Tridiagonal Maximum-Entropy Sampling and Tridiagonal Masks

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Abstract

The NP-hard maximum-entropy sampling problem (MESP) seeks a maximum (log-)determinant principal submatrix, of a given order, from an input covariance matrix $C$.

We give an efficient dynamic-programming algorithm for MESP when $C$ (or its inverse) is tridiagonal and generalize it to the situation where the support graph of $C$ (or its inverse) is a spider graph with a constant number of legs (and beyond). We give a class of arrowhead covariance matrices $C$ for which a natural greedy algorithm solves MESP.

A mask $M$ for MESP is a correlation matrix with which we pre-process $C$, by taking the Hadamard product $M \circ C$. Upper bounds on MESP with $M \circ C$ give upper bounds on MESP with $C$. Most upper-bounding methods are much faster to apply, when the input matrix is tridiagonal, so we consider tridiagonal masks $M$ (which yield tridiagonal $M \circ C$). We make a detailed analysis of such tridiagonal masks, and develop a combinatorial local-search based upper-bounding method that takes advantage of fast computations on tridiagonal matrices.

Keywords: nonlinear combinatorial optimization, covariance matrix, differential entropy, maximum-entropy sampling, dynamic programming, local search, spider, arrowhead, tridiagonal, mask, correlation matrix

1. Introduction

Let $C$ be an order-$n$ symmetric positive semidefinite real matrix, and let $s$ be an integer satisfying $1 \leq s \leq n$. In applications, $C$ is the covariance matrix for

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a multivariate Gaussian random vector \( Y_{N_n} \), where \( N_n := [1, n] := \{1, 2, \ldots, n\} \) — note that we regard \( N_n \) as an ordered set, which will be important later. For nonempty \( S \subseteq N_n \), let \( C[S, S] \) denote the principal submatrix of \( C \) indexed by \( S \). We denote \( \log \det(\cdot) \) by \( \text{ldet}(\cdot) \). Up to constants, \( \text{ldet} C[S, S] \) is the (differential) entropy associated with the subvector \( Y_S \) (see [SW87], for example). The maximum-entropy sampling problem, defined by [SW87], is

\[
  z = \max \{ \text{ldet} C[S, S] : |S| = s, S \subseteq N_n \} \quad \text{(MESP)}
\]

MESP corresponds to choosing a maximum-entropy subvector \( Y_S \) from \( Y_{N_n} \), subject to \( |S| = s \). Later, it will sometimes be convenient to emphasize the dependence of MESP on the data, and in such situations we will write \( \text{MESP}(C, s) \) and \( z(C, s) \).

MESP was introduced in [SW87], it was established to be NP-Hard in [KLQ95] (via reduction from the NP-Complete problem: does an \( n \)-vertex graph \( G \) have a vertex packing of cardinality \( s \)), and there has been considerable work on algorithms. Viable approaches aimed at exact solution of moderate-sized instances employ branch-and-bound (see [KLQ95]). For use in branch-and-bound, we have many methods for efficiently calculating good upper bounds; see [KLQ95, AFLW96, AFLW99, HLW01, LW03, AL04, BL07, Ans18, Ans20, CFL21, Nik15, LX20, CFL21] and the survey [Lee12]. Notably, we have developed an R package providing an easy means for instantiating MESP from raw environmental-monitoring data (see [ATL20a, ATL20b]).

In what follows, “\( \circ \)” denotes Hadamard (i.e., elementwise) product of a pair of matrices of the same dimensions. Given a positive integer \( n \), we define a mask as any \( n \times n \) symmetric positive semidefinite matrix \( M \) with all ones on the diagonal. Masks are better known as “correlation matrices”. These were introduced for MESP in [AL04], where it was observed that for any \( S \) and mask \( M \), \( \text{ldet} C[S, S] \leq \text{ldet}(C \circ M)[S, S] \), and so any upper bound on MESP for \( C \circ M \) is valid for the MESP on \( C \). It is a challenge to find a good mask with respect to a particular MESP upper-bounding method — i.e., a mask \( M \) that minimizes the upper bound on \( z(C \circ M, s) \). This topic was investigated in [AL04] and [BL07]. We define a combinatorial mask as any block-diagonal mask \( M \) where the diagonal blocks (which may vary in size) are matrices of all ones. At the extremes, we have \( M := I_n \) (an identity matrix) and \( M := J_n \) (an all ones matrix). As we observed in [AL04], we can view some of [HLW01] and [LW03] in this way; e.g., the “spectral partition bound” of [HLW01]. But there are many possibilities for masks that are not combinatorial masks. For example, a (tridiagonal) \( \frac{1}{2} \)-mask \( M \) has \( M_{i,i+1} = M_{i+1,i} := \frac{1}{2} \) for \( i = 1, \ldots, n-1 \) (and all other off-diagonal entries are 0). One goal of ours is to investigate computational aspects of tridiagonal masks \( M \), so as to take advantage of the fact that most bounds can be calculated much faster (than on dense matrices) for tridiagonal matrices (in our case, \( M \circ C \)).

In Section 2, we give an \( \mathcal{O}(n^5) \) dynamic-programming algorithm for MESP when \( C \) is tridiagonal. This also solves the problem in the same complexity when instead \( C^{-1} \) is tridiagonal. This is the first progress on identifying significantly polynomially-solvable cases of MESP. We extend our result to the case...
where the support graph of $C$ is a spider with a constant number of legs, and we indicate how it can be further extended when the number of connected components of the support graph of $C$ is polynomial in $n$. Finally, we present the results of computational experiments on matrices having support graphs that are spiders, indicating the superiority of a parallel implementation of our dynamic-programming algorithm as compared with branch-and-bound.

