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Mixing convex-optimization bounds for maximum-entropy sampling

Zhongzhu Chen · Marcia Fampa ·
Amélie Lambert · Jon Lee

February 3, 2020

Abstract The maximum-entropy sampling problem is a fundamental and challenging combinatorial-optimization problem, with application in spatial statistics. It asks to find a maximum-determinant order- s principal submatrix of an order- n covariance matrix. Exact solution methods for this NP-hard problem are based on a branch-and-bound framework. Many of the known upper bounds for the optimal value are based on convex optimization. We present a methodology for “mixing” these bounds to achieve better bounds.

Keywords maximum-entropy sampling · convex optimization

Mathematics Subject Classification (2000) 90C25 · 90C27 · 90C51 · 62K99 · 62H11

Introduction

Let C be an order- n (symmetric) positive-definite real matrix, and let s be an integer satisfying $1 \leq s \leq n$. Let $N := \{1, 2, \dots, n\}$. We interpret C as the covariance matrix for a multivariate Gaussian random vector Y_N . For nonempty $S \subseteq N$, let $C[S, S]$ denote the principle submatrix of C indexed by S . We

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denote $\log \det(\cdot)$ by $\text{ldet}(\cdot)$. Up to constants, $\text{ldet } C[S, S]$ is the (differential) entropy associated with the subvector Y_S . The *maximum-entropy sampling problem* (MESP) is

$$z(C, s) := \max \{ \text{ldet } C[S, S] : |S| = s, S \subseteq N \}$$

(see [SW87]).

MESP is NP-hard (see [KLQ95]), and the main paradigm for exact solution of moderate-sized instances is branch-and-bound (see [KLQ95]). In this context, there has been considerable work on efficiently calculating good upper bounds for MESP; see [KLQ95, AFLW96, AFLW99, HLW01, LW03, AL04, BL07, Ans18b, Ans18a], the survey [Lee12], and the closely related works [LL19, AFLW01].

A very relevant point for us is the following identity:

$$\det C[S, S] = \det C \times \det C^{-1}[\bar{S}, \bar{S}],$$

where \bar{S} denotes the complement of S in $\{1, 2, \dots, n\}$. With this identity, we have $z(C, s) = \text{ldet } C + z(C^{-1}, n - s)$, and so upper bounds for $z(C^{-1}, n - s)$ yield upper bounds for $z(C, s)$, shifting by $\text{ldet } C$. This idea gives something for bounds that are *not* invariant under complementation (see [AFLW99, HLW01, LW03, AL04, Ans18b]). It does not give us anything for bounds that are invariant under complementation (see [KLQ95, Ans18a]).

In §1, we describe a very simple general idea for “mixing” bounds. In §2, we apply the simple idea to MESP by mixing the so-called “BQP bound” (see [Ans18b]) with the same bound applied to the complementary problem. In §3, we mix the so-called “NLP bound” (see [AFLW99]) with the same bound applied to the complementary problem. Because the BQP bound and the NLP bound are not invariant under complementation, we can get improved bounds with these mixings. In §4, we look at tuning the so-called “linx bound” (see [Ans18a]). In §5, we investigate mixing the NLP bound (or its complement) with a “non-NLP bound” (e.g., the linx bound, the BQP bound, or the complementary BQP bound). In §6, we make some concluding remarks.

Throughout, when we carry out computational experiments with the BQP bound, the complementary BQP bound, and the linx bound, we use SDPT3 (see [TTT99, TTT12]) via Matlab and Yalmip (a Matlab toolbox for optimization; see [Löf04]). SDPT3 has an efficient way of handling ldet , and this functionality is exposed via Yalmip (not, at this writing, by CVX). But when we work with the NLP bound, we employ our own tailored interior-point solver.

Further notation: We denote transpose of a vector x by x' , and likewise for matrices. $S^n(\mathbb{R})$ denotes the set of real order- n symmetric matrices. $A \circ B$ denotes Hadamard (element-wise) product of compatible matrices A and B , while $A \bullet B := \text{Trace}(AB')$ denotes the matrix dot-product. For $X \in \mathbb{R}^{n \times n}$, $\text{Diag}(X) := (X_{1,1}, X_{2,2}, \dots, X_{n,n})' \in \mathbb{R}^n$. For $x \in \mathbb{R}^n$, $\text{diag}(x) \in \mathbb{R}^{n \times n}$ is defined by $\text{diag}(x)_{i,i} := x_{i,i}$ and $\text{diag}(x)_{i,j} := 0$ for $i \neq j$.

1 General mixing

The idea is so simple that we do not dare claim that it is original. We are however confident that it is new in the context of the MESP. In this section, we describe the general idea.

We start with a combinatorial maximization problem

$$z := \max\{f(S) : S \in \mathcal{F}\},$$

where \mathcal{F} is an arbitrary subset of the power set of $\{1, 2, \dots, n\}$. We consider m upper bounds for z based on convex relaxations in a possibly lifted space of variables.

As is standard, for $x \in \mathbb{R}^n$, we denote the *support* of x by $\underline{x} := \{i \in \{1, 2, \dots, n\} : x_i \neq 0\}$. Also, if $x \in \{0, 1\}^n$, then x is the *characteristic vector* of \underline{x} .

For $i = 1, 2, \dots, m$, the convex set \mathcal{P}_i uses variables (x, \mathcal{X}^i) . The vector $x \in [0, 1]^n$ relaxes $x \in \{0, 1\}^n$ and is used to model \mathcal{F} . Specifically, we assume that if we project \mathcal{P}_i onto \mathbb{R}^n , we get a subset of $[0, 1]^n$, and then if we intersect with \mathbb{Z}^n , we get precisely the characteristic vectors of \mathcal{F} . Next, for $i = 1, 2, \dots, m$, we have a concave function f_i , taking $(x, \mathcal{X}^i) \in \mathcal{P}_i$ to \mathbb{R} . We assume that for $(x, \mathcal{X}^i) \in \mathcal{P}_i$ such that $x \in \mathbb{Z}^n$, we have $f_i(x, \mathcal{X}^i) = f(\underline{x})$. In this sense, each \mathcal{P}_i is an *exact relaxation* (possibly in an extended space) of $\text{conv}(\{x \in \mathbb{R}^n : \underline{x} \in \mathcal{F}\})$.

Now, for $i = 1, 2, \dots, m$, we have the convex programs

$$v_i := \max\{f_i(x, \mathcal{X}^i) : (x, \mathcal{X}^i) \in \mathcal{P}_i\},$$

yielding m upper bounds on z .

Next, for $\alpha \in \mathbb{R}^m$, such that $\alpha \geq 0$, $e'\alpha = 1$, we define the *mixing bound*

$$v(\alpha) := \max\left\{\sum_{i=1}^m \alpha_i f_i(x, \mathcal{X}^i) : (x, \mathcal{X}^i) \in \mathcal{P}_i, 1 = 1, 2, \dots, m\right\}.$$

The following is very simple to establish.

Proposition 1 The function $v(\alpha)$ is convex on $\{\alpha \in \mathbb{R}^m : \alpha \geq 0\}$, and for all $\alpha \in \mathbb{R}^m$ such that $e'\alpha = 1$, we have $v(\alpha) \geq z$.

Owing to this, a natural goal is to minimize the convex $v(\alpha)$, over $\{\alpha \in \mathbb{R}^m : e'\alpha = 1, \alpha \geq 0\}$. *The power of the mixing bound is that the same variable x is appearing in each of the \mathcal{P}_i .* If it were not for this, then the minimum value of $v(\alpha)$, over $\{\alpha \in \mathbb{R}^m : e'\alpha = 1, \alpha \geq 0\}$, would trivially be $\max_{i=1}^m v_i$.

Of course each \mathcal{P}_i can be strengthened to improve the mixing bound. But very importantly, we note that the mixing bound can be strengthened by introducing valid equations and inequalities across the entire variable space: $x, \mathcal{X}_1, \dots, \mathcal{X}_m$. We exploit both of these observations in the next section.

Before continuing, we wish to mention that a slightly different formulation for finding an optimal mixing is as the following convex program.

$$\begin{aligned}
& \max v \\
& \text{subject to:} \\
& v \leq f_i(x, \mathcal{X}^i), \quad i = 1, 2, \dots, m; \\
& (x, \mathcal{X}^i) \in \mathcal{P}_i, \quad i = 1, 2, \dots, m.
\end{aligned}$$

The equivalence can easily be seen by Lagrangian duality. We prefer our formulation because by aggregating the nonlinearities into the objective, in the style of a surrogate dual, we get a formulation that is more easily handled by solvers and more easily optimized in terms of selecting good mixing (and other bound) parameters. Related to this, in the context of branch-and-bound, we can expect that child subproblems will be able to inherit good parameters from their parents, leading to faster computations.

2 Mixing the BQP bound with the complementary BQP bound

In this section, we apply the simple mixing idea from §1, mixing the (scaled) BQP bound for MESP (see [Ans18b]) with the same bound applied to the complementary problem. We will see that minimizing this bound over α gives us a bound that is sometimes stronger than the two bounds that it is based upon — it is always at least as strong. In fact, we will see that the bound will tend to be stronger when the two bounds being mixed have similar values.

