

## A Geodesic convexity

Recall that we are using the notation

$$P \#_t Q := P^{1/2} (P^{-1/2} Q P^{-1/2})^t P^{1/2}, \quad t \in [0, 1], \text{ and } P, Q \succ 0,$$

to denote the *geodesic* between positive definite matrices  $P$  and  $Q$  under the Riemannian metric  $g_P(X, Y) = \text{tr}(P^{-1} X P^{-1} Y)$ . The midpoint of this geodesic is  $P \#_{1/2} Q$ , and it is customary to drop the subscript and just write  $P \# Q$ .

### A.1 Proof of Lemma 3.3

Here we prove the log-g-convexity of  $E_\ell$  on the set of psd matrices. As far as we are aware, this result is novel. By continuity, it suffices to prove midpoint log-g-convexity; that is, it suffices to prove

$$E_\ell(P \# Q) \leq \sqrt{E_\ell(P) E_\ell(Q)}.$$

From basic multilinear algebra (see e.g., [5, Ch. 1]) we know that for any  $n \times n$  matrix  $P$ , there exists a projection matrix  $W$  such that  $E_\ell(P) = \text{tr} \wedge^\ell P = \text{tr} W^* P^{\otimes n} W$ . [40, Lemma 2.23] shows that

$$(P \# Q)^{\otimes n} = P^{\otimes n} \# Q^{\otimes n}.$$

Thus, it follows that

$$\begin{aligned} E_\ell(P \# Q) &= \text{tr} W^* (P \# Q)^{\otimes n} W = \text{tr} W^* [P^{\otimes n} \# Q^{\otimes n}] W \\ &\leq [\text{tr} W^* P^{\otimes n} W]^{1/2} [\text{tr} W^* Q^{\otimes n} W]^{1/2} \\ &= [E_\ell(P) E_\ell(Q)]^{1/2}, \end{aligned}$$

where the inequality follows from log-g-convexity of the trace map [40, Cor. 2.9].  $\square$

Observe that this result is *stronger* than the usual log-convexity result, which it yields as a corollary.

### A.2 Proof of Corollary 3.4

We present now a short new proof of the log-convexity of the map  $Z \mapsto E_\ell(A^\top Z A)^{-1}$ ; we assume that  $A$  has full column rank. As before, it suffices to prove midpoint convexity. Let  $Z, Y \succ 0$ . We must then show that

$$\log E_\ell \left( A^\top \left( \frac{Z+Y}{2} \right) A \right)^{-1} \leq \frac{1}{2} \log E_\ell(A^\top Z A)^{-1} + \frac{1}{2} \log E_\ell(A^\top Y A)^{-1}.$$

Since (e.g., [6, Ch. 5])  $(A^\top Z A) \# (A^\top Y A) \leq \frac{A^\top Z A + A^\top Y A}{2}$ , we get  $[A^\top (\frac{Z+Y}{2}) A]^{-1} \leq [(A^\top Z A) \# (A^\top Y A)]^{-1}$ . Since  $\log E_\ell$  is monotonic in Löwner order (Prop. 2.1-(i)), we see that

$$\log E_\ell \left( A^\top \left( \frac{Z+Y}{2} \right) A \right)^{-1} \leq \log E_\ell [(A^\top Z A) \# (A^\top Y A)]^{-1} = \log E_\ell [(A^\top Z A)^{-1} \# (A^\top Y A)^{-1}].$$

But from Lemma 3.3 we know that  $E_\ell(P \# Q) \leq \sqrt{E_\ell(P) E_\ell(Q)}$ , which allows us to write

$$\log E_\ell [(A^\top Z A)^{-1} \# (A^\top Y A)^{-1}] \leq \frac{1}{2} \log E_\ell(A^\top Z A)^{-1} + \frac{1}{2} \log E_\ell(A^\top Y A)^{-1},$$

which completes the proof.  $\square$

## B Bounding the support of the continuous relaxation

As mentioned in the main paper, this proof is identical to the proof provided by [44, Lemma 3.5] for A-optimal design once we derive  $\nabla f_\ell(z)$ ; we reproduce it here for completeness.

