply the variable-fixing procedure described in Theorem 9 in a B&B algorithm to solve **CGMESP**, we need a feasible solution for **DGFact**. To avoid wrong variable fixing by using dual information from near-optimal solutions to **DDGFact**, we will show how to construct a rigorous feasible solution for **DGFact** from a feasible solution \hat{x} of **DDGFact** with finite objective value, with the goal of producing a small gap.

Although in **CGMESP**, the lower and upper bounds on the variables are zero and one, we will derive the construction of the dual solution considering the more general problem with

lower and upper bounds on the variables given respectively by l and u , that is, we consider the constraints $l \leq x \leq u$ in **DDGFact**, instead of $0 \leq x \leq \mathbf{e}$. The motivation for this, is to derive the technique to fix variables at any subproblem considered during the execution of the B&B algorithm, when some of the variables may already be fixed. Instead of redefining the problem with less variables in our numerical experiments, we found it more efficient to change the upper bound u_i from one to zero, when variable i is fixed at zero in a subproblem, and similarly, change the lower bound l_i from zero to one, when variable i is fixed at one.

We consider the spectral decomposition $F(\hat{x}) = \sum_{\ell=1}^k \hat{\lambda}_\ell \hat{u}_\ell \hat{u}_\ell^\top$, with $\hat{\lambda}_1 \geq \hat{\lambda}_2 \geq \dots \geq \hat{\lambda}_{\hat{r}} > \hat{\lambda}_{\hat{r}+1} = \dots = \hat{\lambda}_k = 0$. Notice that $\text{rank}(F(\hat{x})) = \hat{r} \geq t$. Following [20], we set $\hat{\Theta} := \sum_{\ell=1}^k \hat{\beta}_\ell \hat{u}_\ell \hat{u}_\ell^\top$, where

$$(9) \quad \hat{\beta}_\ell := \begin{cases} 1/\hat{\lambda}_\ell, & 1 \leq \ell \leq \hat{i}; \\ 1/\hat{\delta}, & \hat{i} < \ell \leq \hat{r}; \\ (1 + \epsilon)/\hat{\delta}, & \hat{r} < \ell \leq k, \end{cases}$$

for any $\epsilon > 0$, where \hat{i} is the unique integer defined in Lemma 10 for $\lambda_\ell = \hat{\lambda}_\ell$, and $\hat{\delta} := \frac{1}{t-\hat{i}} \sum_{\ell=\hat{i}+1}^k \hat{\lambda}_\ell$. From Lemma 10, we have that $\hat{i} < t$. Then,

$$(10) \quad -\sum_{\ell=1}^t \log(\hat{\beta}_\ell) = \sum_{\ell=1}^{\hat{i}} \log(\hat{\lambda}_\ell) + (t - \hat{i}) \log(\hat{\delta}) = \Gamma_t(F(\hat{x})).$$

Therefore, the minimum duality gap between \hat{x} in **DDGFact** and feasible solutions of **DGFact** of the form $(\hat{\Theta}, v, \nu, \pi, \tau)$ is the optimal value of

$$(G(\hat{\Theta})) \quad \begin{aligned} & \min \quad -v^\top l + \nu^\top u + \pi^\top b + \tau s - t \\ & \text{subject to:} \quad v - \nu - A^\top \pi - \tau \mathbf{e} = -\text{diag}(F\hat{\Theta}F^\top), \\ & \quad \quad \quad v \geq 0, \nu \geq 0, \pi \geq 0. \end{aligned}$$