In Section 3, we characterize a class of positive-semidefinite “arrowhead matrices” (i.e., having the support graph of $C$ being a star), such that a certain natural greedy algorithm optimally solves MESP.

In Section 4, we characterize for each $n$, masks that differ from $\frac{1}{2}$-masks in two (symmetric) pairs of off-diagonal positions. These results are useful in identifying good masks for MESP bounds, in the context of local search in the space of masks.

In Section 5, we develop a combinatorial local-search algorithm that seeks a good tridiagonal mask $M$ for the so-called ‘linx’ upper bound (which is one of the best known upper-bounding method for MESP). Some computational experiments validate our approach.

2. Tridiagonal covariance matrices

The inverse covariance matrix, known as the precision matrix, captures the conditional covariances between pairs of random variables, conditioning on the remaining $n - 2$ random variables. For a spatial process with random variables placed in a line, a reasonable model may have the precision matrix being tridiagonal, when the random variables are numbered in a natural order (along the line); intuitively, such a model would assume that no extra information can be obtained from a non-neighbor of a random variable $Y_i$, over and above the information obtainable from the neighbors of $Y_i$.

To see how the inverse covariance matrix plays a role for MESP, we employ the identity

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

(see [HJ85, Section 0.8.4]). With this identity, we have $z(C,s) = \text{ldet} C + z(C^{-1}, n - s)$, and so the MESP for choosing $s$ elements with respect to $C$ is equivalent to the MESP for choosing $n - s$ elements with respect to $C^{-1}$.

The determinant of a tridiagonal matrix can be calculated in linear time, via a simple recursion (see [Dem97]), which we write for the symmetric case as that is our need. Let $T_1 = (a_1)$, and for $r \geq 2$, let

$$T_r := \begin{pmatrix} a_1 & b_1 & b_2 \\ b_1 & a_2 & b_2 \\ & \ddots & \ddots \\ & & b_{r-1} & b_{r-1} \\ & & & b_r \\ & & & a_r \end{pmatrix}.$$
Lemma 1. Defining \( \det T_0 := 1 \), we have \( \det T_r =: a_r \det T_{r-1} - b_r^2 \det T_{r-2} \), for \( r \geq 2 \).

Theorem 2. MESP is polynomially solvable when \( C \) or \( C^{-1} \) is tridiagonal, or when there is a symmetric permutation of \( C \) or \( C^{-1} \) so that it is tridiagonal.

Proof. Suppose that \( C \) is tridiagonal. Let \( S \) be an ordered subset of \( N_n \). Then we can write \( C[S, S] \) uniquely as \( C[S, S] = \text{Diag}(C[S_1, S_1], C[S_2, S_2], \ldots, C[S_p, S_p]) \), with \( p \geq 1 \), where each \( S_i \) is a maximal ordered contiguous subset of \( S \), and for all \( 1 \leq i < j \leq p \), all elements of \( S_i \) are less than all elements of \( S_j \). We call the \( S_i \) the pieces of \( S \), and in particular \( S_p \) is the last piece. It is easy to see that

\[
\det C[S, S] = \prod_{i=1}^{p} \det C[S_i, S_i] = \det C[S_p, S_p] \times \det C[S \setminus S_p, S \setminus S_p].
\]

Of course every \( S \) has a last piece, and for an optimal \( S \) to MESP, if the last piece is \( S_p =: [k, \ell] \), then we have the “principle of optimality”:

\[
\lde C[S \setminus [k, \ell], S \setminus [k, \ell]] = z(C[N_{k-2}, N_{k-2}], s - (\ell - k + 1)).
\]

With this way of thinking, we define

\[
f(k, \ell, t) := \max \left\{ \lde C[S, S] : |S| = t, S \subset N_n, \text{ and the last piece of } S \text{ is } [k, \ell] \right\},
\]

for \( 1 \leq \ell - k + 1 \leq t \leq s \). Note that the last block of \( S \) (in the definition of \( f \)) has \( \ell - k + 1 \) elements, which is why \( t \) must be at least that large. We have that

\[
z(C, s) = \max_{k, \ell} \left\{ f(k, \ell, s) : 1 \leq k \leq \ell \leq n, \ \ell - k + 1 \leq s \right\},
\]

where we are simply maximizing over the possible (quadratic number of) last pieces.

Our dynamic-programming recursion is

\[
f(k, \ell, t) = \lde C[[k, \ell], [k, \ell]] + \max_{i,j} \left\{ f(i, j, t - (\ell - k + 1)) : 1 \leq i \leq j \leq k - 2, \ j - i + 1 \leq t - (\ell - k + 1) \right\},
\]

The idea is that if \([k, \ell]\) is the last block of an optimal selection of \( t \) elements, then we have to pick \( t - (\ell - k + 1) \) more elements, and element \( k - 1 \) is ruled out (because \([k, \ell]\) is maximal).

To get the recursion started, we calculate

\[
f(k, \ell, \ell - k + 1) = \lde C[[k, \ell], [k, \ell]],
\]

for \( 1 \leq k \leq \ell \leq n, \ \ell - k + 1 \leq s \), observing that in such a boundary case, there is only one feasible solution. Already, it appears that the initialization requires \( \mathcal{O}(n^3) \) basic arithmetic operations, but in fact we can do this part in \( \mathcal{O}(n^2) \) operations, using the tridiagonal-determinant formula (Lemma 1).
Next, we compute, using the recursion, for $t = 1, 2, \ldots, s$, $f(k, \ell, t)$ for all $1 \leq k \leq \ell \leq n$ such that $\ell - k + 1 < t$. It is not hard to see that this gives an $O(n^5)$ algorithm for MESP, when $C$ is tridiagonal, and by earlier observations, we also get an $O(n^5)$ algorithm for MESP, when $C^{-1}$ is tridiagonal.