2.1 Mixing BQP and its complement

Let

$$\begin{aligned}
P(n, s) & := \{(x, X) \in \mathbb{R}^n \times S^n(\mathbb{R}) : \\
& \quad X - xx' \succeq 0, \quad \text{Diag}(X) = x, \quad e'x = s, \quad Xe = sx\} \\
Q(n, n-s) & := \{(y, Y) \in \mathbb{R}^n \times S^n(\mathbb{R}) : \\
& \quad Y - yy' \succeq 0, \quad \text{Diag}(Y) = y, \quad e'y = n-s, \quad Ye = (n-s)y\}.
\end{aligned}$$

The set $P(n, s)$ (respectively, $Q(n, n-s)$) is the well-known SDP relaxation of the binary solutions to $X - xx' = 0$, $e'x = s$ (respectively, $Y - yy' = 0$, $e'y = n-s$).

We introduce the *mixed BQP (mBQP) bound*:

$$\begin{aligned}
v(C, s; \alpha, \gamma_1, \gamma_2) & := \\
& \max (1 - \alpha) (\text{l det}(\gamma_1 C \circ X + I - \text{diag}(x)) - \text{s log} \gamma_1) \\
& \quad + \alpha (\text{l det}(\gamma_2 C^{-1} \circ Y + I - \text{diag}(y)) - (n-s) \text{log} \gamma_2 + \text{l det} C), \\
& \text{subject to:} \\
& (x, X) \in P(n, s), \quad (y, Y) \in Q(n, n-s), \quad x + y = e,
\end{aligned}$$

where $0 \leq \alpha \leq 1$ is a “weighting” parameter, and $\gamma_1, \gamma_2 > 0$ are “scaling parameters”. We will see that this mBQP bound is a manifestation of the idea from §1, mixing the scaled BQP bound with its complement.

It is almost immediate that the mBQP bound is a mixing in the precise sense of §1, but because of the way that we have formulated it with different variables for the complementary part, there is a little checking to do.

We define an invertible linear map Φ by

$$\Phi(x, X) = (e - x, X + ee' - ex' - xe').$$

Notice that if $(\hat{y}, \hat{Y}) := \Phi(\hat{x}, \hat{X})$, then $\hat{Y}_{ij} = \hat{X}_{ij} + 1 - \hat{x}_j - \hat{x}_i$.

We have the following useful result.

Lemma 2 $(\hat{x}, \hat{X}) \in P(n, s)$ if and only if $\Phi(\hat{x}, \hat{X}) \in Q(n, n - s)$.

Proof We check the constraints:

$$\hat{Y} - \hat{y}\hat{y}' = \hat{X} + ee' - e\hat{x}' - \hat{x}e' - (e - \hat{x})(e - \hat{x})' = \hat{X} - \hat{x}\hat{x}' \succeq 0'.$$

$$\text{Diag}(\hat{Y}) = \text{Diag}(\hat{X}) + \text{Diag}(ee') - \text{Diag}(e\hat{x}') - \text{Diag}(\hat{x}e') = \hat{x} + e - \hat{x} - \hat{x} = \hat{y}.$$

$$e'\hat{y} = e'(e - \hat{x}) = n - s.$$

$$\hat{Y}e = (\hat{X} + ee' - e\hat{x}' - \hat{x}e')e = s\hat{x} + ne - se - n\hat{x} = (n - s)(e - \hat{x}) = (n - s)\hat{y}.$$

The other direction is similar. \square

For $\alpha = 0$ and $\alpha = 1$, the mBQP reduces to the bounds of [Ans18b]¹:

Proposition 3 $v(C, s; \alpha = 0, \gamma_1, \gamma_2)$ is equal to the scaled BQP bound

$$-\log \gamma_1 + \max \text{ldet}(\gamma_1 C \circ X + I - \text{diag}(x)),$$

subject to:

$$(x, X) \in P(n, s),$$

and $v(C, s; \alpha = 1, \gamma_1, \gamma_2)$ is equal to the scaled complementary BQP bound

$$\text{ldet} C - (n - s)\log \gamma_2 + \max \text{ldet}(\gamma_2 C^{-1} \circ Y + I - \text{diag}(y))$$

subject to:

$$(y, Y) \in Q(n, n - s).$$

Proof When $\alpha = 0$, for any $(\hat{x}, \hat{X}) \in P(n, s)$, Lemma 2 allows us to always be able to choose a (\hat{y}, \hat{Y}) , which together with (\hat{x}, \hat{X}) is feasible for the mBQP optimization formulation. And because $\alpha = 0$, the choice of (\hat{y}, \hat{Y}) has no impact on the mBQP objective function. Similarly, when $\alpha = 1$, for any $(\hat{y}, \hat{Y}) \in Q(n, n - s)$, Lemma 2 allows us to always be able to choose a (\hat{x}, \hat{X}) which together with (\hat{y}, \hat{Y}) is feasible for the mBQP optimization formulation. And because $\alpha = 1$, the choice of (\hat{x}, \hat{X}) has no impact on the mBQP objective function. \square

¹ Helmberg suggested (essentially) the BQP bound in 1995 (see [Lee12, FL00]) to Anstreicher and Lee, but no one developed it at all until [Ans18b] did so extensively, drawing in and significantly extending some techniques from [AFLW99].

Of course we have

Proposition 4

$$z(C, s) \leq v(C, s; \alpha, \gamma_1, \gamma_2) .$$

We can see from the convexity of v that there is a good potential to improve on the minimum of the scaled BQP bound and the scaled complementary BQP bound precisely when these two bounds are similar. See Figure 1 where this is illustrated the well-known “ $n = 63$ ” benchmark covariance matrix. A simple univariate search can find a good value for α . Moreover, in the context of branch-and-bound for exact solution of the MESP, a good (starting) value of α can be inherited from a parent.

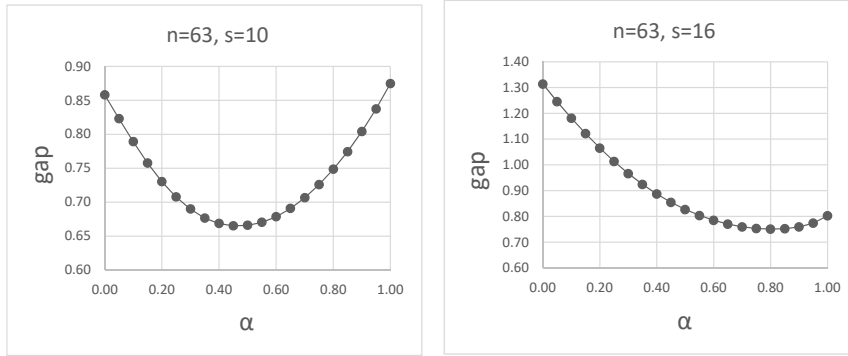


Fig. 1 Gap vs. α (optimized γ_i)

2.2 Valid equations in the extended spaces

Next, we will see that we can strengthen the mBQP bound, using equations that link the extended variables from the two bounds that we mix, and then even eliminate the variables (y, Y) .

Proposition 5

$$\begin{aligned}
 v(C, s; \alpha, \gamma_1, \gamma_2) &\geq \check{v}(C, s; \alpha, \gamma_1, \gamma_2) := \\
 &\max (1 - \alpha) (\text{ldet} (\gamma_1 C \circ X + I - \text{diag}(x)) - s \log \gamma_1) \\
 &\quad + \alpha (\text{ldet} (\gamma_2 C^{-1} \circ (X + ee' - ex' - xe') + I - \text{diag}(e - x)) \\
 &\quad \quad - (n - s) \log \gamma_2 + \text{ldet} C), \\
 &\text{subject to:} \\
 &\quad (x, X) \in P(n, s).
 \end{aligned}$$

The result follows from Lemma 2 and the following simple lemma.

Lemma 6 For the solutions of $x + y = e$, $X = xx'$, $Y = yy'$, the equations $Y = X + ee' - ex' - xe'$ are valid.

Proof Under $x + y = e$, we have that

$$0 = Y - yy' = Y - (e - x)(e - x)' = Y - ee' + ex' + xe' - xx'.$$

Subtracting $0 = X - xx'$, we obtain the desired equations. \square

We experimented further with the “ $n = 63$ ” covariance matrix. Considering now Figure 2, the unmixed bounds are indicated by the lines for “ $\alpha = 0$ ” and “ $\alpha = 1$ ”. We optimized the γ_i for these bounds (see §2.3). We chose an interesting range of s , where the unmixed bounds transition between which is stronger (i.e., the lines cross). The line indicated by “ α^* ” is the optimal mixing of the BQP bound and its complement. Note that we only optimized $v(C, s; \alpha, \gamma_1, \gamma_2)$ on α , keeping the optimal γ_i from the unmixed bounds. A (probably small) further improvement could be obtained by iterating between optimizing on α and the γ_i . The line indicated by “ α^* strengthened” is the optimal mixing of the BQP bound and its complement, but now with the valid equations in the extended space. Note that again we only optimized $\check{v}(C, s; \alpha, \gamma_1, \gamma_2)$ on α , keeping the optimal γ_i from the unmixed bounds.