*Proof. (Theorem 3.6).* It is easy to show from (5.1) and Prop. 2.1-(iii) that

$$\frac{\partial f_\ell(z)}{\partial z_i} = -\frac{1}{\ell} x_i^\top \underbrace{U (\Lambda^{-1} - \nabla e_{m-\ell}(\Lambda) / e_{m-\ell}(\Lambda)) U^\top}_{W} x_i$$

and that  $W$  is positive definite.

Assume now that all choices of  $m(m+1)/2$  distinct rows of  $X$  have their mapping under  $\tilde{\phi}$  be independent. We now consider the Lagrangian multiplier version of (3.2):

$$f(z, u_i, v_i, \lambda) = f_\ell(z) - \sum_i u_i z_i + \sum_i (z_i - 1) + \lambda(\sum_i z_i - k)$$

Let  $z^*$  be the optimal solution, and let  $A \subseteq [n]$  be the indices  $i$  such that  $0 < z_i < 1$ . Assume by contradiction that  $|A| > m(m+1)/2$ . By KKT conditions, we have for  $i \in A$ ,

$$-\frac{\partial f(z^*)}{\partial z_i} = x_i^\top W x_i = \langle \phi(x) \mid \psi(W) \rangle = \mu \quad (\text{B.1})$$

where  $\phi$  is the mapping defined in Theorem 3.6 and  $\psi$  takes the upper triangle of a symmetric matrix and maps it to a vector of size  $m(m+1)/2$ . Then, (B.1) can be rewritten for  $m(m+1)/2$  indices in  $A$  as the following linear system of variables:

$$\begin{pmatrix} \tilde{\phi}(x_1) \\ \vdots \\ \tilde{\phi}(x_{m(m+1)/2+1}) \end{pmatrix} \begin{pmatrix} \psi(W) \\ -\lambda \end{pmatrix} = 0. \quad (\text{B.2})$$

By hypothesis, the first matrix is invertible and hence  $\psi(W)$  and  $\lambda$  must be 0, which contradicts the strict positive definiteness of  $W$ .  $\square$

## C Greedy algorithm details

To analyze our greedy algorithm, we need the following lemma, which is an extension of [2, Lemma 3.9] to all elementary symmetric polynomials:

**Lemma C.1.** *Let  $X \in \mathbb{R}^{n \times m}$  ( $n \geq m$ ) be a matrix with full column rank, and let  $k$  be a budget  $m \leq k \leq n$ . Let  $S$  be a random variable with probability*

$$P_S = \frac{\det(X_S^\top X_S)}{\sum_{T \subseteq [n], |T|=k} \det(X_T^\top X_T)}.$$

Then

$$\mathbb{E} \left[ E_\ell \left( (X_S^\top X_S)^{-1} \right) \right] \leq \left( \prod_{i=1}^{\ell} \frac{n-m+i}{k-m+i} \right) E_\ell \left( (X^\top X)^{-1} \right). \quad (\text{C.1})$$

*Proof.* The below calculations depend heavily on the Cauchy-Binet formula, of which we reproduce a special case here for  $X \in \mathbb{R}^{n \times m}$ :

$$\det(X^\top X) = \sum_{S \subseteq [n], |S|=m} \det(X_S^\top X_S). \quad (\text{C.2})$$

We also use the representation (2.2). By definition we have

$$\mathbb{E} \left[ E_\ell \left( (X_S^\top X_S)^{-1} \right) \right] = \frac{\sum_{S \subseteq [n], |S|=k} \det(X_S^\top X_S) E_\ell \left( (X_S^\top X_S)^{-1} \right)}{\sum_{S \subseteq [n], |S|=k} \det(X_S^\top X_S)}$$