For an arbitrary symmetric $C$, with rows and columns indexed from $N_n$, we consider the support graph $G(C)$, with node set $V(G(C)) := N_n$, and edge set $E(G(C)) := \{(i, j) : i, j \in N_n, i < j, C[i, j] \neq 0\}$. If $C$ is a generic tridiagonal matrix (i.e., $C[i, i + 1] \neq 0$ for $i \in N_{n-1}$), then $G(C)$ is the path $P_n := \{1, 2, \ldots, n\}$. If $C$ is tridiagonal but not generic, then $G(C)$ is a subgraph of $P_n$. Because we can efficiently solve MESP when $C$ is tridiagonal (and also when $C$ is tridiagonal after symmetric permutation), it is natural to consider broader classes of $C$, and natural exploitable structure is encoded in the support graph $G(C)$.

We are interested in “spiders” with $r \geq 1$ legs on an $n$-vertex set (see [MMW08], for example): for convenience, we let the vertex set be $N_n$, and let vertex 1 be the body of the spider; the non-body vertex set $V_i$ of leg $i$, is a non-empty contiguously numbered subset of $N_n \setminus \{1\}$, such that distinct $V_i$ do not intersect, and the union of all $V_i$ is $N_n \setminus \{1\}$; we number the legs $i$ in such a way that: (i) the minimum element of $V_1$ is 2, and (ii) the minimum element of $V_{i+1}$ is one plus the maximum element of $V_i$, for $i \in [1, r - 1]$. A small example clarifies all of this; see Figures 1–2. Note that with one leg, the spider is the path $P_n$, and with two legs, the vertices can be re-numbered so that the spider is the path $P_n$. So, we may as well assume that the spider has $r \geq 3$ legs.

Consider how a MESP solution $S$ intersects with the vertices of the spider. As before, the solution has pieces. Note how at most one piece contains the body, and every other piece is a contiguous set of vertices of a leg. The number of

![Figure 1: Spider with five legs](attachment:image.png)
distinct possible pieces containing the body is $O(n^r)$. And the number of other pieces is $O(n^2)$. Overall, we have $O(n^r)$ pieces. In any solution, we can order the pieces by the minimum vertex in each piece. Based on this, we have a well-defined last piece. From this, we can devise an efficient dynamic-programming algorithm, when we consider $r$ to be constant.

**Theorem 3.** MESP is polynomially solvable when $G(C)$ or $G(C^{-1})$ is a spider with a constant number of legs.

In fact, we can easily organize a dynamic-programming scheme to exploit parallel computation. We can compute $\text{ldet} C[S_1,S_1]$ for all possible pieces containing the body 1. In parallel, we can compute optimal MESP solution values for all possible budgets $t \leq s$ for each leg, keeping track of the minimum vertex used for each such solution. With all of that information, we can then calculate an overall optimal solution.

We conducted some experiments to get some evidence that our dynamic-programming algorithm can be practical, compared to branch-and-bound. For each of $k = 13, 18, 23, 28, 33, 38, 43$, we constructed ten positive-semidefinite matrices $C$, with $G(C)$ being a spider with three legs and $k$ vertices per leg. So we have $n = 3k + 1$, and we chose $s \sim \ell n/4$, for $\ell = 1, 2, 3$. For the matrix constructions, we built a cvx (see [GB17]) semidefinite-programming model that takes a random choice of positive diagonal elements (constructed using \texttt{rand} of Matlab). The objective of the semidefinite-program was to maximize the sum of the off-diagonal elements of $C$, subject to $C$ is positive semidefinite, and $G(C)$ being the spider described above.

In Table 3, we report on our numerical experiments. We compare our parallel dynamic-programming algorithm, implemented in Matlab, with the serial
branch-and-bound Matlab code of [Ans20], which in turn uses the conic solver SDPT3 (see [TTT12, TTT99]). For our dynamic-programming algorithm, we use the Matlab parallel for-loop instruction `parfor`, for easy parallelization across spider legs. Parallelizing branch-and-bound would be a much more difficult task, and load balancing is highly nontrivial. We note that the running time of Matlab is highly variable (particularly for branch-and-bound), even with the same data and deterministic implementations of the algorithms. But because we average over ten experiments for each choice of \( n \) and \( s \), our results are meaningful. In the individual experiments it is clear that the dynamic-programming algorithm has more consistent time performance, while the time taken by the branch-and-bound fluctuates considerably. For most of the experiments, we set an upper limit of 2 hours (7200 seconds), except for the hardest one, the \( n = 130, s = 97 \) experiment, where we increased the time limit to 4 hours. In the table, * indicates that the time limit was reached. Overall the dynamic-programming algorithm performed much better than branch-and-bound, and it scales much better.

| \( n \) (k) | \( s \) | No. of trials | Avg. time for DP (sec.) | Avg. time for B&B (sec.) |
|------------|-----|-------------|------------------|-------------------|
| 40 (13)    | 10  | 10          | < 1              | 90                |
| 40 (13)    | 20  | 10          | 5                | 21                |
| 40 (13)    | 30  | 10          | 7                | 678               |
| 55 (18)    | 13  | 10          | 1                | 5642              |
| 55 (18)    | 27  | 10          | 21               | 173               |
| 55 (18)    | 41  | 10          | 33               | 8150              |
| 70 (23)    | 17  | 10          | 4                | 7200*             |
| 70 (23)    | 35  | 10          | 86               | 241               |
| 70 (23)    | 52  | 10          | 146              | 7200*             |
| 85 (28)    | 21  | 10          | 12               | 7200*             |
| 85 (28)    | 42  | 10          | 260              | 347               |
| 85 (28)    | 63  | 10          | 519              | 7200*             |
| 100 (33)   | 25  | 10          | 32               | 7200*             |
| 100 (33)   | 50  | 10          | 858              | 7200*             |
| 100 (33)   | 75  | 10          | 1364             | 7200*             |
| 115 (38)   | 28  | 10          | 68               | 7200*             |
| 115 (38)   | 57  | 10          | 1654             | 7200*             |
| 115 (38)   | 86  | 10          | 3250             | 7200*             |
| 130 (43)   | 32  | 10          | 163              | 7200*             |
| 130 (43)   | 65  | 10          | 4086             | 7200*             |
| 130 (43)   | 97  | 10          | 7093             | 14400*            |