We note that $G(\hat{\Theta})$ is always feasible (e.g., $v := 0, \nu := \text{diag}(F\hat{\Theta}F^\top), \pi := 0, \tau := 0$). Also, $G(\hat{\Theta})$ has a simple closed-form solution for **GMESP**, that is when there are no $Ax \leq b$ constraints. To construct this optimal solution, we consider the permutation σ of the indices in N , such that $\text{diag}(F\hat{\Theta}F^\top)_{\sigma(1)} \geq \dots \geq \text{diag}(F\hat{\Theta}F^\top)_{\sigma(n)}$. If $u_{\sigma(1)} + \sum_{i=2}^n l_{\sigma(i)} > s$, we let $\varphi := 0$, otherwise we let $\varphi := \max\{j \in N : \sum_{i=1}^j u_{\sigma(i)} + \sum_{i=j+1}^n l_{\sigma(i)} \leq s\}$. We define $P := \{\sigma(1), \dots, \sigma(\varphi)\}$ and $Q := \{\sigma(\varphi+2), \dots, \sigma(n)\}$. Then, we can verify that the following solution is optimal for $G(\hat{\Theta})$ when there are no side constraints (see the full version [22] for the proof of optimality of the solution).

$$\begin{aligned} \tau^* &:= \text{diag}(F\hat{\Theta}F^\top)_{\sigma(\varphi+1)}, \\ \nu_\ell^* &:= \begin{cases} \text{diag}(F\hat{\Theta}F^\top)_\ell - \tau^*, & \text{for } \ell \in P; \\ 0, & \text{otherwise,} \end{cases} \\ v_\ell^* &:= \begin{cases} \tau^* - \text{diag}(F\hat{\Theta}F^\top)_\ell, & \text{for } \ell \in Q; \\ 0, & \text{otherwise.} \end{cases} \end{aligned}$$

Although we are not able to prove the following conjecture concerning the dual solution for **DGFact** constructed as described above, it was supported by our numerical experiments. The conjecture is open even for the special cases of **MESP** and **binary D-Opt**.

► **Conjecture 17.** *Considering **GMESP**, that is, considering the case when there are no $Ax \leq b$ constraints, if \hat{x} is an optimal solution to **DDGFact**, then $(\hat{\Theta}, v^*, \nu^*, \tau^*)$ is an optimal solution to **DGFact**.*

4 Experiments

Our initial experiments are only for [GMESP](#). For all instances, we use a benchmark covariance matrix of dimension $n = 63$, originally obtained from J. Zidek (University of British Columbia), coming from an application for re-designing an environmental monitoring network; see [10] and [11]. This matrix has been used extensively in testing and developing algorithms for MESP; see [13, 15, 4, 17, 11, 5, 6, 1, 2, 7, 8].

4.1 Lower bounds

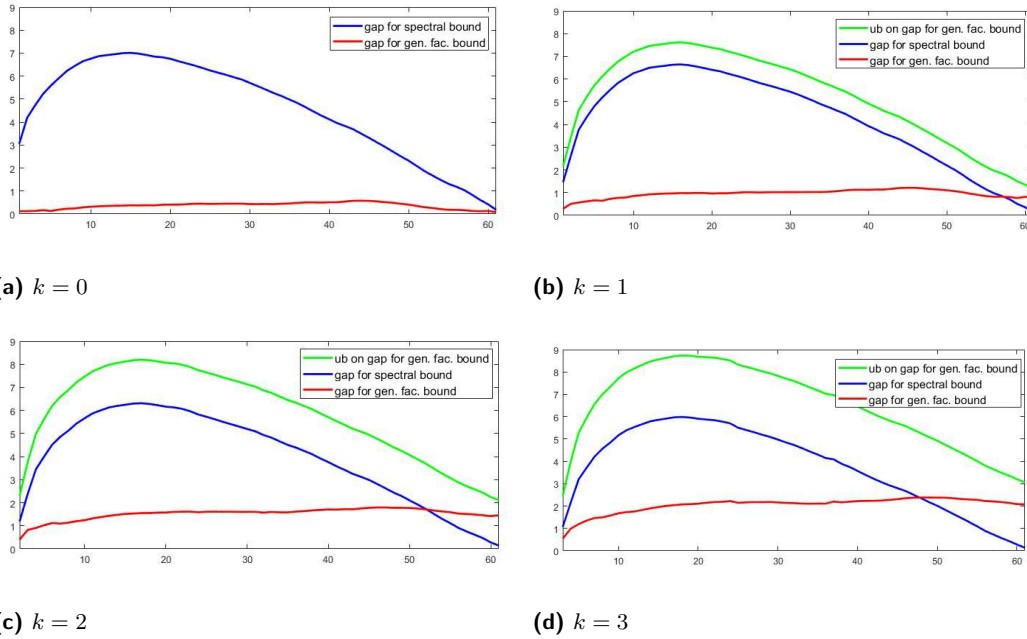
To get an idea of the performance of upper bounds, we wish to present gaps to good lower bounds. For good lower bounds for [GMESP](#), we carry out an appropriate local search, in the spirit of [13, Sec. 4], starting from various good feasible solutions. Our local search is classical: Starting from some S with $|S| = s$, we iteratively replace S with $S + j - i$ when $\prod_{\ell=1}^t \lambda_\ell(C[S + j - i, S + j - i]) > \prod_{\ell=1}^t \lambda_\ell(C[S, S])$. We return at the end $x(S)$, the characteristic vector of S .