For the denominator, we have

$$\begin{aligned} \sum_{S \subseteq [n], |S|=k} \det(X_S^\top X_S) &= \sum_{S \subseteq [n], |S|=k} \det(X_S^\top X_S) \\ &\stackrel{(a)}{=} \sum_{S \subseteq [n], |S|=k} \sum_{T \subseteq S, |T|=m} \det(X_T^\top X_T) \\ &\stackrel{(b)}{=} \binom{n-m}{k-m} \sum_{T \subseteq [n], |T|=m} \det(X_T^\top X_T) \\ &\stackrel{(c)}{=} \binom{n-m}{k-m} \det(X^\top X) \end{aligned}$$

where (a) is obtained using the Cauchy-Binet formula (C.2), (b) by noticing that there are  $\binom{n-m}{k-m}$  sets of size  $k$  that contain a set  $T$  of size  $m$ , and (c) by reapplying (C.2).

For the numerator, we first use the fact that  $E_\ell(A^{-1}) = \frac{1}{\det A} E_{m-\ell}(A)$ :

$$\begin{aligned}
\sum_{S \subseteq [n], |S|=k} \det(X_S^\top X_S) E_\ell \left( (X_S^\top X_S)^{-1} \right) &\stackrel{(a)}{\leq} \sum_{S \subseteq [n], |S|=k} E_{m-\ell}(X_S^\top X_S) \\
&= \sum_{S \subseteq [n], |S|=k} \sum_{L \subseteq [m], |L|=m-\ell} (X_S^\top X_S)[L|L] \\
&\stackrel{(b)}{=} \sum_{S \subseteq [n], |S|=k} \sum_{L \subseteq [m], |L|=m-\ell} \det((Y_L)_S^\top (Y_L)_S) \\
&\stackrel{(c)}{=} \sum_{S \subseteq [n], |S|=k} \sum_{L \subseteq [m], |L|=m-\ell} \sum_{T \subseteq S, |T|=m-\ell} \det((Y_L)_T^\top (Y_L)_T) \\
&= \binom{n-m+\ell}{k-m+\ell} \sum_{L \subseteq [m], |L|=m-\ell} \sum_{T \in [n], |T|=m-\ell} \det((Y_L)_T^\top (Y_L)_T) \\
&\stackrel{(d)}{=} \binom{n-m+\ell}{k-m+\ell} \sum_{L \subseteq [m], |L|=m-\ell} \det((Y_L)^\top (Y_L)) \\
&= \binom{n-m+\ell}{k-m+\ell} \sum_{L \subseteq [m], |L|=m-\ell} (X^\top X)[L|L] \\
&= \binom{n-m+\ell}{k-m+\ell} E_{m-\ell}(X^\top X)
\end{aligned}$$

Here, (a) is just (2.2); we have equality if all subsets  $S$  of size  $k$  produce strictly positive definite matrices  $X_S^\top X_S$ . For (b), we note  $Y_L$  the submatrix of  $X$  with all columns but those in  $L$  removed; then,  $(Y_L)_S^\top (Y_L)_S = [X_S^\top X_S]$  for all subsets  $S$ . (d) is an application of Cauchy-Binet. Hence,

$$\begin{aligned}
\mathbb{E} \left[ E_\ell \left( (X_S^\top X_S)^{-1} \right) \right] &= \frac{\sum_{S \subseteq [n], |S|=k} \det(X_S^\top X_S) E_\ell \left( (X_S^\top X_S)^{-1} \right)}{\sum_{S \subseteq [n], |S|=k} \det(X_S^\top X_S)} \\
&= \frac{\binom{n-m+\ell}{k-m+\ell} E_{m-\ell}(X^\top X)}{\binom{k-m}{n-m} \det(X^\top X)} \\
&= \left( \prod_{i=1}^{\ell} \frac{n-m+i}{k-m+i} \right) E_\ell((X^\top X)^{-1})
\end{aligned}$$

□

We can now prove Theorem 4.3:

*Proof.* We recursively show that greedily removing  $j$  items constructs a set  $S$  (of size  $(n-j)$ ) s.t.

$$E_\ell \left( (X_S^\top X_S)^{-1} \right) \leq \left( \prod_{i=1}^{\ell} \frac{n-m+i}{n-j-m+i} \right) E_\ell \left( (X^\top X)^{-1} \right). \quad (\text{C.3})$$

(C.3) is trivially true for  $j = 0$ . Assume now that (C.3) holds for  $j \geq 0$ , and let  $S_j$  be the corresponding set of size  $(n-j)$ . Let now  $S_{j+1}$  be the set of size  $|S_j| - 1$  that minimizes  $E_\ell(X_{S_{j+1}}^\top X_{S_{j+1}})$ .