We can seek to improve the mBQP bound by adding RLT, triangle and other inequalities, valid for the BQP, for both (x, X) and (y, Y) . We could do it directly (like [Ans18b]), but the conic-bundle method (see [FGRS06]) seems more promising, due to the large number of inequalities to be potentially exploited. So we dynamically include triangle inequalities via a bundle method; specifically we use the solver SDPT3 (see [TTT99]) together with the Conic Bundle Library (see [Hel19]) for solving the associated semidefinite programs, as described in [BELW17]. In the figure, the line “ α^* strengthened + triangles” indicates the bound obtained.

We repeated this experiment for a the well-known larger “ $n = 124$ ” benchmark covariance matrix. The results, exhibiting a similar behavior, are indicated in Figure 3. Note that in this figure, gaps are to a lower bound generated by a heuristic.

2.3 Choosing good parameters $(\alpha, \gamma_1, \gamma_2)$

Toward designing a reasonable algorithm for minimizing $\check{v}(C, s; \alpha, \gamma_1, \gamma_2)$, over $\alpha \in [0, 1]$ and $\gamma_1, \gamma_2 > 0$, we establish convexity properties.

2.3.1 Convexity properties

Theorem 7 For fixed $\gamma_1, \gamma_2 > 0$, the function $\check{v}(C, s; \alpha, \gamma_1, \gamma_2)$ is convex in $\alpha \in [0, 1]$. For fixed $\alpha \in [0, 1]$, the function $\check{v}(C, s; \alpha, \exp(\psi_1), \exp(\psi_2))$ is jointly convex in $(\psi_1, \psi_2) \in \mathbb{R}^2$.

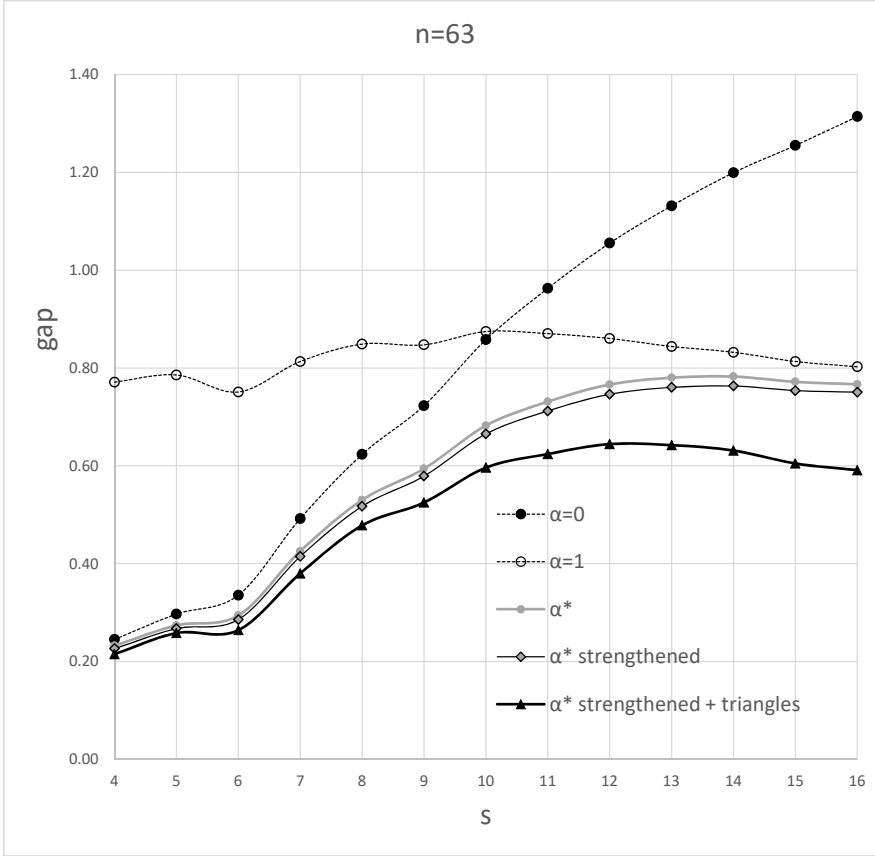


Fig. 2 Gap vs. s (optimized α and γ_i)

Proof We already know from general principles that our mixing bounds are convex in α . So in this section, we begin by establishing joint convexity in the logarithms of the scaling parameters γ_1, γ_2 .

Let

$$F_1(C, s; \gamma_1, (x, X)) := (\gamma_1 C - I) \circ X + I = \gamma_1 C \circ X + I - \text{diag}(x), \quad (1)$$

$$F_2(C, s; \gamma_2, (x, X)) := \gamma_2 C^{-1} \circ (X + ee' - ex' - xe') + \text{diag}(x), \quad (2)$$

$$f_1(C, s; \gamma_1, (x, X)) := \text{ldet } F_1(C, s; \gamma_1, (x, X)) - s \log \gamma_1,$$

$$f_2(C, s; \gamma_2, (x, X)) := \text{ldet } F_2(C, s; \gamma_2, (x, X)) - (n - s) \log \gamma_2 + \text{ldet } C,$$

$$f(C, s; \alpha, \gamma_1, \gamma_2, (x, X)) := (1 - \alpha)f_1(C, s; \gamma_1, (x, X)) + \alpha f_2(C, s; \gamma_2, (x, X)).$$

So, with this notation,

$$\check{v}(C, s; \alpha, \gamma_1, \gamma_2) = \max_{(x, X) \in P(n, s)} (1 - \alpha)f_1(C, s; \gamma_1, (x, X)) + \alpha f_2(C, s; \gamma_2, (x, X)).$$

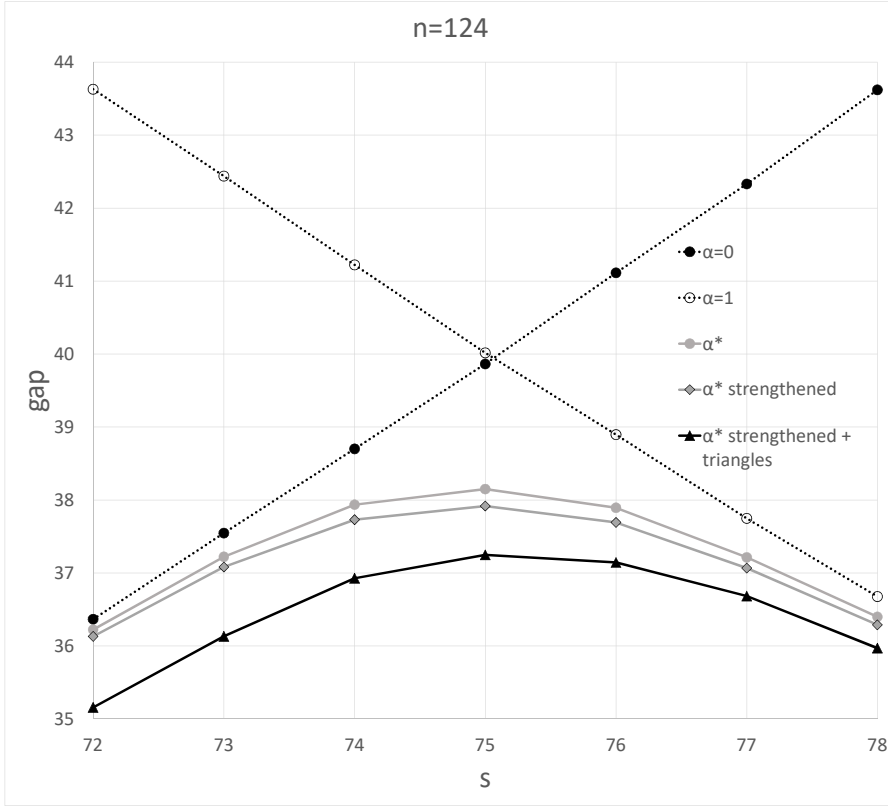


Fig. 3 Gap vs. s (optimized α and γ_i)

The function $\check{v}(C, s; \alpha, \exp(\psi_1), \exp(\psi_2))$ is the point-wise maximum of $f(C, s; \alpha, \exp(\psi_1), \exp(\psi_2), (x, X))$, over $(x, X) \in P(n, s)$. So it suffices to show that $f(C, s; \alpha, \exp(\psi_1), \exp(\psi_2), (x, X))$ is itself convex for each fixed $(x, X) \in P(n, s)$.

