Convex relaxation for generalized maximum-entropy sampling problem

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MOM26

The generalized maximum-entropy sampling problem

From [Williams, 1998; Lee and Lind, 2020], we consider

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

and

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

where $C \in \mathbb{S}_+^n$, with $\text{rank}(C) =: r$, $0 < t \leq r$, and $t \leq s < n$.

- GMESP is motivated by a selection problem in the context of PCA (principal component analysis): maximize the geometric mean of the t greatest principal components from a selection of size s.
- GMESP is a generalization of the NP-hard MESP ("maximum-entropy sampling problem)", with application to environmental monitoring, for example. $[t := s]$
- GMESP is a generalization of the NP-hard binary D-Opt ("D-Optimality") problem, with very broad application to experimental design. $[\mathcal{A}_{n\times m}\,,\ C := \mathcal{A}\mathcal{A}^\top,\ t := m = r(\mathcal{A})]$
- constrained version is useful in the applications (e.g., budget constraints).

The generalized factorization problem

Let $C = FF^\top$, with $F \in \mathbb{R}^{n\times k}$, $r \le k \le n$. This could be:

- a Cholesky-type factorization (see [Nikolov, 2015; Li and Xie, 2023]), where F is lower triangular and $k := r$,
- 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, $i = 1, \ldots, k := r$,
- derived from the matrix square root of C, where $F := C^{1/2}$, and $k := n$.

For $x \in [0,1]^n$, we define

$$F(x) := \sum_{i=1}^{n} F_{i\cdot}^\top F_{i\cdot}\; x_i \;= F^\top \operatorname{Diag}(x) F,$$

and

$$z_{\text{GFact}}(C, s, t, A, b; F) := \begin{array}{ll} \max & \sum_{\ell=1}^{t} \log\left(\lambda_\ell(F(x))\right) \\ \text{s.t.} & \mathbf{e}^\top x = s, \\ & Ax \le b, \\ & 0 \le x \le \mathbf{e}. \end{array} \qquad \text{(GFact)}$$

A relaxation for CGMESP

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

$$z_{\text{GFact}}(C,s,t,A,b;F) := \max\left\{\sum_{\ell=1}^{t} \log\left(\lambda_\ell(F(x))\right) \;:\; \mathbf{e}^\top x = s,\;\; Ax \le b,\;\; 0 \le x \le \mathbf{e}\right\} \quad (\text{GFact})$$

Theorem

GFact gives an upper bound for CGMESP: $z(C,s,t,A,b) \le z_{\mathrm{GFact}}(C,s,t,A,b;F)$.

Proof.

It suffices to show that for any feasible solution x of CGMESP with finite objective value, we have

$$\sum_{\ell=1}^{t} \log\left(\lambda_\ell(C[S(x),S(x)])\right) = \sum_{\ell=1}^{t} \log\left(\lambda_\ell(F(x))\right).$$

Let $S := S(x)$. Then, for $S \subset \{1,\dots,n\}$ with $|S| = s$ and $\operatorname{rank}(C[S,S]) \ge t$, we have

$$F(x) = \sum_{i=1}^{n} F_{i\cdot}^\top F_{i\cdot}\, x_i \;= \sum_{i\in S} F_{i\cdot}^\top F_{i\cdot} = F[S,\cdot]^\top F[S,\cdot] \in \mathbb{S}_+^k\,, \text{ and}$$

$$C[S,S] = F[S,\cdot]F[S,\cdot]^\top \in \mathbb{S}_+^s\,.$$

The nonzero eigenvalues of $F[S,\cdot]^\top F[S,\cdot]$ and $F[S,\cdot]F[S,\cdot]^\top$ are identical, and their rank is at least t. So, the t largest eigenvalues of these matrices are positive and identical. □

Remark

GFact is not generally a convex program, so we cannot make direct use of the Theorem above.

$$z_{\text{GFact}}(C, s, t, A, b; F) := \max \left\{ \sum_{\ell=1}^{t} \log \left(\lambda_\ell(F(x)) \right) \ : \ \mathbf{e}^\top x = s, \ Ax \le b, \ 0 \le x \le \mathbf{e} \right\} \quad \text{(GFact)}$$

Using Lagrangian duality, we will obtain an upper bound for z_{GFact} . We first re-cast GFact as