From lemma 4.2, we know that for sets  $S$  of size  $|S_j| - 1$  drawn according to dual volume sampling,

$$\mathbb{E} \left[ E_\ell \left( (X_S^\top X_S)^{-1} \right) \right] \leq \left( \prod_{i=1}^{\ell} \frac{|S_j| - m + i}{(|S_j| - 1) - m + i} \right) E_\ell \left( (X_{S_j}^\top X_{S_j})^{-1} \right).$$

In particular, the minimum of  $E_\ell(X_S^T X_S)$  over all sets of size  $|S_j| - 1$  is upper bounded by the expectancy:  $E_\ell(X_{S_{j+1}}^T X_{S_{j+1}}) \leq \left( \prod_{i=1}^\ell \frac{n-j-m+i}{n-j-1-m+i} \right) E_\ell \left( (X_{S_j}^\top X_{S_j})^{-1} \right)$ .

By recursion hypothesis applied to  $S_j$ , we then have

$$\begin{aligned} E_\ell(X_{S_{j+1}}^T X_{S_{j+1}}) &\leq \left( \prod_{i=1}^\ell \frac{n-j-m+i}{n-j-1-m+i} \right) E_\ell \left( (X_{S_j}^\top X_{S_j})^{-1} \right) \\ &\leq \left( \prod_{i=1}^\ell \frac{n-j-m+i}{n-j-1-m+i} \right) \left( \prod_{i=1}^\ell \frac{n-m+i}{n-j-m+i} \right) E_\ell \left( (X^\top X)^{-1} \right) \\ &\leq \left( \prod_{i=1}^\ell \frac{n-m+i}{n-(j+1)-m+i} \right) E_\ell \left( (X^\top X)^{-1} \right), \end{aligned}$$

which concludes the recursion. Then, constructing a set of size  $k$  amounts to setting  $j = n - k$  in Eq.(C.3), which proves Eq. (4.2).  $\square$

## D Obtaining the dual formulation

We first show that (5.2) has  $H \succ 0$ : by contradiction, assume that there exists  $x$  such that  $x^\top H x < 0$  and  $\|x\| = 1$ . Then setting  $A = I - \frac{t}{1+t} x x^\top$  has  $g(A)$  go to infinity with  $t$ .

Next,  $g(A) = -\frac{1}{\ell} \log E_\ell(A) - \text{tr}(H A^{-1})$  reaches its maximum on  $\mathbb{S}_m^{++}$ : if  $\|A\| \rightarrow \infty$ , we easily have  $g \rightarrow -\infty$ . The same holds for  $A \rightarrow \partial \mathbb{S}_m^{++}$ .

We now derive the dual form:

$$\begin{aligned} (5.2) &\iff \inf_{\substack{\mu \in \mathbb{R}, \\ H \in \mathbb{R}^{m \times m}}} \sup_{A \succ 0, z \geq 0} -\frac{1}{\ell} \log E_\ell(A) - \text{tr}(H A^{-1}) + \text{tr}(H X^\top \text{Diag}(z) X) - \mu(\mathbf{1}^\top z - k) \\ (5.2) &\iff \inf_{\mu \in \mathbb{R}, H \succeq 0} \left[ f_\ell^*(-H) + \sup_{z \geq 0} \text{tr}(H X^\top \text{Diag}(z) X) - \mu(\mathbf{1}^\top z - k) \right] \\ (5.2) &\iff \inf_{\mu \in \mathbb{R}, H \succeq 0} \left[ f_\ell^*(-H) + \sup_{z \geq 0} \sum_i z_i (x_i^\top H x_i - \mu) + \mu k \right] \\ (5.2) &\iff \inf_{\substack{x_i^\top H x_i \leq \mu, \\ H \succeq 0}} f_\ell^*(-H) + k\mu \\ (5.2) &\iff \sup_{\substack{x_i^\top H x_i \leq 1, \\ H \succeq 0, \mu > 0}} -f_\ell^*(-\mu H) - k\mu \\ (5.2) &\stackrel{*}{\iff} \sup_{\substack{x_i^\top H x_i \leq 1, \\ H \succeq 0}} -f_\ell^*(-H) \end{aligned}$$