In what follows, for $i = 1, 2$, we use f_i as a short form for $f_i(C, s; \gamma_i, (x, X))$, and we use $F_i(\gamma_i, (x, X))$ as a short form for $F_i(C, s; \gamma_i, (x, X))$. We have

$$\begin{aligned}
 \frac{\partial f_1}{\partial \gamma_1} &= \frac{\partial}{\partial \gamma_1} (\text{ldet } F_1(\gamma_1, (x, X)) - s \log \gamma_1) \\
 &= \frac{\partial}{\partial \gamma_1} (\text{ldet}(\gamma_1 C \circ X + I - \text{diag}(x)) - s \log \gamma_1) \\
 &= F_1(\gamma_1, (x, X))^{-1} \bullet (C \circ X) - \frac{s}{\gamma_1} \\
 &= \frac{1}{\gamma_1} (F_1(\gamma_1, (x, X))^{-1} \bullet (\gamma_1 C \circ X) - s) \\
 &= \frac{1}{\gamma_1} (F_1(\gamma_1, (x, X))^{-1} \bullet F_1(\gamma_1, (x, X)) - F_1(\gamma_1, (x, X))^{-1} \bullet (I - \text{diag}(x)) - s)
 \end{aligned}$$

$$= \frac{1}{\gamma_1} (n - s - F_1(\gamma_1, (x, X))^{-1} \bullet (I - \text{diag}(x))) .$$

Letting $\psi_1 := \log \gamma_1$, by the chain rule we have

$$\frac{\partial f_1}{\partial \gamma_1} = \frac{\partial f_1}{\partial \psi_1} \frac{d\psi_1}{d\gamma_1} = \frac{\partial f_1}{\partial \psi_1} \frac{1}{\gamma_1} .$$

So we have

$$\frac{\partial f_1}{\partial \psi_1} = \gamma_1 \frac{\partial f_1}{\partial \gamma_1} = n - s - F_1(\exp(\psi_1), (x, X))^{-1} \bullet (I - \text{diag}(x)) =: g_1(\gamma_1) .$$

Next, we calculate

$$\begin{aligned} \frac{\partial^2 f_1}{\partial \gamma_1^2} &= \frac{\partial}{\partial \gamma_1} \left(\frac{1}{\gamma_1} (n - s - F_1(\gamma_1, (x, X))^{-1} \bullet (I - \text{diag}(x))) \right) \\ &= -\frac{1}{\gamma_1^2} (n - s - F_1(\gamma_1, (x, X))^{-1} \bullet (I - \text{diag}(x))) \\ &\quad + \frac{1}{\gamma_1} (e - x)' \text{diag}(F_1(\gamma_1, (x, X))^{-1} (C \circ X) F_1(\gamma_1, (x, X))^{-1}) . \end{aligned}$$

So we have

$$\begin{aligned} \gamma_1^2 \frac{\partial^2 f_1}{\partial \gamma_1^2} &= -n + s + F_1(\gamma_1, (x, X))^{-1} \bullet (I - \text{diag}(x)) \\ &\quad + \gamma_1 (e - x)' \text{diag}(F_1(\gamma_1, (x, X))^{-1} (C \circ X) F_1(\gamma_1, (x, X))^{-1}) . \end{aligned}$$

Finally, again taking $\psi_1 := \log \gamma_1$, using the chain rule we have

$$\begin{aligned} \frac{\partial^2 f_1}{\partial \psi_1^2} &= \frac{\partial g_1}{\partial \psi_1} = \gamma_1 \frac{\partial g_1}{\partial \gamma_1} = \gamma_1 \left(\frac{\partial f_1}{\partial \gamma_1} + \gamma_1 \frac{\partial^2 f_1}{\partial \gamma_1^2} \right) = \gamma_1 \frac{\partial f_1}{\partial \gamma_1} + \gamma_1^2 \frac{\partial^2 f_1}{\partial \gamma_1^2} \\ &= n - s - F_1(\exp(\psi_1), (x, X))^{-1} \bullet (I - \text{diag}(x)) \\ &\quad - n + s + F_1(\exp(\psi_1), (x, X))^{-1} \bullet (I - \text{diag}(x)) \\ &\quad + \exp(\psi_1) (e - x)' \text{diag}(F_1(\exp(\psi_1), (x, X))^{-1} (C \circ X) F_1(\exp(\psi_1), (x, X))^{-1}) \\ &= \exp(\psi_1) (e - x)' \text{diag}(F_1(\exp(\psi_1), (x, X))^{-1} (C \circ X) F_1(\exp(\psi_1), (x, X))^{-1}) . \end{aligned}$$

It remains to demonstrate that this last expression is nonnegative. We have $C \succ 0$ and $X \succeq 0$, and therefore $C \circ X \succeq 0$ (see [Zha05, page 175]). Then, it is also clear from (1) that $F_1(\exp(\psi_1), (x, X)) \succ 0$. Therefore

$$F_1(\exp(\psi_1), (x, X))^{-1} (C \circ X) F_1(\exp(\psi_1), (x, X))^{-1} \succeq 0 .$$

So we have

$$\frac{\partial^2 f_1}{\partial \psi_1^2} \geq 0 ,$$

and we can conclude that $f_1(\exp(\psi_1), (x, X))$ is convex in ψ_1 .

Similarly, $f_2(\exp(\psi_2), (x, X))$ is convex in ψ_2 . Finally, for fixed α and (x, X) , $F(\alpha, \exp(\psi_1), \exp(\psi_2), (x, X))$ is jointly convex in ψ_1 and ψ_2 because it is a weighted sum of $f_1(\exp(\psi_1), (x, X))$ and $f_2(\exp(\psi_2), (x, X))$. \square

Remark 8 By working with the $\psi_i := \log(\gamma_i)$ and establishing convexity, we are able to rigorously find the best values of the γ_i . [Ans18b] does not work that way. Working directly with the scaling parameters, γ_i , (of course separately for the BQP bound and the complementary BQP bound), he heuristically sought good values for the γ_i .

2.3.2 Optimizing the parameters

The (strengthened) mBQP bound depends on the parameters $(\alpha, \gamma_1, \gamma_2)$. We do not have any type of full joint convexity. But based on Theorem 7, to find a good upper bound, we are motivated to formulate two convex problems.

First, for given $\hat{\psi}_1$ and $\hat{\psi}_2$, we consider the convex optimization problem

$$\min\{V_{\hat{\psi}_1, \hat{\psi}_2}(\alpha) : \alpha \in [0, 1]\}, \quad (3)$$

where

$$\begin{aligned} V_{\hat{\psi}_1, \hat{\psi}_2}(\alpha) &:= \check{v}(C, s; \alpha, \exp(\hat{\psi}_1), \exp(\hat{\psi}_2)) \\ &= (1 - \alpha)f_1(C, s; \exp(\hat{\psi}_1), (x^*, X^*)) + \alpha f_2(C, s; \exp(\hat{\psi}_2), (x^*, X^*)), \end{aligned}$$

and $(x^*, X^*) = (x^*(\alpha), X^*(\alpha))$ solves the maximization problem in Proposition 5 for the given α , when $\gamma_1 = \exp(\hat{\psi}_1)$, and $\gamma_2 = \exp(\hat{\psi}_2)$.

Next, for $i = 1, 2$, we use $f_i^*(\alpha)$ as a short form for $f_i(C, s; \exp(\hat{\psi}_i), (x^*, X^*))$.

We solve (3) with a primal-dual interior-point method, considering the following barrier problem

$$\min\left\{V_{\hat{\psi}_1, \hat{\psi}_2}(\alpha) - \mu(\log(\alpha) + \log(1 - \alpha)) : \alpha \in (0, 1)\right\}, \quad (4)$$

where $\mu > 0$ is the barrier parameter. Let

$$L_{\mu, \hat{\psi}_1, \hat{\psi}_2}(\alpha) := V_{\hat{\psi}_1, \hat{\psi}_2}(\alpha) - \mu(\log(\alpha) + \log(1 - \alpha)).$$

We motivate our algorithm, by assuming some differentiability. The optimality conditions for the barrier problem is obtained by differentiating $L_{\mu, \hat{\psi}_1, \hat{\psi}_2}$ with respect to α , and can be written as

$$G_{\mu, \hat{\psi}_1, \hat{\psi}_2}(\alpha) := \frac{\partial V_{\hat{\psi}_1, \hat{\psi}_2}(\alpha)}{\partial \alpha} - \frac{\mu}{\alpha} + \frac{\mu}{1 - \alpha} = 0.$$

We aim at improving the mBQP bound by taking Newton steps to solve the nonlinear equation above. The search direction δ_α , is defined by

$$H_{G_{\mu, \hat{\psi}_1, \hat{\psi}_2}}(\alpha)(\delta_\alpha) = -G_{\mu, \hat{\psi}_1, \hat{\psi}_2}(\alpha),$$

where

$$H_{G_{\mu, \hat{\psi}_1, \hat{\psi}_2}}(\alpha) = \frac{\partial^2 V_{\hat{\psi}_1, \hat{\psi}_2}(\alpha)}{\partial \alpha^2} + \frac{\mu}{\alpha^2} + \frac{\mu}{(1 - \alpha)^2}.$$

We note that

$$\frac{\partial V_{\hat{\psi}_1, \hat{\psi}_2}(\alpha)}{\partial \alpha} = -f_1^*(\alpha) + (1 - \alpha) \frac{\partial f_1^*(\alpha)}{\partial \alpha} + f_2^*(\alpha) + \alpha \frac{\partial f_2^*(\alpha)}{\partial \alpha}.$$

However, we cannot analytically compute $\partial f_i^*(\alpha)/\partial \alpha$, for $i = 1, 2$. Indeed, we do not even know that the f_i^* are differentiable. In the implementation of the interior-point method, we consider the following approximations:

$$\begin{aligned} -f_1^*(\alpha) + (1 - \alpha) \frac{\partial f_1^*(\alpha)}{\partial \alpha} &\approx -f_1^*(\alpha), \\ f_2^*(\alpha) + \alpha \frac{\partial f_2^*(\alpha)}{\partial \alpha} &\approx f_2^*(\alpha). \end{aligned} \quad (5)$$

We then approximate the second partial derivative $\partial^2 V_{\hat{\psi}_1, \hat{\psi}_2}(\alpha)/\partial \alpha^2$, also considering (5). At the first iteration of the interior-point method, we approximate it by $b_0 = 1$, and in iteration $k \geq 0$, we compute

$$b_{k+1} = -\frac{\Delta f_1^*(\alpha)^{k+1}}{\Delta \alpha} + \frac{\Delta f_2^*(\alpha)^{k+1}}{\Delta \alpha},$$

where, for $i = 1, 2$, $\Delta f_i^*(\alpha)^{k+1}/\Delta \alpha := (f_i^*(\alpha^{k+1}) - f_i^*(\alpha^k))/(\alpha^{k+1} - \alpha^k)$ is the finite-difference approximation of the first-order partial derivative $\partial f_i^*(\alpha)/\partial \alpha$. Following what is commonly applied in a BFGS scheme, we update the approximation of the second partial derivative at iteration k only if b_{k+1} is non-negative.