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

and consider the Lagrangian function

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

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

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

and the corresponding Lagrangian dual problem is

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

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

The generalized factorization bound

We note that

$$\sup_{W\in\mathbb{S}_+^{k,t},\,x} \left\{\sum_{\ell=1}^{t} \log\left(\lambda_\ell\left(W\right)\right) + \Theta \bullet \left(F(x) - W\right) + \upsilon^\top x + \nu^\top(\mathbf{e} - x) + \pi^\top(b - Ax) + \tau(s - \mathbf{e}^\top x)\right\}$$

$$= \sup_{W\in\mathbb{S}_+^{k,t}} \left\{\sum_{\ell=1}^{t} \log\left(\lambda_\ell\left(W\right)\right) - \Theta \bullet W\right\} \quad (1)$$

$$+ \sup_{x} \left\{\Theta \bullet F(x) + \upsilon^\top x - \nu^\top x - \pi^\top Ax - \tau\mathbf{e}^\top x + \nu^\top\mathbf{e} + \pi^\top b + \tau s\right\}. \quad (2)$$

Next, we analytically characterize the suprema in (1) and (2) (see [Li and Xie, 2023, Lemma 1]).

Theorem (proof in [Ponte, Fampa, and Lee, 2024])

For $\Theta \in \mathbb{S}^k$, we have

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

Theorem

For $(\Theta, \upsilon, \nu, \pi, \tau) \in \mathbb{S}^k \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}$, we have

$$\sup_{x} \left(\Theta \bullet F(x) + \upsilon^\top x - \nu^\top x - \pi^\top Ax - \tau\mathbf{e}^\top x + \nu^\top\mathbf{e} + \pi^\top b + \tau s\right)$$

$$= \begin{cases} \nu^\top\mathbf{e} + \pi^\top b + \tau s, & \textit{if } \operatorname{diag}(F\Theta F^\top) + \upsilon - \nu - A^\top\pi - \tau\mathbf{e} = 0; \\ +\infty, & \textit{otherwise.} \end{cases}$$

The Lagrangian dual of GFact

$$z_{\text{GFact}}(C,s,t,A,b;F) := \max\left\{\sum_{\ell=1}^{t} \log\left(\lambda_\ell(F(x))\right) \;:\; \mathbf{e}^\top x = s,\; Ax \le b,\; 0 \le x \le \mathbf{e}\right\} \qquad \text{(GFact)}$$

$$\begin{array}{rll} z_{\text{DGFact}}(C,s,t,A,b;F) := & \min & -\sum_{\ell=k-t+1}^{k} \log\left(\lambda_\ell\left(\Theta\right)\right) + \nu^\top \mathbf{e} + \pi^\top b + \tau s - t \\ & \text{subject to:} & \operatorname{diag}(F\Theta F^\top) + \upsilon - \nu - A^\top \pi - \tau \mathbf{e} = 0, \qquad \text{(DGFact)} \\ & & \Theta \succ 0,\; \upsilon \ge 0,\; \nu \ge 0,\; \pi \ge 0. \end{array}$$

Remark

From Lagrangian duality, we have that DGFact is a convex program. However, GFact is not generally a convex program, so strong duality between GFact and DGFact does not hold in general.

We establish properties for the generalized factorization bound (see [Chen, Fampa, and Lee, 2023] for similar results for MESP).

Theorem

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

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

Comparing the factorization bound to the spectral bound for GMESP

$$z_{\mathrm{DGFact}}(C,s,t,A,b\,;F) := \min\Big\{-\sum_{\ell=k-t+1}^{k}\log\left(\lambda_\ell\left(\Theta\right)\right) + \nu^{\mathsf T}\mathbf{e} + \pi^{\mathsf T} b + \tau s - t :$$
$$\mathrm{diag}(F\Theta F^{\mathsf T}) + \upsilon - \nu - A^{\mathsf T}\pi - \tau\mathbf{e} = 0,\ \Theta \succ 0,\ \upsilon \geq 0,\ \nu \geq 0,\ \pi \geq 0\Big\}$$

The *spectral bound* for GMESP is given by $z_{\mathcal{S}}(C,t) := \sum_{\ell=1}^{t}\log\lambda_\ell(C)$ ([Lee and Lind, 2020]).

Theorem

Let $C \in \mathbb{S}_+^n$, $r := \mathrm{rank}(C)$, $0 < t \leq r$, $t \leq s < n$. Then, for all factorizations $C = FF^{\mathsf T}$, we have

$$z_{\mathrm{DGFact}}(C,s,t,\cdot,\cdot\,;F) \;-\; z_{\mathcal{S}}(C,t) \;\leq\; t\log\left(\tfrac{s}{t}\right).$$

Proof.