Table 3: DP vs B&B on spiders

Finally, we observe that for any class of \( n \)-vertex graphs for which the number of connected components is bounded above by a polynomial in \( n \), we can use the same ideas as above to build an efficient dynamic-programming algorithm,
assuming that we can enumerate the connected components in polynomial time. We do note that the class of \(n\)-vertex “stars” (i.e., spiders with \(n - 1\) single-edge legs) has \(2^{n-1}\) subtrees containing the body, and so we do not in this way get an efficient algorithm for MESP when \(G(C)\) is a star. But see the next section for an efficient algorithm for a subclass of the positive-semidefinite \(C\) for which \(G(C)\) is a star.

We could perhaps hope that what is generally needed for a tree (to lead to an efficient dynamic programming algorithm of this type) is a degree bound. But even for a degree bound of three, we get bad behavior: for binary trees, the number of subtrees can be exponential in the number of vertices.\(^4\)

3. Stars

In this section, we present an algorithm that computes the exact optimum of MESP, when \(C\) is an arrowhead matrix (i.e., when the support graph \(G(C)\) is a star with center 1) under an easily-checkable sufficient condition.

We define the arrowhead matrix

\[
A(\alpha_1, \alpha, D) := \begin{pmatrix}
\alpha_1 & \alpha^T \\
\alpha & D
\end{pmatrix},
\]

with \(\alpha_1 \in \mathbb{R}\), \(\alpha := (\alpha_2, \ldots, \alpha_n) \in \mathbb{R}^{n-1}\), \(d := (d_2, \ldots, d_n) \in \mathbb{R}^{n-1}_+\), and \(D := \text{Diag}(d) \in \mathbb{R}^{(n-1) \times (n-1)}\); see [OS90], for example.

**Lemma 4.** \(A(\alpha_1, \alpha, D) \succeq 0\) if and only if \(\alpha_1 \geq \sum_{i=2}^n \frac{\alpha_i^2}{d_i}\).

**Proof.** By symmetric row/column scaling, it is easy to see that \(A(\alpha_1, \alpha, D) \succeq 0\) if and only if \(A(\alpha_1, \tilde{\alpha}, \alpha_1 I) \succeq 0\), where \(\tilde{\alpha}_i := \alpha_i \sqrt{\frac{\alpha_i}{d_i}}\), for \(i = 2, \ldots, n\). From [AG01], we have that \(A(\alpha_1, \tilde{\alpha}, \alpha_1 I) \succeq 0\) if and only if \(\alpha_1 \geq \|\tilde{\alpha}\|\) — this is how the “ice-cream cone” constraint is typically modeled as a semidefinite-programming constraint. Now plugging in the definition of \(\tilde{\alpha}\) and simplifying, we obtain our result. \(\square\)

We consider now MESP\((A(\alpha_1, \alpha, D), s)\), where we assume that \(\alpha_1 \geq \sum_{i=2}^n \frac{\alpha_i^2}{d_i}\), so that \(A(\alpha_1, \alpha, D) \succeq 0\). We will employ a greedy algorithm to solve MESP\((A(\alpha_1, \alpha, D), s)\), but we do not simply apply such an algorithm directly. Rather, we will branch on element 1, and then apply a greedy algorithm to the two subproblems, selecting the best solution so found.

Our greedy algorithm is a manifestation of a generic greedy maximization algorithm for the more general problem: Given \(f : 2^N \mapsto \mathbb{R}\), find an \(s\) element set \(S \subset N\) with maximum value of \(f(S)\).

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\(^4\)Consider a full binary tree with \(\ell\) levels, and hence \(2^\ell - 1\) vertices. Such a graph has \(2^{\ell-1}\) chains (on \(\ell - 1\) edges) from the top to the bottom. Taking the union of any subset of these chains gives a distinct subtree, so we have at least \(2^{2^{\ell-1}}\) subtrees, which is exponential in the number of vertices.
Algorithm 0: Generic greedy for max \( \{ f(S) : |S| = s \} \)

Input: \( f : 2^N \mapsto \mathbb{R} ; 1 < s < n \);  
Output: \( S \);  
\( S := \emptyset \);  
while \( |S| < s \) do  
  let \( j^* := \text{argmax} \ \{ f(S + j) : j \in N \setminus S \} \);  
  let \( S := S + j \);  
end while

We let \( S_0 = \emptyset, S_1, \ldots, S_s \) be the sequence of iterates \( S \) that are created, iteration by iteration, in Algorithm 0. We have the following nice property that we can exploit.

Lemma 5. Suppose that \( f : 2^N \mapsto \mathbb{R} \) satisfies the following stability property:  
\( f(T \cup \{ i \}) \leq f(T \cup \{ j \}) \) for all \( T \subset N \setminus \{ i, j \} \), whenever distinct \( i, j \) in \( N \) satisfy \( f(i) \leq f(j) \). Then the iterates of Algorithm 0 are maximizing sets for each cardinality.