We emphasize that to compute the search direction at each iteration of the interior-point method, we need to compute $f_i^*(\alpha)$, $i = 1, 2$, and therefore we need the optimal solution $(x^*, X^*) = (x^*(\alpha), X^*(\alpha))$ of the (strengthened) mBQP relaxation for the current α , when $\gamma_1 = \exp(\hat{\psi}_1)$, and $\gamma_2 = \exp(\hat{\psi}_2)$. The relaxation is thus solved at each iteration of the algorithm, each time for a new α . As α is a real variable, the time to minimize the mBQP bound is dominated by solving mBQP relaxations, the remaining effort for computing the bound is negligible.

In Algorithm 1, we present, in detail, an iteration of the interior-point method. The iteration presented is repeated for a fixed value of the barrier parameter μ , for a prescribed number of times or until the absolute value of the residual r is small enough. The parameter μ is then reduced and the process repeated, until μ is also small enough.

In what follows, we also define for given $\hat{\alpha} \in [0, 1]$, the convex problem

$$\min\{V_{\hat{\alpha}}(\psi_1, \psi_2) : (\psi_1, \psi_2) \in \mathbb{R}^2\}, \quad (6)$$

$$\begin{aligned} V_{\hat{\alpha}}(\psi_1, \psi_2) &:= \check{v}(C, s; \hat{\alpha}, \exp(\psi_1), \exp(\psi_2)) \\ &= (1 - \hat{\alpha})f_1(C, s; \exp(\psi_1), (x^*, X^*)) + \hat{\alpha}f_2(C, s; \exp(\psi_2), (x^*, X^*)), \end{aligned}$$

and $(x^*, X^*) = (x^*(\psi_1, \psi_2), X^*(\psi_1, \psi_2))$ solves the maximization problem in Proposition 5 for $\alpha = \hat{\alpha}$, $\gamma_1 = \exp(\psi_1)$, and $\gamma_2 = \exp(\psi_2)$.

Algorithm 1: Updating α , with $\gamma_1 = \exp(\hat{\psi}_1)$, $\gamma_2 = \exp(\hat{\psi}_2)$

Input: $k, \alpha^k, (x^*(\alpha^k), X^*(\alpha^k)), f_1^*(\alpha^k), f_2^*(\alpha^k), b_k, \mu^k, \tau_\alpha := 0.9, \tau_\mu := 0.1$.
 Compute the residual:

$$r := -f_1^*(\alpha^k) + f_2^*(\alpha^k) - \frac{\mu^k}{\alpha^k} + \frac{\mu^k}{1 - \alpha^k}.$$

Compute the search direction δ_α :

$$\delta_\alpha = -r / \left(b_k + \frac{\mu^k}{(\alpha^k)^2} + \frac{\mu^k}{(1 - \alpha^k)^2} \right).$$

Update α :

$$\alpha^{k+1} := \alpha^k + \hat{\theta} \delta_\alpha,$$

where

$$\hat{\theta} := \tau_\alpha \times \min\{1, \operatorname{argmax}_\theta \{\alpha^k + \theta \delta_\alpha \geq 0\}, \operatorname{argmax}_\theta \{\alpha^k + \theta \delta_\alpha \leq 1\}\}.$$

Obtain the optimal solution $(x^*(\alpha^{k+1}), X^*(\alpha^{k+1}))$ of the mBQP relaxation, considering $\alpha := \alpha^{k+1}$, $\gamma_1 := \exp(\hat{\psi}_1)$, and $\gamma_2 := \exp(\hat{\psi}_2)$.

For $i = 1, 2$, set:

$$f_i^*(\alpha^{k+1}) := f_i(C, s; \exp(\hat{\psi}_i), (x^*(\alpha^{k+1}), X^*(\alpha^{k+1}))),$$

$$\Delta_i := (f_i^*(\alpha^{k+1}) - f_i^*(\alpha^k)) / (\alpha^{k+1} - \alpha^k).$$

if $(-\Delta_1 + \Delta_2 > 0)$ then

$$b_{k+1} = -\Delta_1 + \Delta_2,$$

else

$$b_{k+1} := b_k.$$

Output: $\alpha^{k+1}, (x^*(\alpha^{k+1}), X^*(\alpha^{k+1})), f_1^*(\alpha^{k+1}), f_2^*(\alpha^{k+1}), b_{k+1}$.

Next, for $i = 1, 2$, we use $f_i^*(\psi_1, \psi_2)$ as a short form for $f_i(C, s; \exp(\psi_i), (x^*, X^*))$, and we use F_i as a short form for $F_i(C, s; \exp(\psi_i), (x^*, X^*))$.

The optimality condition for (6) is given by

$$\begin{cases} \frac{\partial V_{\hat{\alpha}}(\psi_1, \psi_2)}{\partial \psi_1} = (1 - \hat{\alpha}) \frac{\partial f_1^*(\psi_1, \psi_2)}{\partial \psi_1} + \hat{\alpha} \frac{\partial f_2^*(\psi_1, \psi_2)}{\partial \psi_1} = 0, \\ \frac{\partial V_{\hat{\alpha}}(\psi_1, \psi_2)}{\partial \psi_2} = (1 - \hat{\alpha}) \frac{\partial f_1^*(\psi_1, \psi_2)}{\partial \psi_2} + \hat{\alpha} \frac{\partial f_2^*(\psi_1, \psi_2)}{\partial \psi_2} = 0. \end{cases}$$

Here we should observe that we cannot analytically compute $\partial f_1^*(\psi_1, \psi_2) / \partial \psi_2$ nor $\partial f_2^*(\psi_1, \psi_2) / \partial \psi_1$. Again, we cannot even be sure that these derivatives exist. In the implementation of the interior-point method, we consider the following approximations:

$$\begin{cases} (1 - \hat{\alpha}) \frac{\partial f_1^*(\psi_1, \psi_2)}{\partial \psi_1} + \hat{\alpha} \frac{\partial f_2^*(\psi_1, \psi_2)}{\partial \psi_1} \approx (1 - \hat{\alpha}) \frac{\partial f_1^*(\psi_1, \psi_2)}{\partial \psi_1}, \\ (1 - \hat{\alpha}) \frac{\partial f_1^*(\psi_1, \psi_2)}{\partial \psi_2} + \hat{\alpha} \frac{\partial f_2^*(\psi_1, \psi_2)}{\partial \psi_2} \approx \hat{\alpha} \frac{\partial f_2^*(\psi_1, \psi_2)}{\partial \psi_2}. \end{cases} \quad (7)$$

We obtain then the following approximation for the optimality conditions for (6):

$$G_{\hat{\alpha}}(\psi_1, \psi_2) := \begin{pmatrix} n - s - F_1^{-1} \bullet (I - \text{diag}(x^*)) \\ s - F_2^{-1} \bullet \text{diag}(x^*) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \quad (8)$$

We aim now at improving the bound by taking Newton steps to solve the nonlinear system above. The search direction is defined by

$$\nabla G_{\hat{\alpha}}(\psi_1, \psi_2) \begin{pmatrix} \delta_{\psi_1} \\ \delta_{\psi_2} \end{pmatrix} = -G_{\hat{\alpha}}(\psi_1, \psi_2),$$

where,

$$\nabla G_{\hat{\alpha}}(\psi_1, \psi_2) = \left(\frac{\partial G_{\hat{\alpha}}(\psi_1, \psi_2)}{\partial \psi_1}, \frac{\partial G_{\hat{\alpha}}(\psi_1, \psi_2)}{\partial \psi_2} \right), \quad (9)$$

$$\frac{\partial G_{\hat{\alpha}}(\psi_1, \psi_2)}{\partial \psi_1} = \begin{pmatrix} \exp(\psi_1)(e - x^*)' \text{diag}(F_1^{-1}(C \circ X^*)F_1^{-1}) \\ 0 \end{pmatrix},$$

$$\frac{\partial G_{\hat{\alpha}}(\psi_1, \psi_2)}{\partial \psi_2} = \begin{pmatrix} 0 \\ \exp(\psi_2)x^{*'} \text{diag}(F_2^{-1}(C^{-1} \circ (X^* + ee' - ex^{*'} - x^*e')F_2^{-1})) \end{pmatrix}.$$

In Algorithm 2, we present an iteration of the Newton method applied to update the parameters ψ_1 and ψ_2 in the mBQP relaxation. The iteration presented is repeated for a prescribed number of times or until the absolute value of the residuals, components of $G_{\hat{\alpha}}(\psi_1, \psi_2)$, are small enough.