Where  $\stackrel{*}{\iff}$  follows from  $f_\ell^*(-\mu H) = \sup_{A \succ 0} -\text{tr}(H A) - f_\ell(A/\mu) = f_\ell^*(-H) - \log \mu$ .

Finally, we saw that by definition of  $a(H)$ ,  $f_\ell^*(-H) = g(a(H)) = -E_\ell(a(H)) - \text{tr}(H(a(H))^{-1})$ , and that the eigenvalues  $\Lambda$  of  $a(H)$  verify

$$\lambda_i^2 \frac{e_{\ell-1}(\lambda_1, \dots, \lambda_{i-1}, \lambda_{i+1}, \dots, \lambda_m)}{e_\ell(\lambda_1, \dots, \lambda_m)} = h_i, \quad 1 \leq i \leq m.$$

Then,

$$\begin{aligned}
e_\ell(\lambda_1, \dots, \lambda_m) \operatorname{tr}(H (a(H))^{-1}) &= \sum_i \frac{1}{\lambda_i} \lambda_i^2 e_{\ell-1}(\lambda_1, \dots, \lambda_{i-1}, \lambda_{i+1}, \dots, \lambda_m) \\
&= \sum_i \lambda_i e_{\ell-1}(\lambda_1, \dots, \lambda_{i-1}, \lambda_{i+1}, \dots, \lambda_m) \\
&= \sum_i \sum_{J \subseteq [n], |J|=\ell, i \in J} \prod_{j \in J} \lambda_j
\end{aligned}$$

Each subset  $J$  is hence going to appear  $\ell$  times, once for each of its elements; finally

$$\operatorname{tr}(H (a(H))^{-1}) = \ell \sum_{J \subseteq [n], |J|=\ell} \prod_{j \in J} \lambda_j / e_\ell(\lambda_1, \dots, \lambda_m) = \ell$$

and hence

$$\sup_{\substack{x_i^\top H x_i \leq 1, \\ H \succeq 0}} -f_\ell^*(-H) \iff \sup_{\substack{x_i^\top H x_i \leq 1, \\ H \succeq 0}} -g(a(H)) = \sup_{\substack{x_i^\top H x_i \leq 1, \\ H \succeq 0}} \frac{1}{\ell} \log E_\ell(a(H)) + \ell.$$

## E Additional synthetic experimental results

To compare to [44], we generated the experimental matrix  $X$  by sampling  $n$  vectors of size  $m$  from the multivariate Gaussian distribution of mean 0 and covariance  $\Sigma = \operatorname{Diag}(1^{-\alpha}, \dots, m^{-\alpha})$  for various sizes of  $\alpha$  and multiple budgets  $k$ , with  $m = 50, n = 1000$ ;  $\alpha$  controls hows *skewed* the distribution is.

Table 4:  $\|z\|_0$  for  $n = 500, m = 30, \ell = 15$

	$k = 60$	$k = 120$	$k = 180$	$k = 240$	$k = 300$
$\alpha = 1$	$167 \pm 9$	$192 \pm 6$	$241 \pm 5$	$290 \pm 4$	$335 \pm 4$
$\alpha = 2$	$160 \pm 4$	$187 \pm 5$	$240 \pm 2$	$284 \pm 3$	$331 \pm 6$
$\alpha = 3$	$160 \pm 4$	$190 \pm 3$	$237 \pm 5$	$281 \pm 4$	$333 \pm 3$