We have three methods for generating initial solutions for the local search.

- *Rounding a continuous solution.* Let $\lambda_\ell(C)$ be the ℓ -th greatest eigenvalue of C , and u_ℓ be the corresponding eigenvector, normalized to have Euclidean length 1. We define $\bar{x} \in \mathbb{R}^n$ by $\bar{x}_j := \sum_{\ell=1}^t u_{\ell j}^2$. It is easy to check (similar to [15, Sec. 3]) that $0 \leq \bar{x} \leq \mathbf{e}$ and $\mathbf{e}^\top \bar{x} = t$. Next, we simply choose S to comprise the indices j corresponding to the s biggest \bar{x}_j ; we note that this rounding method can be adapted to [CGMESP](#), by instead solving a small integer linear optimization problem (see [15, Sec. 4]).
- *Greedy.* Starting from $S := \emptyset$, we identify the element $j \in N \setminus S$ that maximizes the product of the $\min\{t, |S| + 1\}$ biggest eigenvalues of $C[S + j, S + j]$. We let $S := S + j$, and we repeat while $|S| < s$.
- *Dual greedy.* Starting from $S := N$, we identify the element $j \in S$ that maximizes the product of the t biggest eigenvalues of $C[S - j, S - j]$. We let $S := S - j$, and we repeat while $|S| > s$.