Proof. Without loss of generality, we assume that \( f(1) \geq f(2) \geq \cdots \geq f(n) \). Under our hypothesis, the sequence of sets \( S_k := \{ 1, 2, \ldots, k \}, k = 0, 1, 2, \ldots, s \), is a valid sequence of sets to be produced by the greedy algorithm. By way of a proof by contradiction, suppose that some \( S_k \), with \( k \geq 2 \), is not a maximizing set of its cardinality. Among all maximizing solutions of cardinality \( k \), let \( S^* \) be a maximizer that has the maximum number of elements in common with \( S_k \). We have \( f(S^*) > f(S_k) \), and so we can choose \( j \in S^* \setminus S_k \) and \( i \in S_k \setminus S^* \). Clearly, by how \( S_k \) is chosen and by the hypothesis of the lemma, we have \( f(j) \leq f(i) \). But now the hypothesis of the lemma give us that \( f((S^* \setminus \{ j \}) \cup \{ j \}) \geq f((S^* \setminus \{ j \}) \cup \{ i \}) \). Therefore \( S^* \setminus \{ j \} \cup \{ i \} \) is also optimal, but it has more elements in common with \( S_k \) than \( S^* \) does — a contradiction.

In fact, we are interested in \( \text{MESP}(C, s) \), whereupon Algorithm 0 particularizes as follows:

Algorithm 1: Greedy for \( \text{MESP}(C, s) \)

Input: \( C \in S_n^+ ; 1 < s < n \);  
Output: \( S \);  
\( S := \emptyset \);  
while \( |S| < s \) do  
  let \( j^* := \text{argmax} \ \{ \text{ldet} C[S + j, S + j] : j \in N \setminus S \} \);  
  let \( S := S + j \);  
end while

Remark. In fact, using the Schur complement of \( C[S, S] \) in \( C[S + j, S + j] \), we have

\[
\text{ldet} C[S + j, S + j] = \text{ldet} C[S, S] + \log \left( C[j, j] - C[j, S] (C[S, S])^{-1} C[S, j] \right).
\]
So, to calculate $j^*$ in Algorithm 1, we simply find the largest diagonal element from the Schur complement of $C[S,S]$ in $C$:

$$C[N \setminus S, N \setminus S] - C[N \setminus S, S] (C[S,S])^{-1} C[S, N \setminus S].$$

**Branching on element 1.**

- If $1$ is not in some optimal solution of $\text{MESP}(A(\alpha_1, \alpha, D), s)$, then
  $$z(A(\alpha_1, \alpha, D), s) = z(D, s) = \sum_{i=1}^{s} \log d_{[i]}.$$  
  That is, if $1$ is not in some optimal solution, then such an optimal solution contains $s$ values of $i$ (from $\{2, \ldots, n\}$) with largest $d_i$. Or, to put it another way, an optimal solution is found by applying Algorithm 1 to $\text{MESP}(D, s)$.

- Alternatively, if $1$ is in some optimal solution of $\text{MESP}(A(\alpha_1, \alpha, D), s)$, then
  $$z(A(\alpha_1, \alpha, D), s) = \log \alpha_1 + z(D - \frac{1}{\alpha_1} \alpha \alpha^T, s - 1).$$
  So, then
  $$z(A(\alpha_1, \alpha, D), s) = \max \left\{ \sum_{i=1}^{s} \log d_{[i]}, \log \alpha_1 + z(D - \frac{1}{\alpha_1} \alpha \alpha^T, s - 1) \right\},$$
  and it remains only to calculate $z(D - \frac{1}{\alpha_1} \alpha \alpha^T, s - 1)$. So in what follows, we employ Algorithm 1, although we will apply it to $\text{MESP}(D - \frac{1}{\alpha_1} \alpha \alpha^T, s - 1)$.

Now, we are prepared to describe our sufficient condition for Algorithm 1 to correctly solve $\text{MESP}(D - \frac{1}{\alpha_1} \alpha \alpha^T, s - 1))$. What we will show is that as we take successive Schur complements in $D - \frac{1}{\alpha_1} \alpha \alpha^T$, the ordering of the remaining diagonal elements is not affected.

**Definition 1.** Let $r_k := \frac{\alpha_2^2}{\alpha_1}$ for $2 \leq k \leq n$, and we choose a (sorting) bijection $\pi : \{1, \ldots, n-1\} \to \{2, \ldots, n\}$, such that $r_{\pi(1)} \geq r_{\pi(2)} \geq \cdots r_{\pi(n-1)}$. Let $\Phi(s - 1) := \{ \pi(k) : 1 \leq k \leq s - 1 \}$.

So, $\pi$ sorts the ratios $r_i$, and then $\Phi$ selects the original indices of the $s - 1$ largest.

**Theorem 6.** Let

$$\hat{\alpha}_1 := \sum_{k \in \Phi(s-1)} r_k + \max_{i,j \in \{2, \ldots, n\} \setminus \Phi(s-1)} \left\{ \frac{\alpha_i^2 - \alpha_j^2}{d_i - d_j} : d_i > d_j, \, \alpha_i^2 > \alpha_j^2 \right\}.$$  

If $A(\alpha_1, \alpha, D) \succeq 0$, $\alpha_1 \geq \hat{\alpha}_1$, then Algorithm 1 produces an optimal solution of $\text{MESP}(D - \frac{1}{\alpha_1} \alpha \alpha^T, s - 1)$.
Proof. Let \( \tilde{D} := D - \frac{1}{\alpha_1} \alpha_1 \alpha^T \). If the Schur complement of \( \tilde{D}[T, T] \) in \( \tilde{D} \) has the same ordering of its diagonal elements as \( \tilde{D}[N \setminus T, N \setminus T] \), for all \( T \subset N \setminus \{1\} \), then Algorithm 1 applied to \( \text{MESP}(\tilde{D}, s - 1) \) will choose \( s - 1 \) values of \( \alpha \) corresponding to the \( s - 1 \) greatest diagonal elements of \( \tilde{D} \), and that will be optimal for \( \text{MESP}(\tilde{D}, s - 1) \). By Lemma 5 Algorithm 0, and hence Algorithm 1, generates the optimal solution.