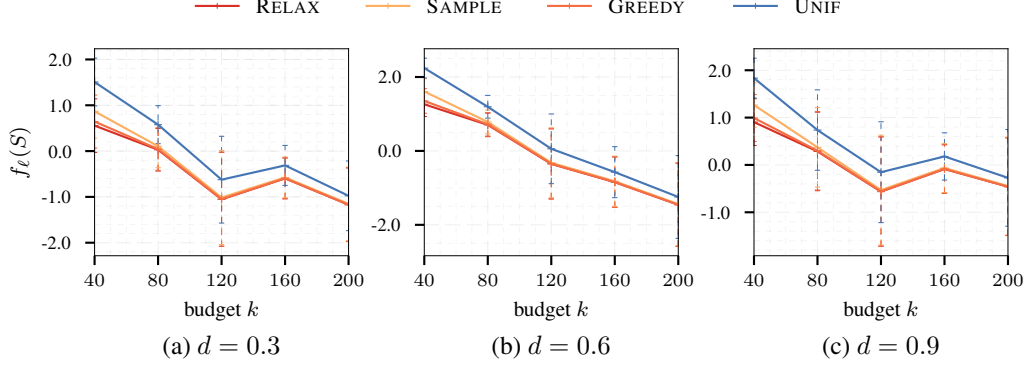


Figure 3: Synthetic experiments,  $n = 500$ ,  $m = 30$ ,  $\ell = 1$ .

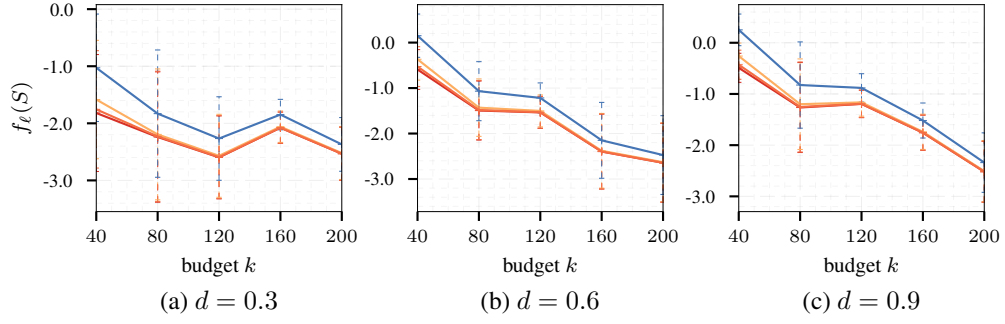


Figure 4: Synthetic experiments,  $n = 500$ ,  $m = 30$ ,  $\ell = 10$ .

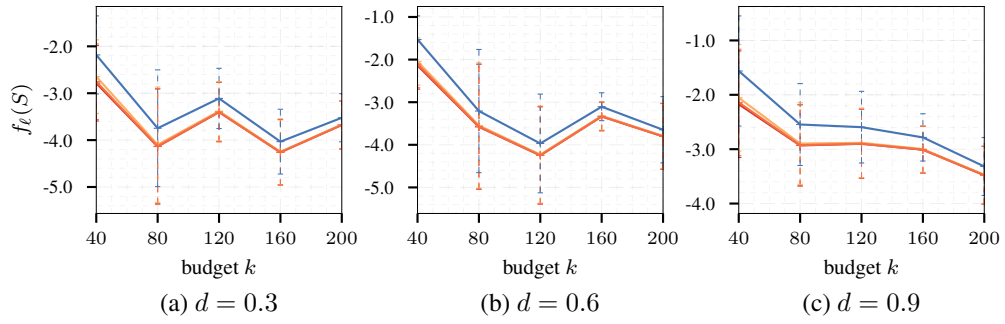


Figure 5: Synthetic experiments,  $n = 500$ ,  $m = 30$ ,  $\ell = 30$ .