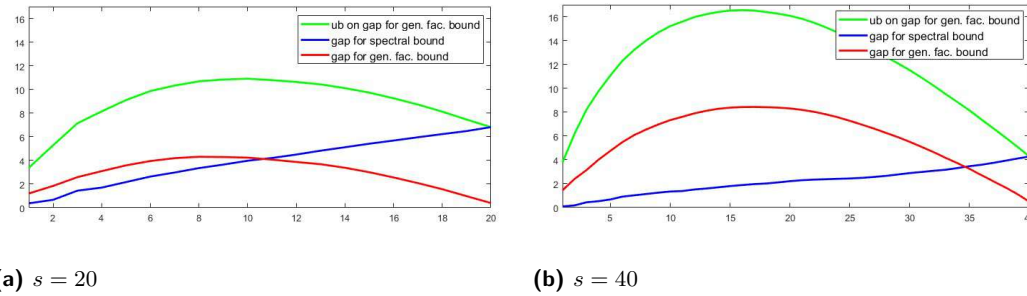
4.2 Behavior of upper bounds

To analyze the generalized factorization bound for [GMESP](#) and compare it to the spectral bound, we conducted two experiments using our covariance matrix with $n = 63$. In the first experiment, for each integer k from 0 to 3, we consider the instances obtained when we vary s from $k + 1$ to 61, and set $t := s - k$. In Figure 1, we depict for each k , the gaps given by the difference between the lower bounds for [GMESP](#) computed as described in §4.1, and the generalized factorization bound and the spectral bound for each pair $(s, t := s - k)$. We also depict the upper bound on the gap for the generalized factorization bound determined in Theorem 6, specifically given by the gap for the spectral bound added to $t \log(s/t)$. When $k = 0$ (instances of MESP), $t \log(s/t)$ is zero, confirming that the generalized factorization bound dominates the spectral bound as already proved in [8]. When k increases, the generalized factorization bound becomes weaker and gets worse than the spectral bound when s and t get large enough. Nevertheless, the generalized factorization bound is still much stronger than the spectral bound for most of the instances considered, and we see that the upper bound on it given in Theorem 6 is, in general, very loose, specially for $s \in [10, 20]$. The variation on the gaps for generalized factorization bounds for the different values of s is very small when compared to the spectral bound, showing its robustness.



■ **Figure 1** Gaps, varying $t = s - k$ ($n = 63$)

In the second experiment, for $s = 20$ and $s = 40$, we consider the instances obtained when we vary t from 1 to s . Similarly to what we show in Figure 1, in Figure 2 we show the gaps for each instance, and the upper bound on the gap corresponding to the generalized factorization bound.



■ **Figure 2** Gaps, varying t , with s fixed ($n = 63$)

In both plots in Figure 2, we see that after a certain value of t , the generalized factorization bound becomes stronger than the spectral bound. The interval for t on which the generalized factorization bound is stronger is bigger when $s = 20$. The last two observations are expected. We note that from the formulae to calculate the bounds, the spectral bound does not take s into account, so it should become worse as s becomes smaller, compared to the dimension of C , and the generalized factorization bound take into account all the s eigenvalues of the submatrix of C , so it should become worse as t becomes smaller, compared to s . When $t = s$, we see again in both plots that the generalized factorization bound dominates the spectral bound. We observe that the bound on the gap for the generalized factorization bound is

always very loose for the values of s considered. The plots confirm the analysis in Figure 1, showing now, for fixed s , that the generalized factorization bound becomes more promising when the difference between t and s is small.

4.3 Branch-and-bound

We coded a B&B algorithm using the generalized factorization bound and initializing it with the lower bound computed as described in §4.1. Branching is the standard fixing of a variable at 0 or 1 for the two child subproblems. We never create child subproblems if there is a unique feasible solution of a subproblem relaxation. For GMESP (no side constraints), such a solution will always be integer; for CGMESP, details on how to handle this are in [4, Sec. 4].

Because DDGFact is not an exact relaxation, we have to make some accommodations that are not completely standard for B&B. When we get an *integer optimum* solution \bar{x} for a relaxed subproblem: (i) if the objective value of the relaxation of the subproblem being handled is above the lower bound, then we have to create child subproblems; (ii) we have to evaluate the true objective value of \bar{x} in CGMESP, to determine if we should increase the lower bound.

We ran our B&B experiments on a 16-core machine (running Windows Server 2016 Standard): two Intel Xeon CPU E5-2667 v4 processors running at 3.20GHz, with 8 cores each, and 128 GB of memory. We coded our algorithms in Julia v.1.9.0. To solve the convex relaxation DDGFact, we apply Knitro v0.13.2. To solve GMESP, we employ the B&B algorithm in Juniper [14].

In Table 1, we present statistics for the B&B applied to instances where C is the leading principal submatrix of order 32 of our 63-dimensional covariance matrix and s varies from 2 to 31. For each s , we solve an instance of GMESP with $t = s - 1$ and an instance of MESP ($t = s$). For all instances, the initial lower bounds computed were optimal, so the B&B worked on proving optimality by decreasing the upper bound. In the first column of Table 1, we show s , and in the other columns, we show the following statistics for GMESP and MESP: the initial gap given by difference between the upper and lower bounds at the root node (root gap), the number of convex relaxations solved (nodes), the number of nodes pruned by bound (pruned bound), the number of variables fixed at 0 (1) by the procedure described in Theorem 9 (var fix 0 (1)), and the elapsed time (in seconds) for the B&B (B&B time). We observe that the difficulty of the problem significantly increases when t becomes smaller than s as the upper bounds become weaker, confirming the analysis of Figure 1. Nevertheless, the largest root gap for GMESP is about one, and we can solve all the instances in a time limit of 36,000 seconds. The quality of the generalized factorization bound for these instances of GMESP can be evaluated by the number of nodes pruned by bound in the B&B. For the most difficult instances (that took more than 9,000 seconds to be solved), about 20% of the nodes were pruned by bound. Moreover, we see that the generalized factorization bound led to an effective application of the variable-fixing procedure described in Theorem 9.