So, it remains to demonstrate that if \( \alpha_1 \geq \hat{\alpha}_1 \), then the Schur complement of \( \tilde{D}[T, T] \) in \( \tilde{D} \) has the same ordering of its diagonal elements as \( \tilde{D}[N \setminus T, N \setminus T] \), for all \( T \subset N \setminus \{1\} \). In what follows, it is notationally easier to work with \( D \) rather than \( \tilde{D} \), so we consider \( 1 \in T \subset N \) rather than \( T \subset N \setminus \{1\} \).

For \( 1 \in T \subset N \), with \( |T| = t \), the Schur complement of \( A[T, T] \) in \( A := A(\alpha_1, \alpha, D) \) is

\[
A[N \setminus T, N \setminus T] - A[N \setminus T, T] (A[T, T])^{-1} A[T, N \setminus T] = D[N \setminus T, N \setminus T] - (\alpha[N \setminus T, 0_{(n-t) \times 1}) (A[T, T])^{-1} (\alpha[N \setminus T, 0_{(n-t) \times 1})^T
\]

\[
= D[N \setminus T, N \setminus T] - (A[T, T])^{-1}_{11} \alpha[N \setminus T] \alpha[N \setminus T]^T.
\]

Now, for \( i \in N \setminus T \), the diagonal entry indexed by \( i \) of this Schur complement is

\[
d_{ii} - \left( \frac{1}{\alpha_1 - \sum_{k \in T\{1\}} \frac{\alpha_k^2}{\alpha_k}} \right) \alpha_i^2,
\]

where we have extracted \( (A[T, T])^{-1}_{11} \) using the standard block-matrix inverse formula on

\[
A[T, T] = \begin{pmatrix} \alpha_1 & \alpha[T \setminus \{1\}]^T \\
\alpha[T \setminus \{1\}] & D[T \setminus \{1\}, T \setminus \{1\}] \end{pmatrix}.
\]

If \( T = \{1\} \), then diagonal element \( i \) of the Schur complement is \( d_i - \frac{1}{\alpha_1} \alpha_i^2 \). So we want to demonstrate that, for all \( T \supset 1 \) and \( i, j \in T \setminus N \), if

\[
d_i - \frac{1}{\alpha_1} \alpha_i^2 \geq d_j - \frac{1}{\alpha_1} \alpha_j^2,
\]

then

\[
d_i - \frac{\alpha_i^2}{\alpha_1 - \sum_{k \in T\{1\}} \frac{\alpha_k^2}{\alpha_k}} \geq d_j - \frac{\alpha_j^2}{\alpha_1 - \sum_{k \in T\{1\}} \frac{\alpha_k^2}{\alpha_k}}.
\]

Note that (\*) implies that either \( d_i \geq d_j \) and \( \alpha_i^2 \leq \alpha_j^2 \), in which case (\**) is trivially true, or \( d_i > d_j \) and \( \alpha_i^2 > \alpha_j^2 \). In this latter case, (\**) reduces to

\[
\alpha_1 \geq \sum_{k \in T\{1\}} \frac{\alpha_k^2}{\alpha_k} + \frac{\alpha_i^2 - \alpha_j^2}{d_i - d_j}.
\]

The result now follows.
Example 1. If the sufficient condition of Theorem 6 does not hold, then indeed the greedy algorithm may not find an optimum. For example, Let

\[
A = \begin{pmatrix}
12 & 3.5 & 1.9 & 0.04 & 4.9 \\
3.5 & 4 & 0 & 0 & 0 \\
1.9 & 0 & 3 & 0 & 0 \\
0.04 & 0 & 0 & 2.5 & 0 \\
4.9 & 0 & 0 & 0 & 5
\end{pmatrix}
\]

and take \( s = 3 \). It is easy to check that

\[
\alpha_1 = 12 < \hat{\alpha} = 15.0831 = \frac{4.9^2}{5} + \frac{3.5^2}{4} + \frac{1.9^2 - 0.04^2}{3 - 2.5}.
\]

The diagonal elements of the Schur complements of \( A[T,T] \) for \( T := \{1\} \) and \( T := \{1,5\} \) respectively are

\[
\begin{pmatrix}
2 & \left( 4 - \frac{3.5^2}{12} \right) \\
3 & \left( 3 - \frac{1.9^2}{12} \right) \\
4 & \left( 2.5 - \frac{0.04^2}{12} \right) \\
5 & \left( 5 - \frac{4.9^2}{12} \right)
\end{pmatrix} = \begin{pmatrix}
2.9792 \\
2.6992 \\
2.4999 \\
2.9992
\end{pmatrix}
\quad \text{and} \quad
\begin{pmatrix}
2 & \left( 4 - \frac{3.5^2}{12-4.9^2/5} \right) \\
3 & \left( 3 - \frac{1.9^2}{12-4.9^2/5} \right) \\
4 & \left( 2.5 - \frac{0.04^2}{12-4.9^2/5} \right)
\end{pmatrix} = \begin{pmatrix}
2.2981 \\
2.4985 \\
2.4998
\end{pmatrix}.
\]

The ordering implied by the first Schur complement is \( 5, 2, 3, 4 \) and for the second it is \( 4, 3, 2 \). The greedy solution appends \( 5 \) and then \( 4 \) to \( \{1\} \), but the optimal solution turns out to be \( S^* = \{1, 2, 3\} \).