$C = \sum_{\ell=1}^{r}\lambda_\ell(C)u_\ell u_\ell^{\mathsf T}$ (spectral decomposition of C). It suffices to take $F := \sum_{\ell=1}^{r}\sqrt{\lambda_\ell(C)}u_\ell u_\ell^{\mathsf T}$.
Let: $\hat\Theta := \frac{t}{s}\left(C^\dagger + \frac{1}{\lambda_r(C)}\left(I - CC^\dagger\right)\right)$, $\hat\nu := 0$, $\hat\pi := 0$, $\hat\tau := \frac{t}{s}$. The equality constraint of DGFact is satisfied at this solution. The eigenvalues of $\hat\Theta$ are $\frac{t}{s}\left(\frac{1}{\lambda_1(C)},\frac{1}{\lambda_2(C)},\ldots,\frac{1}{\lambda_r(C)},\ldots,\frac{1}{\lambda_r(C)}\right) > 0$.
So, $\hat\Theta \succ 0$. We have $F\hat\Theta F^{\mathsf T} = \frac{t}{s}\sum_{\ell=1}^{r}u_\ell u_\ell^{\mathsf T}$, $\sum_{\ell=1}^{r}u_\ell u_\ell^{\mathsf T} \preceq I$. So, $\mathrm{diag}(F\hat\Theta F^{\mathsf T}) \leq \frac{t}{s}\mathbf{e}$, and $\hat\upsilon \geq 0$.
Then, $(\hat\Theta,\hat\upsilon,\hat\nu,\hat\pi,\hat\tau)$ is feasible to DGFact with objective value $t\log\left(\frac{s}{t}\right) + \sum_{\ell=1}^{t}\log\lambda_\ell(C)$. □

Remark

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

Concavity related to the bounds

$$z_{\mathrm{DGFact}}(C,s,t,A,b\,;F) := \min\Big\{-\sum_{\ell=k-t+1}^{k}\log\left(\lambda_\ell\left(\Theta\right)\right) + \nu^{\mathsf{T}}\mathbf{e} + \pi^{\mathsf{T}}b + \tau s - t :$$
$$\mathrm{diag}(F\Theta F^{\mathsf{T}}) + \upsilon - \nu - A^{\mathsf{T}}\pi - \tau\mathbf{e} = 0, \Theta \succ 0, \upsilon \ge 0, \nu \ge 0, \pi \ge 0\Big\}\,.$$

$z_{\mathcal{S}}(C,t) := \sum_{\ell=1}^{t}\log\lambda_\ell(C)$.

$z_{\mathrm{DGFact}}(C,s,t,\cdot,\cdot\,;F) \;-\; z_{\mathcal{S}}(C,t) \;\le\; t\log\left(\frac{s}{t}\right).$

Theorem

(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* $\{1,2,\ldots,r\}$*;*

(c) $z_{\mathrm{DGFact}}(C,s,t,A,b\,;F)$ *is discrete concave in* t *on* $\{1,2,\ldots,k\}$*.*

Proof.

(a) we see that the second derivative of the function is $-1/t$, which is negative on $\mathbb{R}_{++}$.

(b) we verify that discrete concavity is equivalent to $\lambda_t(C) \ge \lambda_{t+1}(C)$, for all integers t satisfying $1 \le t < r$, which we have.

(c) we view $z_{\mathrm{DGFact}}(C,s,t,A,b\,;F)$ as the point-wise minimum of $-\sum_{\ell=k-t+1}^{k}\log\left(\lambda_\ell\left(\Theta\right)\right) + \nu^{\mathsf{T}}\mathbf{e} + \pi^{\mathsf{T}}b + \tau s - t$ over the points in the convex feasible region of DGFact. So it suffices to show that this function is discrete concave in t. We verify that this is equivalent to $\lambda_{k-t+1}(C) \ge \lambda_{k-t+2}(C)$, for all integers t satisfying $1 < t \le k$, which we have. □

The Lagrangian spectral bound for CGMESP ([Lee and Lind, 2020])

$$v^* := \min_{\pi \in \mathbb{R}^m_+} v(\pi) := \sum_{\ell=1}^{t} \log \lambda_\ell \left(D_\pi C D_\pi\right) + \pi^\top b \; - \min_{K \subset N, |K|=s-t} \sum_{j \in K} \sum_{i \in M} \pi_i a_{ij} \,,$$

where $D_\pi \in \mathbb{S}^n_{++}$ is the diagonal matrix defined by

$$D_\pi[\ell, j] := \begin{cases} \exp\{-\frac{1}{2} \sum_{i=1}^m \pi_i a_{ij}\}, & \text{for } \ell = j; \\ 0, & \text{for } \ell \neq j. \end{cases}$$

Theorem (see [Ponte, Fampa, and Lee, 2024])

v^* is discrete concave in t on $\mathbb{Z}_{++}$.