Algorithm 2: Updating ψ_1, ψ_2 , with $\alpha = \hat{\alpha}$

Input: $k, (x^*(\psi_1^k, \psi_2^k), X^*(\psi_1^k, \psi_2^k)); \psi_i^k, F_i^k, f_i^*(\psi_1^k, \psi_2^k), i = 1, 2.$

Compute $G_{\hat{\alpha}}(\psi_1^k, \psi_2^k)$ and $\nabla G_{\hat{\alpha}}(\psi_1^k, \psi_2^k)$ as defined in (8) and (9).

Solve the linear system to obtain the search direction $(\delta_{\psi_1}, \delta_{\psi_2})'$:

$$\nabla G_{\hat{\alpha}}(\psi_1^k, \psi_2^k) \begin{pmatrix} \delta_{\psi_1} \\ \delta_{\psi_2} \end{pmatrix} = -G_{\hat{\alpha}}(\psi_1^k, \psi_2^k),$$

For $i = 1, 2$, update ψ_i :

$$\psi_i^{k+1} := \psi_i^k + \delta_{\psi_i}.$$

Obtain the optimal solution $(x^*(\psi_1^{k+1}, \psi_2^{k+1}), X^*(\psi_1^{k+1}, \psi_2^{k+1}))$ of the mBQP relaxation, considering $\alpha := \hat{\alpha}$, $\gamma_1 := \exp(\psi_1^{k+1})$, and $\gamma_2 := \exp(\psi_2^{k+1})$.

For $i = 1, 2$, set:

$$F_i^{k+1} := F_i(C, s; \exp(\psi_i^{k+1}), (x^*(\psi_1^{k+1}, \psi_2^{k+1}), X^*(\psi_1^{k+1}, \psi_2^{k+1}))),$$

$$f_i^*(\psi_1^{k+1}, \psi_2^{k+1}) := f_i(C, s; \exp(\psi_i^{k+1}), (x^*(\psi_1^{k+1}, \psi_2^{k+1}), X^*(\psi_1^{k+1}, \psi_2^{k+1}))).$$

Output: $(x^*(\psi_1^{k+1}, \psi_2^{k+1}), X^*(\psi_1^{k+1}, \psi_2^{k+1})); \psi_i^{k+1}, F_i^{k+1}, f_i^*(\psi_1^{k+1}, \psi_2^{k+1}), i = 1, 2.$

Finally, in order to obtain a good bound, we propose an algorithmic approach where we start from given values for the parameters α , ψ_1 , and ψ_2

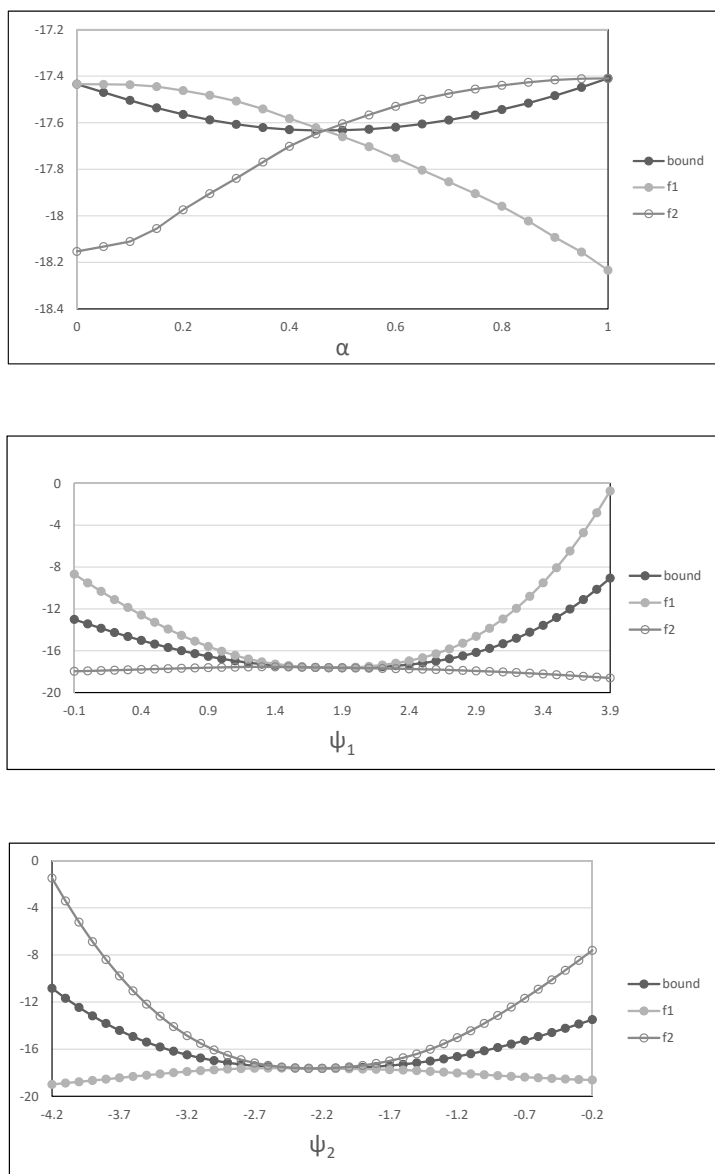


Fig. 4 Variation of f_1, f_2 , and the overall bound, with $\alpha, \psi_1, \psi_2 (n = 63, s = 10)$

and alternate between solving problems (3) and (6), applying respectively, the procedures described in Algorithms 1 and 2.

In Figure 4 we illustrate how f_1, f_2 , and the (strengthened) mBQP bound vary with each of the parameters α, ψ_1 , and ψ_2 , separately, for the instance with $n = 63, s = 10$. To construct each plot in Figure 4, we fix two of the

parameters and vary the other. The values of the two parameters that are fixed were obtained by the procedure described above, i.e., alternating between the execution of Algorithms 1 and 2. The interval in which the third parameter varies is centered in the value also obtained with the alternating algorithm, so the best bound obtained by the algorithm is depicted in the figure. The plots in Figure 4 were considered to support the approximations pointed in (5) and (7), used in the computation of the search directions of Algorithms 1 and 2.

3 Mixing the NLP bound with the complementary NLP bound

Now, we introduce the *mixed NLP (mNLP) bound*:

$$\begin{aligned} w(C, s; \alpha, \gamma_1, \gamma_2) := & \\ \max & (1 - \alpha) \left(\text{ldet} \left(\gamma_1 X^{p/2} (C - D) X^{p/2} + (\gamma_1 D)^x \right) - s \log \gamma_1 \right) \\ & + \alpha \left(\text{ldet} \left(\gamma_2 Y^{\bar{p}/2} (C^{-1} - \bar{D}) Y^{\bar{p}/2} + (\gamma_2 \bar{D})^y \right) - (n - s) \log \gamma_2 + \text{ldet} C \right), \end{aligned}$$

subject to:

$$e'x = s, \quad x + y = e,$$

where $0 \leq \alpha \leq 1$ is a weighting parameter.

The objective function of the mNLP relaxation is defined over the order- n diagonal matrices D and \bar{D} , the order- n vectors p and \bar{p} , and the scaling parameters $\gamma_1, \gamma_2 > 0$. The following notation is also employed in its definition: $X := \text{diag}(x)$, $Y := \text{diag}(y)$, and $(V^u)_{i,i} := V_{i,i}^{u_i}$, $i = 1, \dots, n$, for a diagonal matrix V and a vector u .

In [AFLW99], three different strategies are presented for choosing D , p , and γ_1 , in order to have the NLP relaxation proven convex. Analogously, the strategies also applies to the selection of the parameters \bar{D} , \bar{p} , and γ_2 , for the complementary problem. In our numerical experiments with the NLP bound, we have chosen these parameters based on the so-called ‘‘NLP-Trace’’ strategy, where D minimizes the trace of $D - C$, subject to $D - C$ being positive semidefinite. Once D is chosen, the scaling parameter γ_1 should be selected in the interval $[1/d_{\max}, 1/d_{\min}]$ (see [AFLW99]). In our experiments, we have tested 100 values for γ_1 in this interval and report results for the best one. The same strategy is applied to the complementary problem. We note that the optimal scaling factors for the mBQP bound were obtained with Newton steps in the previous section, as described in Algorithm 2. The same methodology could not be applied here, because the objective function of the mNLP relaxation is neither convex in the scaling parameters nor in the logarithms of the scaling parameters. Therefore, for the results we present on the mNLP bound, we choose γ_1 to be the best scaling parameter for the original NLP bound ($\alpha = 0$), among the 100 values tested, we choose γ_2 to be the best scaling parameter for the complementary NLP bound ($\alpha = 1$), among the 100 values tested. To select α for each instance, we obtained the mNLP

bound for all $\alpha = 0.1i$, $i = 0, 1, \dots, 10$. The results reported correspond to the best such α .