4. Tridiagonal masks

It may well be that neither \( G(C) \) nor \( G(C^{-1}) \) is a spider with a constant number of legs. Even then, we can use our dynamic-programming algorithm to get a bound on \( z(C, s) \), because \( \text{ldet} C[S,S] \leq \text{ldet}(C \circ M)[S,S] \), for all \( S \subset N \). It is evident that when \( M \) is sparse and \( C \) is fully dense, \( G(C \circ M) = G(M) \), and so when \( G(M) \) is a spider with a constant number of legs, we can apply our dynamic-programming algorithm to \( C \circ M \) to efficiently get an upper bound on \( z(C, s) \). Furthermore, upper bounds for \( z(C^{-1}, n - s) \) yield upper bounds for \( z(C, s) \), shifting by \( \text{ldet} C \), and upper bounds (under this complementation) are not always equivalent. So we can as well profitably apply masking to \( C^{-1} \).

For simplicity of exposition and because we have developed the theory in more detail for tridiagonal masks \( M \) (i.e., when \( G(M) \) is a collection of disjoint paths), we confine our attention to tridiagonal masks \( M \). To set some notation,
a tridiagonal mask $M \in \mathbb{R}^{n \times n}$ has the form

$$M := \begin{pmatrix}
1 & \mu_1 & & & \\
& 1 & \mu_2 & & \\
& & \ddots & \ddots & \\
& & & \ddots & \mu_{n-1} \\
& & & & 1
\end{pmatrix},$$

with $M_{ij} := 0$ when $|i - j| > 1$.

For $M$ to be a mask, we need it to be positive semidefinite. For example, we can check that if we have all $\mu_i := 1$, then $M$ is not positive semidefinite (for all $n > 2$); but if we have all $|\mu_i| \leq \frac{1}{2}$, then $M$ is diagonally dominant and hence positive semidefinite for all $n$. A $\frac{1}{2}$-mask is such an $M$ with all $|\mu_i| = \frac{1}{2}$. In fact, we can do better than this, in the sense that we can increase some entries from $\frac{1}{2}$, which seems empirically to be valuable for getting better bounds. For example: for $n = 2$, we can set $\mu_1 = 1$; and for $n = 3$, we could set $\mu_1 = \frac{1}{2}$ and $\mu_2 = \sqrt{\frac{3}{4}}$. For practical purposes, we will limit the number of pairs of symmetric entries that are increased from $\frac{1}{2}$ to two, and we want to see how much we can increase such entries up from $\frac{1}{2}$. Clearly an upper bound on the maximum value of each $\mu_i$ is 1, because $(\frac{1}{\mu_i}, \frac{1}{1})$ is always a principal submatrix.

For $1 \leq p < q < n$, and $a, b \in \mathbb{R}$, let $M := M(n, p, a, q, b)$ be an order-$n$ matrix that differs from the order-$n$ $\frac{1}{2}$-mask in that $M_{p+1, p} = M_{p, p+1} = \mu_p := a$ and $M_{q+1, q} = M_{q, q+1} = \mu_q := b$. We will also denote $M(n, p, a) := M(n, p, a, p, a)$ and $M_{1/2}(n) := M(n, p, 1/2) \forall 1 \leq p \leq n - 1$.

The following lemma has a somewhat lengthy technical proof, which can be found in Appendix 1.

**Lemma 7.** For $1 \leq p < q < n$, and $a, b \in \mathbb{R}$,

$$\text{det} \ M(n, p, a, q, b) = \frac{1}{2^n} (n - q + 1) (p + 1)(q - p + 1) - 4a^2 p(q - p) - \frac{1}{2^n} (n - q) 4b^2 ((p + 1)(q - p) - 4a^2 p(q - p - 1)).$$

From this, we can see how large we can make $a$, when $b$ is held at $1/2$. In particular, we will see that if $b$ is held at $1/2$, we can make $a$ at least $\sqrt{2}/2$ by positioning $a$ at the first off-diagonal pair.

**Proposition 8.** The maximum value of $a$ such that $M(n, p, a) \succeq 0$ is

$$a^*(n, p) := \frac{1}{2} \sqrt{\left(1 + \frac{1}{p}\right) \left(1 + \frac{1}{n - p}\right)}.$$

Furthermore, $a^*(n, p)$ is convex and decreasing in $n$ and $\lim_{n \to \infty} a^*(n, p) = \frac{1}{2} \sqrt{1 + 1/p}$. In particular, $\max_{1 \leq p < n-1} \lim_{n \to \infty} a^*(n, p) = \lim_{n \to \infty} a^*(n, 1) = \sqrt{2}/2$. 
Proof. Note that $M(n, p, \frac{1}{2}) = M_{1/2}(n) \succeq 0$, because it is diagonally dominant. Also, we have that $\det M(n, p, \frac{1}{2}) > 0$ (by Lemma 7). Using Lemma 7, we can see that

$$\det M(n, p, a) = \frac{1}{2^n} \left( (p + 1)(n - p + 1) - 4a^2 p(n - p) \right)$$

is decreasing in $a$. Now, solving $\det M(n, p, a) = 0$ for $a$, and carrying out some algebraic manipulations, we obtain the formula for $a^*(n, p)$ stated in the result. What we can conclude, at this point, is that $a^*(n, p)$ is an upper bound on the maximum value of $a$ such that $M(n, p, a) \succeq 0$.

To see that this upper bound is in fact the true maximum, we need to verify that $M(n, p, a^*) \succeq 0$. To do this, we will check that all leading principal submatrices of order $1 \leq k < n$ have positive determinant. This, together with the nonnegativity of the determinant of $M(n, p, a^*)$ (it is in fact 0) is sufficient to establish that $M(n, p, a^*) \succeq 0$ (see, for example, [HJ85, Exercise at the bottom of p. 404]).

Now, for $k \leq p$, the $k$-th leading principal submatrix is an order-$k \frac{1}{2}$-mask, which has positive determinant by Lemma 7. For $p < k < n$, the $k$-th leading principal submatrix is $M(k, p, a^*)$. After some algebraic manipulations, we arrive at

$$\det M(k, p, a^*) = \frac{p + 1}{2^k} (k - p) \left( \frac{1}{k - p} - \frac{1}{n - p} \right),$$

which is clearly positive for $p < k < n$.