Proof.

Because v^* is a point-wise minimum, we need only demonstrate that $v(\pi)$ is discrete concave in t, for each fixed $\pi \in \mathbb{R}^m_+$. It is possible to verify that $\sum_{\ell=1}^t \log \lambda_\ell \left(D_\pi C D_\pi\right)$ is discrete concave in t. So, it is enough to demonstrate that

$$\min \left\{ \textstyle\sum_{j \in K} \sum_{i \in M} \pi_i a_{ij} \; : \; K \subset N, |K| = s - t \right\}$$
$$= \min \left\{ \textstyle\sum_{j \in N} \left(\sum_{i \in M} \pi_i a_{ij}\right) x_j \; : \; \mathbf{e}^\top x = s - t, \, 0 \leq x \leq \mathbf{e}, \; x \in \mathbb{Z}^n \right\}$$

is discrete convex in t. Because of total unimodularity, we can drop the integrality requirement, and we see that the last expression is equivalently a minimization linear program, which is well-known to be convex in the right-hand side, which is affine in t. □

Variable fixing

Theorem (see [Anstreicher, Fampa, Lee, and Williams, 1996, 1999; Fampa and Lee, 2022])

Let

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

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

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

$$z_{\text{DGFact}}(C,s,t,A,b\;;F) := \min\Big\{-\textstyle\sum_{\ell=k-t+1}^{k}\log\left(\lambda_\ell\left(\Theta\right)\right)+\nu^{\mathsf{T}}\mathbf{e}+\pi^{\mathsf{T}}b+\tau s-t:$$
$$\operatorname{diag}(F\Theta F^{\mathsf{T}})+\upsilon-\nu-A^{\mathsf{T}}\pi-\tau\mathbf{e}=0,\Theta\succ 0,\upsilon\geq 0,\nu\geq 0,\pi\geq 0\Big\}$$

Consider the Lagrangian function corresponding to DGFact,

$$\mathcal{L}(\Theta,\nu,\pi,\tau,x,y,w) := -\textstyle\sum_{\ell=k-t+1}^{k}\log\left(\lambda_\ell\left(\Theta\right)\right)+\nu^{\mathsf{T}}\mathbf{e}+\pi^{\mathsf{T}}b+\tau s-t$$
$$+x^{\mathsf{T}}\left(\operatorname{diag}(F\Theta F^{\mathsf{T}})-\nu-A^{\mathsf{T}}\pi-\tau\mathbf{e}\right)-y^{\mathsf{T}}\nu-w^{\mathsf{T}}\pi,$$

with $\operatorname{dom}\mathcal{L}=\mathbb{S}^k_{++}\times\mathbb{R}^n\times\mathbb{R}^m\times\mathbb{R}\times\mathbb{R}^n\times\mathbb{R}^n\times\mathbb{R}^m$.

The corresponding dual function is

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

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 $\inf_{\Theta\in\,\mathbb{S}^k_{++},\nu,\pi,\tau}\mathcal{L}(\Theta,\nu,\pi,\tau,x,y,w)=$

$$\inf_{\Theta\in\,\mathbb{S}^k_{++}}\left\{-\textstyle\sum_{\ell=k-t+1}^{k}\log\left(\lambda_\ell\left(\Theta\right)\right)+x^{\mathsf{T}}\operatorname{diag}(F\Theta F^{\mathsf{T}})-t\right\}$$

$$+\inf_{\nu,\pi,\tau}\left\{\nu^{\mathsf{T}}(\mathbf{e}-x-y)+\pi^{\mathsf{T}}(b-Ax-w)+\tau(s-\mathbf{e}^{\mathsf{T}}x)\right\}.$$

The Γ function

Lemma (see [Nikolov, 2015])

Let $\lambda \in \mathbb{R}^k_+$ with $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_k$ and let $0 < t \leq k$. There exists a unique integer ι, with $0 \leq \iota < t$, such that

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

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

With the hypothesis of the lemma, let ι be the unique integer above. We define

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

Next, for $X \in \mathbb{S}^k_+$, [Nikolov, 2015] defines $\Gamma_t(X) := \phi_t(\lambda(X))$.