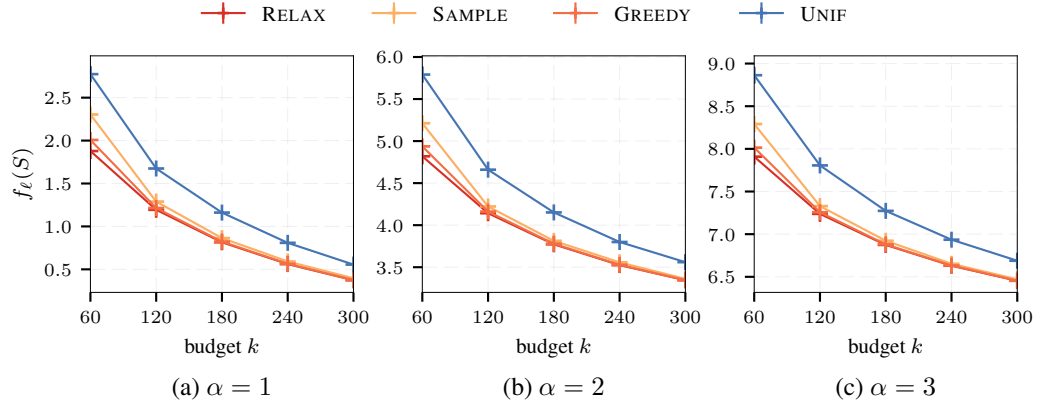


Figure 6: Synthetic experiments,  $n = 500$ ,  $m = 30$ ,  $\ell = 1$ .

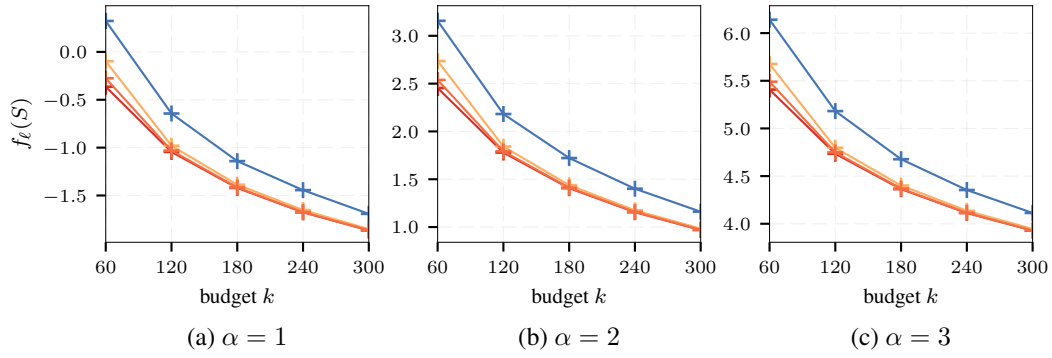


Figure 7: Synthetic experiments,  $n = 500$ ,  $m = 30$ ,  $\ell = 15$ .

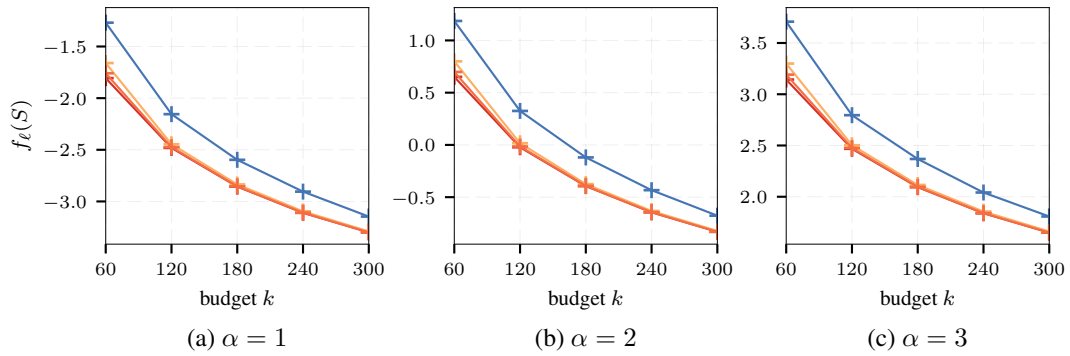


Figure 8: Synthetic experiments,  $n = 500$ ,  $m = 30$ ,  $\ell = 30$ .