Finally, we note that unlike the mBQP bound, the mNLP bound cannot be computed by SDPT3, via Matlab and Yalmip. So, to compute it, we have coded an interior-point algorithm, also in Matlab. The solution procedure is the same as described in [AFLW99, Section 3], where the NLP bound and the complementary NLP bound are considered. Later, the procedure was also applied in the related work [AFLW01]. The procedure employs a long-step path following methodology, using logarithmic barrier terms for the bound constraints on x (i.e., $0 \leq x \leq e$). For a fixed value of the barrier parameter μ , the barrier function is approximately minimized on $\{x \in \mathbb{R}^n : e'x = s\}$. The parameter μ is then reduced and the process is repeated, until μ is small enough for an approximate minimizer to be within a prescribed tolerance of optimality. The tolerance is certified by a dual solution generated by the algorithm, providing a valid upper bound for the optimal value of NLP.

In Figure 5, we illustrate our approach. By mixing the NLP-Trace bound and the complementary NLP-Trace bound, we were able to obtain an improvement for the $n = 124$ problem in the vicinity of $s = 73$.

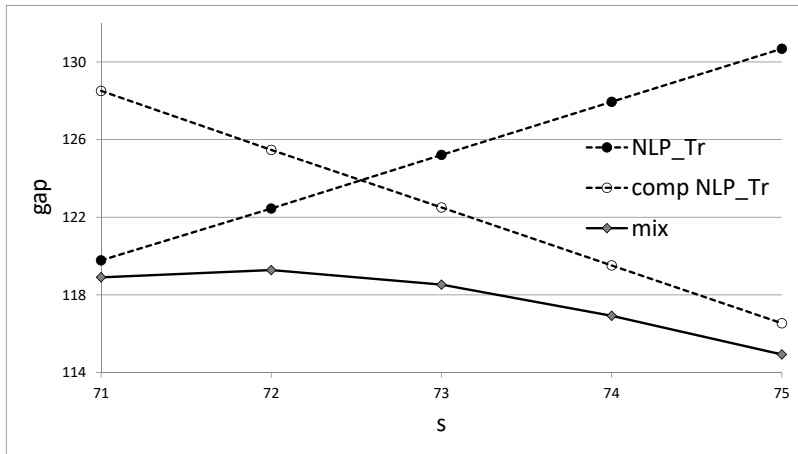


Fig. 5 Mixing the NLP bound with complementary NLP bound

4 On the linx bound

Next, we consider the linx bound introduced by [Ans18a], i.e., the solution of

$$\max\left\{\frac{1}{2}v(\gamma, x) \mid e'x = s, 0 \leq x \leq e\right\} \quad (10)$$

where

$$v(\gamma, x) := \text{ldet } F(\gamma, x) - s \log \gamma$$

and

$$F(\gamma, x) := \gamma C \operatorname{diag}(x) C + I - \operatorname{diag}(x), \quad (11)$$

The linx bound has excellent performance, and it is a challenge to improve upon it. In the remainder of this section, we consider fine tuning the bound via its scaling parameter. In §5, we are able to get an improvement on the linx bound by mixing it with the NLP bound.

4.1 Optimizing the linx bound on the scaling parameter γ

The linx bound depends on the scaling parameter γ . [Ans18a] observed that the linx bound is particularly sensitive to the choice of γ . This is probably due to the fact that the bound is derived by bounding the *square* of the determinant of an order- s principle submatrix of C . So for mixing with the linx bound, it is very useful to be able to optimize on γ .

To find the best bound, we now define $\psi := \log(\gamma)$ and formulate the problem

$$\min_{\psi} \{H(\psi)\}, \quad (12)$$

where

$$H(\psi) := v(\exp(\psi), x^*),$$

and where x^* is a maximizer of (10), with $\gamma (= \exp(\psi))$ fixed.

Theorem 9 The function $H(\psi)$ is convex in $\psi \in \mathbb{R}$.

Proof Based on the same argument used in the proof of Theorem 7, we show that $v(\exp(\psi), x)$ is convex in ψ , for fixed x in the feasible set of (10).

We have

$$\begin{aligned} \frac{\partial}{\partial \gamma} v(\gamma, x) &= F(\gamma, x)^{-1} \bullet (C \operatorname{diag}(x) C) - \frac{s}{\gamma} \\ &= \frac{1}{\gamma} (F(\gamma, x)^{-1} \bullet ((F(\gamma, x) - I + \operatorname{diag}(x)) - s)) \\ &= \frac{1}{\gamma} (F(\gamma, x)^{-1} \bullet (\operatorname{diag}(x) - I) + n - s) \\ \frac{\partial^2}{\partial \gamma^2} v(\gamma, x) &= \frac{\partial}{\partial \gamma} \left(\frac{1}{\gamma} (F(\gamma, x)^{-1} \bullet (\operatorname{diag}(x) - I) + n - s) \right) \\ &= -\frac{1}{\gamma^2} (F(\gamma, x)^{-1} \bullet (\operatorname{diag}(x) - I) + n - s) \\ &\quad + \frac{1}{\gamma} (e - x)' \operatorname{diag}(F(\gamma, x)^{-1} (C \operatorname{diag}(x) C) F(\gamma, x)^{-1}). \end{aligned}$$

Therefore

$$\begin{aligned} \frac{\partial}{\partial \psi} v(\gamma, x) &= \gamma \frac{\partial}{\partial \gamma} v(\gamma, x) \\ &= F(\gamma, x)^{-1} \bullet (\operatorname{diag}(x) - I) + n - s, \end{aligned}$$

and

$$\begin{aligned} \frac{\partial^2}{\partial \psi^2} v(\gamma, x) &= \gamma \frac{\partial}{\partial \gamma} v(\gamma, x) + \gamma^2 \frac{\partial^2}{\partial \gamma^2} v(\gamma, x) \\ &= \gamma (e - x)' \operatorname{diag}(F(\gamma, x)^{-1} (C \operatorname{diag}(x) C) F(\gamma, x)^{-1}). \end{aligned} \quad (13)$$

Now, it remains to show that

$$\frac{\partial^2 v}{\partial \psi^2}(\exp(\psi), x^*) \geq 0, \quad \forall \psi.$$

Considering (13), it suffices to show that

$$\text{diag}(F(\exp(\psi), x^*)^{-1}(C \text{diag}(x^*)C)F(\exp(\psi), x^*)^{-1}) \geq 0.$$

We have $C \succ 0$ and $\text{diag}(x^*) \succeq 0$, therefore $C \text{diag}(x^*)C \succeq 0$. Then, it is also clear from (11) that $F(\exp(\psi), x^*) \succ 0$ and, therefore,

$$F(\exp(\psi), x^*)^{-1}(C \text{diag}(x^*)C)F(\exp(\psi), x^*)^{-1} \succeq 0,$$

which completes the proof. \square

Remark 10 By working with $\psi := \log(\gamma)$ and establishing convexity, we are able to rigorously find the best values of the γ_i . [Ans18b] does not work that way. Working directly with the scaling parameters, γ , he heuristically sought a good value for γ .

4.2 The Newton method on the variable $\psi := \log(\gamma)$

The optimality condition for (12) can be written as

$$G(\psi) := \frac{\partial}{\partial \psi} v(\exp(\psi), x^*) = n - s - F(\exp(\psi), x^*)^{-1} \bullet (I - \text{diag}(x^*)) = 0.$$

We aim at improving the linx bound by taking Newton steps to solve the nonlinear equation above. The Newton direction δ_ψ is then defined by

$$H_G(\psi)\delta_\psi = -G(\psi),$$

where

$$\begin{aligned} H_G(\psi) &:= \frac{\partial^2}{\partial \psi^2} v(\exp(\psi), x^*) \\ &= \exp(\psi)(e - x^*)' \text{diag} \left(F(\exp(\psi), x^*)^{-1}(C \text{diag}(x^*)C)F(\exp(\psi), x^*)^{-1} \right). \end{aligned}$$

5 Mixing the NLP bound and a “non-NLP bound”

A convenient solver for calculating the BQP bound and its complement and also for calculating the linx bound is SDPT3 via Yalmip. But the NLP bound and its complement are not amenable to solution by SDPT3 via Yalmip. So we developed our own IPM for calculating the NLP bound. Because of this dichotomy between available solvers, we need a special approach for mixing the NLP bound or its complement, with any of the BQP bound, its complement, or the linx bound.

We are not very concerned with efficiency. Rather, we only seek a practical method for calculating these mixed bounds to see if we can get an improvement on the unmixed bounds by mixing.