Theorem (see [Nikolov, 2015])

For $x \in \mathbb{R}^n$, we have $\inf_{\Theta \in \mathbb{S}^k_{++}} -\sum_{\ell=k-t+1}^{k} \log\left(\lambda_\ell\left(\Theta\right)\right) + x^\top \mathrm{diag}(F\Theta F^\top) - t$

$$= \begin{cases} \Gamma_t(F(x)), & \text{if } F(x) \succeq 0 \text{ and } \mathrm{rank}(F(x)) \geq t; \\ -\infty, & \text{otherwise.} \end{cases}$$

Theorem

For $(x, y, w) \in \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^m$, we have $\inf_{\nu,\pi,\tau} \nu^\top(\mathbf{e} - x - y) + \pi^\top(b - Ax - w) + \tau(s - \mathbf{e}^\top x)$

$$= \begin{cases} 0, & \text{if } \mathbf{e} - x - y = 0,\ b - Ax - w = 0,\ s - \mathbf{e}^\top x = 0; \\ -\infty, & \text{otherwise.} \end{cases}$$

Lagrangian dual of DGFact

Theorem

The Lagrangian dual of DGFact is equivalent to

$$z_{DDGFact}(C,s,t,A,b;F) = \max\left\{\Gamma_t(F(x)) \;:\; \mathbf{e}^\top x = s,\; Ax \le b,\; 0 \le x \le \mathbf{e}\right\}. \qquad \text{(DDGFact)}$$

Theorem

Let $\lambda \in \mathbb{R}^n_+$ *with* $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_r > \lambda_{r+1} = \cdots = \lambda_n = 0$. *Then,*

$$\begin{array}{lll} \text{(a)} & \phi_t(\lambda) > \sum_{\ell=1}^t \log(\lambda_\ell), & \textit{for } 0 < t < r, \\ \text{(b)} & \phi_t(\lambda) = \sum_{\ell=1}^t \log(\lambda_\ell), & \textit{for } t = r, \\ \text{(c)} & \phi_t(\lambda) = -\infty, & \textit{for } r < t \le n. \end{array}$$

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

Remark

We have $z(C,s,t,A,b) \le z_{DDGFact}(C,s,t,A,b;F)$ *from Lagrangian duality. The theorem above gives an alternative 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.

Remark

$$z_{GFact}(C,s,t,A,b;F) := \max\left\{\sum_{\ell=1}^t \log(\lambda_\ell(F(x))) \;:\; \mathbf{e}^\top x = s,\; Ax \le b,\; 0 \le x \le \mathbf{e}\right\} \qquad \text{(GFact)}$$

is an exact but non-convex relaxation for CGMESP. On the other hand, DDGFact is a convex relaxation for CGMESP, which is non-exact generally, except for the case of $t = s$.

Constructing a dual feasible solution

Let $F(\hat{x}) = \sum_{\ell=1}^{k} \hat{\lambda}_\ell \hat{u}_\ell \hat{u}_\ell^\top$, with $\hat{\lambda}_1 \geq \hat{\lambda}_2 \geq \cdots \geq \hat{\lambda}_{\hat{r}} > \hat{\lambda}_{\hat{r}+1} = \cdots = \hat{\lambda}_k = 0$ and $\hat{r} \geq t$. Following [Nikolov, 2015], let $\hat{\Theta} := \sum_{\ell=1}^{k} \hat{\beta}_\ell \hat{u}_\ell \hat{u}_\ell^\top$, where

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

for any $\epsilon > 0$, where $\hat{\imath} < t$ and $\hat{\delta} := \frac{1}{t-\hat{\imath}} \sum_{\ell=\hat{\imath}+1}^{k} \hat{\lambda}_\ell$. Then, the minimum duality gap between $\hat{x}$ in DDGFact and feasible solutions of DGFact of the form $(\hat{\Theta}, \upsilon, \nu, \pi, \tau)$ is the optimal value of

$$\min \left\{ \nu^\top \mathbf{e} + \pi^\top b + \tau s - t \ : \ \nu + A^\top \pi + \tau \mathbf{e} \geq \operatorname{diag}(F\hat{\Theta}F^\top), \ \nu \geq 0, \pi \geq 0 \right\} \qquad (G(\hat{\Theta}))$$

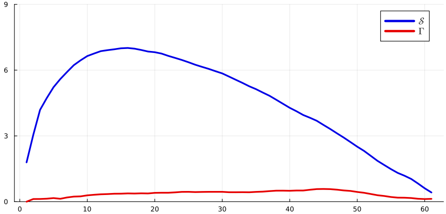
Let σ be the permutation of indices in N, such that $\operatorname{diag}(F\hat{\Theta}F^\top)_{\sigma(1)} \geq \ldots \geq \operatorname{diag}(F\hat{\Theta}F^\top)_{\sigma(n)}$. The following closed-form solution is optimal for $G(\hat{\Theta})$, when there are no $Ax \leq b$ constraints (see [Ponte, Fampa, and Lee, 2024]; also [Fampa and Lee, 2022; Li and Xie, 2023] for similar analysis for MESP).