5 Outlook

We are left with some clear challenges. A key one is to obtain better upper bounds when $s - t$ is large, in hopes of exactly solving GMESP instances by B&B in such cases. In connection with this, we would like a bound that provably dominates the spectral bound (when $t < s$), improving on what we established with Theorem 6.

s	GMESP ($t := s-1$)						MESP ($t := s$)					
	root gap	nodes	pruned bound	var fix 0	var fix 1	B&B time	root gap	nodes	pruned bound	var fix 0	var fix 1	B&B time
2	0.362	186	1	75	6	4.44	0.018	3	2	0	0	0.10
3	0.481	556	14	269	25	12.23	0.058	10	5	52	0	0.38
4	0.594	2048	97	1048	118	45.13	0.120	20	8	55	0	0.84
5	0.699	7385	578	2755	461	169.19	0.129	33	13	58	0	1.03
6	0.731	20766	2183	6826	1599	485.59	0.136	43	16	60	0	1.98
7	0.764	44714	5617	13473	4256	1080.51	0.139	37	14	53	0	1.34
8	0.772	69698	10267	21241	8498	1724.88	0.131	41	16	55	0	1.64
9	0.819	122251	22159	37011	18860	3118.86	0.120	38	15	45	0	1.22
10	0.821	163172	36421	54719	35618	4357.91	0.105	37	17	49	0	1.55
11	0.766	153960	39114	60981	50312	4279.61	0.055	16	8	33	0	0.66
12	0.718	165197	45035	71148	78156	4803.73	0.087	46	21	42	0	2.53
13	0.643	149194	40905	68837	91655	4540.02	0.116	111	49	80	0	5.75
14	0.676	286992	74606	129539	212899	9305.94	0.132	196	83	131	0	10.03
15	0.687	395037	96495	172151	325528	13648.43	0.134	185	81	95	0	10.54
16	0.691	428858	100016	178025	403619	15648.41	0.162	323	149	136	0	16.21
17	0.730	527963	115637	199472	544694	20474.81	0.183	305	140	107	0	16.04
18	0.755	549759	115105	187981	605389	21764.31	0.249	878	391	302	0	40.46
19	0.825	718108	139610	209843	768122	30414.64	0.282	1105	489	380	0	49.41
20	0.862	698011	126972	172900	744406	29224.02	0.320	1421	612	451	0	61.18
21	0.899	639993	109147	131023	672592	25874.41	0.366	2139	852	784	1	90.63
22	0.946	588140	93020	96706	609421	23362.49	0.392	2342	857	808	5	96.33
23	0.992	511571	75387	64191	525923	19582.83	0.388	1812	661	572	0	75.01
24	1.014	369489	51736	35100	388666	13415.42	0.361	1244	463	340	0	51.12
25	1.008	215042	28289	15379	240224	7375.81	0.306	632	230	130	0	24.88
26	0.965	98765	12020	5083	121596	3193.55	0.270	463	160	65	0	17.59
27	0.951	43052	4795	1410	58964	1407.34	0.215	241	74	30	0	8.55
28	0.912	13854	1368	234	22591	451.56	0.168	130	38	10	0	4.58
29	0.900	3404	282	20	6547	112.30	0.134	70	16	4	0	2.77
30	0.873	464	27	1	949	15.45	0.083	19	4	1	0	0.59
31	0.832	32	1	0	30	0.99	0.023	2	1	0	0	0.07

■ **Table 1** Results for B&B with variable fixing

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