Our idea is simply to apply Lagrangian relaxation to the mixing bound, in its form with duplicated variables, as follows:

$$v(\alpha) := \max \{ \alpha f_1(x, \mathcal{X}) + (1 - \alpha) f_2(y, \mathcal{Y}) : (x, \mathcal{X}) \in \mathcal{P}, (y, \mathcal{Y}) \in \mathcal{Q}, x + y = e \}$$

$$\begin{aligned}
&= \min_{\pi \in \mathbb{R}^n} \left\{ \max \{ \alpha f_1(x, \mathcal{X}) + (1 - \alpha) f_2(y, \mathcal{Y}) + \pi' (e - x - y) : \right. \\
&\quad \left. (x, \mathcal{X}) \in \mathcal{P}, (y, \mathcal{Y}) \in \mathcal{Q} \} \right\} \\
&= \min_{\pi \in \mathbb{R}^n} \left\{ \pi' e + \max \{ \alpha f_1(x, \mathcal{X}) - \pi' x : (x, \mathcal{X}) \in \mathcal{P} \} \right. \\
&\quad \left. + \max \{ (1 - \alpha) f_2(y, \mathcal{Y}) - \pi' y : (y, \mathcal{Y}) \in \mathcal{Q} \} \right\}.
\end{aligned}$$

In this form, we apply subgradient optimization to find an optimal $\pi \in \mathbb{R}^n$, and at each step the Lagrangian subproblem decouples into the $(x, \mathcal{X}) \in \mathcal{P}$ maximization problem and the $(y, \mathcal{Y}) \in \mathcal{Q}$ maximization problem. So we can apply separate solvers to each.

In Figure 6, we illustrate some successes with our approach. By mixing the NLP-Trace bound and linx bound, we were able to obtain an improvement for the $n = 63$ problem in the vicinity of $s = 25$.

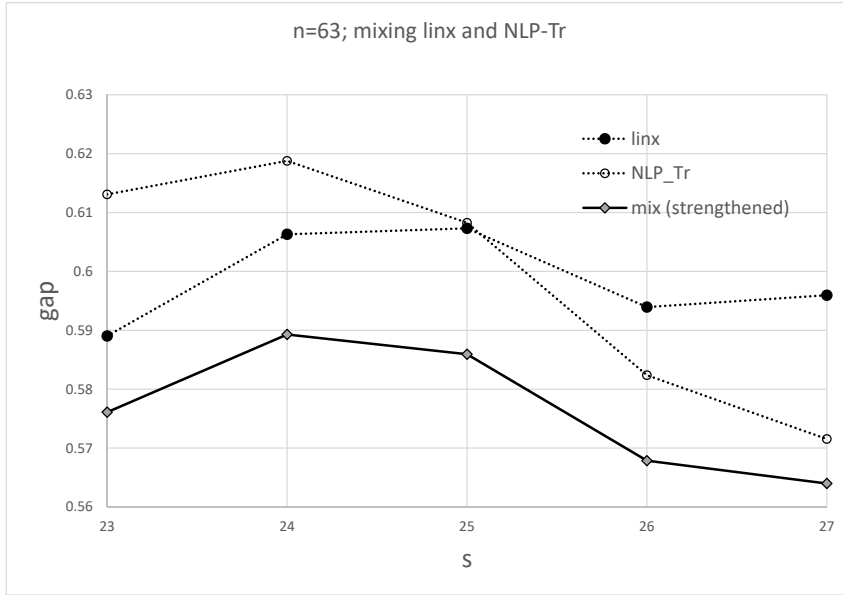


Fig. 6 Mixing the NLP bound with “Non-NLP bounds”

6 Concluding remarks

It is a challenge to *efficiently* employ our ideas in the context of branch-and-bound. We need to find effective mixing parameters α quickly. Note that in our notation, [Ans18b] is using only $\alpha = 0$ or 1 , and in the context of branch-and-bound, each child inherits α from its parent, only updating the choice occasionally. In the context of branch-and-bound, we would now expect that for many subproblems, we would have $\alpha = 0$ or 1 . But we can further expect that for many we will have $0 < \alpha < 1$, and we would then gain from our approach. The guidance of [Ans18b] is: “we use a simple criterion based on the number of fixed variable and depth in the tree to decide when to check the other bound”. So we would proceed similarly, doing a univariate search for a good α after an inherited value becomes stale.

It is not clear at all how our mixing idea could be adapted to “spectral and masked spectral bounds” (see [KLQ95, AL04, BL07, HLW01, LW03]), because these are apparently not based on convex relaxation. We would like to highlight this as an interesting area to explore.

Very recently, [LX20] presented new results on a relaxation and on an approximation algorithm for MESP. It will be interesting to see if some of those results can be exploited in our context.

Finally, our general mixing idea, although well suited for MESP, should find application on other combinatorial-optimization problems with nonlinearities. It is a challenge to find other good applications.

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References

- AFLW96. Kurt M. Anstreicher, Marcia Fampa, Jon Lee, and Joy Williams. Continuous relaxations for constrained maximum-entropy sampling. In *Integer programming and combinatorial optimization (Vancouver, BC, 1996)*, volume 1084 of *Lecture Notes in Comput. Sci.*, pages 234–248. Springer, Berlin, 1996.
- AFLW99. Kurt M. Anstreicher, Marcia Fampa, Jon Lee, and Joy Williams. Using continuous nonlinear relaxations to solve constrained maximum-entropy sampling problems. *Mathematical Programming*, 85(2, Ser. A):221–240, 1999.

- AFLW01. Kurt M. Anstreicher, Marcia Fampa, Jon Lee, and Joy Williams. Maximum-entropy remote sampling. *Discrete Applied Mathematics*, 108(3):211–226, 2001.
- AL04. Kurt M. Anstreicher and Jon Lee. A masked spectral bound for maximum-entropy sampling. In *mODa 7—Advances in model-oriented design and analysis*, Contrib. Statist., pages 1–12. Physica, Heidelberg, 2004.
- Ans18a. Kurt M. Anstreicher. Efficient solution of maximum-entropy sampling problems, 2018. http://www.optimization-online.org/DB_HTML/2018/07/6707.html. To appear in *Operations Research*.
- Ans18b. Kurt M. Anstreicher. Maximum-entropy sampling and the Boolean quadric polytope. *Journal of Global Optimization*, 72(4):603–618, 2018.
- BELW17. A. Billionnet, S. Elloumi, A. Lambert, and A. Wiegele. Using a Conic Bundle method to accelerate both phases of a Quadratic Convex Reformulation. *INFORMS Journal on Computing*, 29(2):318–331, 2017.
- BL07. Samuel Burer and Jon Lee. Solving maximum-entropy sampling problems using factored masks. *Mathematical Programming*, 109(2-3, Ser. B):263–281, 2007.
- FGRS06. Ilse Fischer, Gerald Gruber, Franz Rendl, and Renata Sotirov. Computational experience with a bundle approach for semidefinite cutting plane relaxations of max-cut and equipartition. *Mathematical Programming*, 105:451–469, 2006.
- FL00. Valerii Fedorov and Jon Lee. Design of experiments in statistics. In *Handbook of semidefinite programming*, volume 27 of *Internat. Ser. Oper. Res. Management Sci.*, pages 511–532. Kluwer Acad. Publ., Boston, MA, 2000.
- Hel19. Christoph Helmberg. The ConicBundle Library for Convex Optimization. <https://www-user.tu-chemnitz.de/~helmberg/ConicBundle/>, 2005–2019.
- HLW01. Alan Hoffman, Jon Lee, and Joy Williams. New upper bounds for maximum-entropy sampling. In *mODa 6—advances in model-oriented design and analysis (Puchberg/Schneeberg, 2001)*, Contrib. Statist., pages 143–153. Physica, Heidelberg, 2001.
- KLQ95. Chun-Wa Ko, Jon Lee, and Maurice Queyranne. An exact algorithm for maximum entropy sampling. *Operations Research*, 43(4):684–691, 1995.
- Lee12. Jon Lee. Maximum entropy sampling. In A.H. El-Shaarawi and W.W. Piegorsch, editors, *Encyclopedia of Environmetrics, 2nd ed.*, pages 1570–1574. Wiley, 2012.
- LL19. Jon Lee and Joy Lind. Generalized maximum-entropy sampling. *INFOR: Information Systems and Operational Research*, 2019.
- Löf04. Johan Löfberg. Yalmip : A toolbox for modeling and optimization in Matlab. In *In Proceedings of the CACSD Conference*, 2004.
- LW03. Jon Lee and Joy Williams. A linear integer programming bound for maximum-entropy sampling. *Mathematical Programming, Series B*, 94(2–3):247–256, 2003.
- LX20. Yongchun Li and Weijun Xie. Approximation algorithms for the maximum entropy sampling problem. Technical report, Optimization Online, 2020. http://www.optimization-online.org/DB_FILE/2020/01/7570.pdf.
- SW87. Michael C. Shewry and Henry P. Wynn. Maximum entropy sampling. *Journal of Applied Statistics*, 46:165–170, 1987.
- TTT99. Kim-Chuan Toh, Michael J. Todd, and Reha H. Tütüncü. SDPT3: A Matlab software package for semidefinite programming, version 1.3. *Optimization Methods and Software*, 11(1-4):545–581, 1999.
- TTT12. Kim-Chuan Toh, Michael J. Todd, and Reha H. Tütüncü. On the implementation and usage of sdpt3 – a matlab software package for semidefinite-quadratic-linear programming, version 4.0. In Miguel F. Anjos and Jean B. Lasserre, editors, *Handbook on Semidefinite, Conic and Polynomial Optimization*, pages 715–754. Springer US, Boston, MA, 2012.
- Zha05. Fuzhen Zhang, editor. *The Schur complement and its applications*, volume 4 of *Numerical Methods and Algorithms*. Springer-Verlag, New York, 2005.