$$\tau^* := \operatorname{diag}(F\hat{\Theta}F^\top)_{\sigma(s)},$$

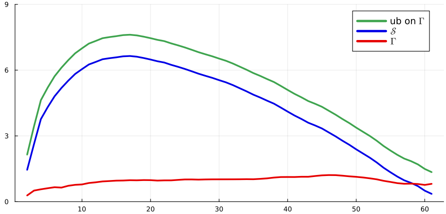
$$\nu^*_{\sigma(\ell)} := \begin{cases} \operatorname{diag}(F\hat{\Theta}F^\top)_{\sigma(\ell)} - \tau^*, & \text{for } 1 \leq \ell \leq s; \\ 0, & \text{for } s < \ell \leq n. \end{cases}$$

Theorem (new, even for MESP and binary D-Opt)

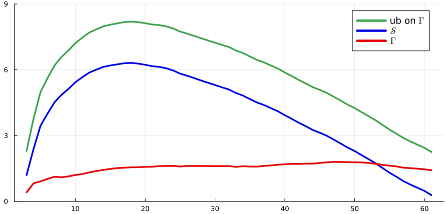
Let $\hat{x}$ be an optimal solution of DDGFact, with no side constraints $Ax \leq b$. Then, $(\hat{\Theta}, \nu^*, \tau^*)$ is an optimal solution to DGFact.



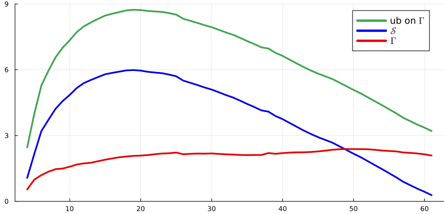
(a) $\kappa = 0$



(b) $\kappa = 1$



(c) $\kappa = 2$

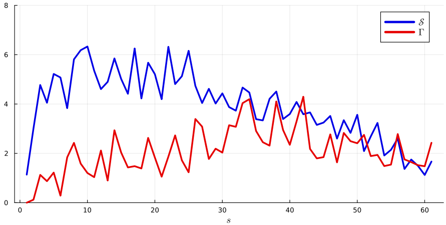


(d) $\kappa = 3$

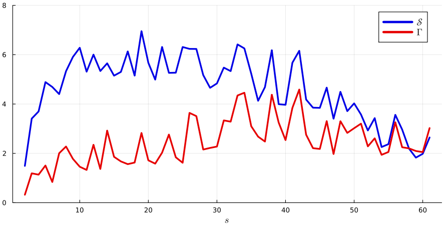
Gaps for GMESP, varying $t = s - \kappa$ ($n = 63$)

Results for B&B with variable fixing: GMESP/MESP

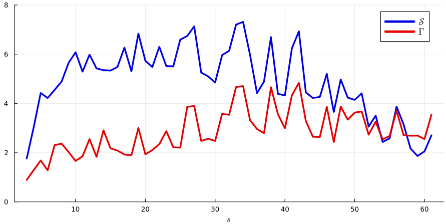
s	GMESP ($t := s-1$) root gap	nodes	tot prun	int prun	tot int	rel avg	rel std	var fix 0	var fix 1	B&B time	MESP root gap	nodes	tot prun	var fix 0	var fix 1	B&B time
2	0.36	186	1	1	179	0.44	0.08	75	6	1.44	0.02	3	2	0	0	0.04
3	0.48	557	14	9	501	0.55	0.07	269	24	4.22	0.06	10	5	52	0	0.08
4	0.59	2037	89	42	1554	0.61	0.07	1022	109	15.45	0.12	20	8	55	0	0.19
5	0.70	7404	579	187	5070	0.64	0.07	2724	483	42.28	0.13	33	13	58	0	0.29
6	0.73	20804	2190	569	13251	0.65	0.07	6668	1657	129.11	0.14	43	16	60	0	0.38
7	0.76	44592	5500	1194	26958	0.66	0.08	12582	4141	278.79	0.14	35	13	53	0	0.32
8	0.77	68682	9697	2056	40021	0.68	0.08	19272	8011	431.56	0.13	41	16	55	0	0.35
9	0.82	119525	20711	3648	67307	0.68	0.08	32902	17728	976.92	0.12	38	15	45	0	0.32
10	0.82	158998	34012	5048	84404	0.69	0.08	47229	32943	1112.10	0.11	37	17	49	0	0.29
11	0.77	147411	35635	4574	72563	0.69	0.08	50893	46972	1160.19	0.06	16	8	33	0	0.14
12	0.72	158170	40735	4522	69865	0.69	0.08	63096	77637	1491.04	0.09	46	21	42	0	0.41
13	0.64	142970	36444	3338	53587	0.70	0.08	67264	100845	1210.29	0.17	111	49	80	0	0.93
14	0.68	279210	66511	5059	88512	0.69	0.08	132296	237550	2821.80	0.13	196	83	131	0	1.72
15	0.69	386507	87553	5638	106718	0.68	0.07	176598	358770	5535.94	0.13	185	81	95	0	1.67
16	0.69	421261	92967	5301	99083	0.69	0.07	181361	430153	5178.73	0.16	323	149	136	0	2.83
17	0.73	519556	109265	5012	103521	0.69	0.06	202088	572510	6399.18	0.18	305	140	107	0	2.77
18	0.76	544073	110176	4483	98168	0.70	0.05	190782	625212	6958.49	0.25	878	391	302	0	7.64
19	0.83	713393	135220	5655	122085	0.72	0.04	212475	787816	10159.16	0.28	1105	489	381	0	9.20
20	0.86	695101	124354	5504	115999	0.75	0.03	174689	757696	9751.58	0.32	1357	586	425	0	11.31
21	0.90	637108	107189	4280	102540	0.76	0.03	132122	682763	8584.51	0.37	2135	850	784	0	17.85
22	0.95	586069	91694	4994	92685	0.78	0.03	97344	615472	7617.47	0.39	2342	855	807	0	20.81
23	0.99	510390	74438	7159	79882	0.79	0.03	64390	528729	6330.14	0.39	1811	660	572	0	15.24
24	1.01	368953	51277	7806	56157	0.80	0.03	35163	389241	4149.70	0.36	1244	463	340	0	10.42
25	1.01	214937	28168	5440	30889	0.81	0.02	15377	240272	2149.56	0.31	632	230	130	0	5.12
26	0.97	98751	12009	2756	13318	0.81	0.02	5084	121572	921.15	0.27	463	160	65	0	3.74
27	0.95	43037	4793	1475	5593	0.82	0.02	1410	58962	389.61	0.22	241	74	30	0	1.99
28	0.91	13854	1367	511	1667	0.82	0.02	234	22591	128.65	0.17	130	38	10	0	1.15
29	0.90	3403	281	134	347	0.82	0.03	20	6547	31.89	0.13	70	16	4	0	0.62
30	0.87	464	27	16	35	0.81	0.05	1	949	4.51	0.08	19	4	1	0	0.17
31	0.83	32	1	1	1	0.74	-	0	30	0.32	0.02	2	1	0	0	0.02



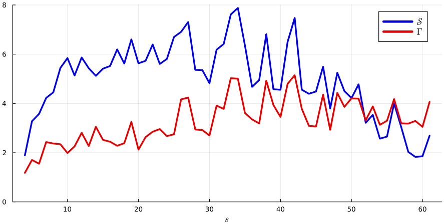
(a) $\kappa = 0$



(b) $\kappa = 1$



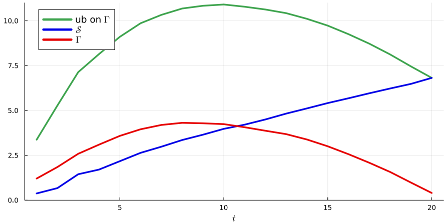
(c) $\kappa = 2$



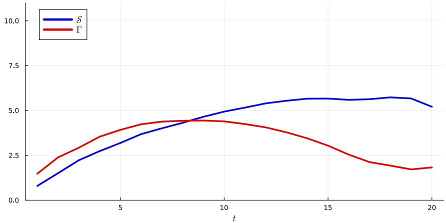
(d) $\kappa = 3$

Gaps for CGMESP, varying $t = s - \kappa$ ($n = 63$, $m = 10$)

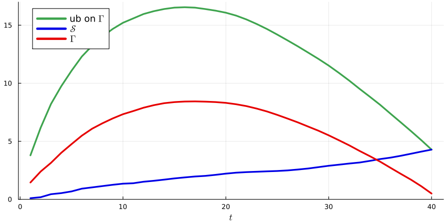
	CGMESP ($t := s-1$)												CMESP					
s	root gap	heur gap	imp inc	nodes	tot prun	int prun	tot int	rel avg	rel std	var fix 0	var fix 1	B&B time	root gap	nodes	tot prun	var fix 0	var fix 1	B&B time
2	0.93	0.37	1	121	2	1	8	0.43	0.06	149	0	6.80	0.85	23	3	63	0	5.63
3	1.18	-	0	27	0	0	3	0.60	0.01	51	0	0.49	0.88	19	2	36	0	0.34
4	0.99	-	0	35	0	0	2	0.60	0.00	93	2	0.59	0.63	17	4	63	2	0.25
5	1.08	-	0	741	76	18	43	0.60	0.08	1213	26	10.85	0.72	144	36	246	3	2.25
6	1.24	0.18	1	419	42	5	21	0.62	0.07	790	32	6.49	0.76	97	24	169	2	1.45
7	1.69	0.03	1	107	1	1	8	0.67	0.04	121	10	1.98	1.36	57	4	92	5	1.04
8	2.12	-	0	122	0	0	1	0.58	-	74	5	2.26	2.02	105	0	108	8	1.86
9	1.15	-	0	625	39	10	70	0.65	0.09	825	160	9.27	0.69	165	41	276	66	2.59
10	1.21	-	0	325	11	0	44	0.69	0.03	372	96	3.59	0.64	84	13	85	15	1.43
11	1.65	-	0	1046	121	6	34	0.68	0.03	1163	452	11.85	1.53	527	127	638	262	8.30
12	2.75	0.22	2	195	0	0	6	0.74	0.02	142	38	2.49	2.56	191	2	153	83	3.20
13	1.77	0.05	1	2904	396	22	106	0.67	0.05	2733	1227	43.59	1.60	1061	319	1432	635	17.42
14	1.71	-	0	47	0	0	3	0.67	0.00	41	23	0.77	1.45	39	0	40	33	0.72
15	1.14	-	0	1653	392	13	58	0.68	0.03	1266	1022	20.46	0.75	343	117	310	225	5.56
16	1.36	0.18	1	11198	2592	208	907	0.70	0.04	7157	6339	132.42	1.04	1898	747	2019	1416	32.60
17	1.97	-	0	876	75	2	9	0.78	0.03	552	668	11.24	1.53	415	79	343	366	7.23
18	1.68	0.31	1	29149	7943	448	1175	0.74	0.04	13686	18518	353.74	1.29	3383	1548	3046	3524	59.50
19	1.64	0.32	2	3664	557	72	252	0.73	0.04	2035	2806	48.31	1.16	1030	353	938	1175	16.49
20	2.55	-	0	209	1	0	4	0.76	0.00	75	215	2.99	2.21	213	3	75	195	3.77
21	1.47	0.04	1	47344	10268	820	2043	0.79	0.03	10281	36017	561.97	0.96	4812	1846	1197	4043	61.19
22	2.91	0.08	1	660	1	0	4	0.79	0.05	100	360	8.70	2.45	526	8	122	473	7.75
23	1.45	-	0	135	8	0	6	0.67	0.01	22	143	1.64	1.03	69	10	21	110	1.18
24	1.38	-	0	1677	163	14	27	0.75	0.06	223	1959	22.66	0.79	434	114	84	572	7.54
25	1.68	-	0	199	1	0	1	0.72	-	24	201	3.04	1.23	158	8	17	193	3.32
26	3.62	-	0	55	0	0	4	0.72	0.00	1	35	0.79	3.18	31	0	1	30	0.53
27	3.47	0.97	3	164	4	1	4	0.73	0.01	5	205	2.23	2.87	131	9	3	213	2.50
28	2.66	-	0	34	0	0	1	0.75	-	1	54	0.55	2.16	32	1	0	49	0.79
29	1.09	-	0	78	5	0	1	0.73	-	1	192	1.17	0.40	39	13	1	127	0.83
30	1.23	-	0	4	0	0	0	-	-	0	10	0.07	0.66	4	0	0	22	0.16
31	0.74	-	0	2	0	0	0	-	-	0	0	0.03	0.00	1	0	0	0	0.02



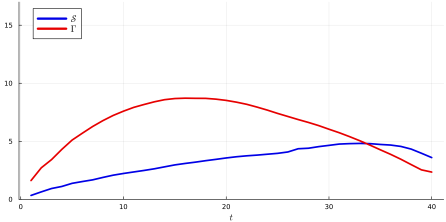
(a) GMESP, $s = 20$



(b) CGMESP, $m = 10$, $s = 20$



(c) GMESP, $s = 40$



(d) CGMESP, $m = 10$, $s = 40$

Gaps for GMESP and CGMESP, varying t, with s fixed ($n = 63$)

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