Thus, we have established that $a^*(n, p)$ is the maximum value of $a$ such that $M(n, p, a) \succeq 0$. The rest of the result is easy to verify. 

Knowing the possible increases of $a$ from $1/2$, we can determine the maximum of $b$ (given $a$) and the general behavior of the maximum as we vary $p$ and $q$.

Theorem 9. For $1 \leq p < q < n$ and $a \in [\frac{1}{2}, a^*(n, p)]$, we have that $M(n, p, a, q, b) \succeq 0$ if and only if $b \in [\frac{1}{2}, b^*(n, p, a, q)]$, where

$$b^*(n, p, a, q) := \frac{1}{2} \sqrt{\frac{(n - q + 1)((p + 1)(q - p + 1) - 4a^2 p(q - p))}{(n - q)((p + 1)(q - p) - 4a^2 p(q - p - 1))}}.$$

Proof. It is easy to verify, from Lemma 7, that the formula given for $b^*(n, p, a, q)$ is the unique nonnegative solution of $\det M(n, p, a, q, b) = 0$.

We claim that $\det M(n, p, a, q, b)$ is decreasing in $b$ when $a \in [\frac{1}{2}, a^*(n, p)]$ (i.e., the the range of $a$ that ensures $M(n, p, a) \succeq 0$). It is evident, from Lemma 7, that this is when

$$(p + 1)(q - p) - 4a^2 p(q - p - 1) > 0,$$
or simply when
\[
a < \tilde{a}(q, p) := \frac{1}{2} \sqrt{(1 + \frac{1}{p}) \left( 1 + \frac{1}{(q-1) - p} \right)}.
\]
Notice that with \( q < n \), we clearly have \( \tilde{a}(q, p) > a^*(n, p) \), and therefore \( \det M(n, p, a, q, b) \) is decreasing in \( b \) when \( a \in [\frac{1}{2}, a^*(n, p)] \).

We can conclude that for \( a \in [\frac{1}{2}, a^*(n, p)] \), the maximum value of \( b \) such that \( \det(M(n, p, a, q, b)) \geq 0 \) is \( b^*(n, p, a, q) \).

Now, it only remains to demonstrate that \( M(n, p, a, q, b) \succeq 0 \), for all \( b \in \left[ \frac{1}{2}, b^*(n, p, a, q) \right] \). It suffices to demonstrate that all proper leading principal submatrices of \( M(n, p, a, q, b^*) \) have a positive determinant. Because \( \det(M(n, p, a, q, b)) \) is decreasing in \( b \) (for the relevant \( n, p, a, q \)), we will then have that all proper leading principal submatrices of \( M(n, p, a, q, b) \) have a positive determinant, for all \( b \in [\frac{1}{2}, b^*(n, p, a, q)] \). This will then imply that \( M(n, p, a, q, b) \succeq 0 \), for all \( b \in [\frac{1}{2}, b^*(n, p, a, q)] \).

From Proposition 8, we have that principal submatrices that take the form \( M_{1/2}(k) \) and \( M(k, p, a) \) with \( p < k < n \) are positive semidefinite, for \( a \in [\frac{1}{2}, a^*] \). So it remains to show that \( M(k, p, a, q, b^*) \) has a positive determinant, for \( 1 \leq p < q < k < n \).

Plugging in the formula for \( b^*(n, p, a, q) \) into the formula for \( \det M(k, p, a, q, b^*) \), after some simplifications we have
\[
\frac{1}{2k} \left( (p + 1)(q - p + 1) - 4a^2p(q - p) \right) \left( (k - q + 1)(n - q) - (n - q + 1)(k - q) \right).
\]

It is easy to check that \((*)\) is positive because \( a < \tilde{a}(q, p) \), and \((***)\) is positive because \( (k - q + 1)/(k - q) > (n - q + 1)/(n - q) \), for \( 1 < q < k < n \).

With the next two results (proofs deferred to Appendix 1), we see that insofar as maximizing the value of \( b \) in \( M(n, p, a, q, b) \), if \( n, q, a \) are fixed, we should set \( p = 1 \); and then with \( p = 1 \), we should set \( q = n - 1 \).

**Theorem 10.** For each \( 1 \leq p < q < n, a \in [\frac{1}{2}, a^*(n, p)] \), and \( n \geq 4 \), we have that \( b^*(n, 1, a, q) \geq b^*(n, p, a, q) \).

**Theorem 11.** \( b^*(n, 1, a, q) \) is maximized over \( q \) for \( 1 < q < n \) at \( q^*(n, 1, a) = n - 1 \). Note that by Theorems 10 and 11, \( b^*(n, p, a, n - 1) \geq b^*(n, p, a, q) \). Symmetrically, corresponding to the last four results, we can establish: (i) a formula for the maximum value of \( b \) when \( a = 1/2 \), (ii) a formula for the maximum value \( a^* \) of \( a \), (iii) that the \( a^* \) is increasing in \( q \), and (iv) that \( a^* \) is maximized over \( p \) at \( p^* = 1 \).
5. Local search on tridiagonal masks

Our goal is to do a local search in the space of tridiagonal masks, so as to get a (tridiagonal) mask $M$ that leads to a low value of $f(C \circ M, s)$ for some upper-bounding method $f(\cdot, s)$ applied to MESP. Besides exact calculation by dynamic programming of $z(C \circ M)$, we work with the following additional bounding methods:

- The (masked) spectral bound for $z(C \circ M, s)$:
  \[
  \sum_{\ell=1}^{s} \log \lambda_{\ell}(C \circ M),
  \]
  where $\lambda_{\ell}(\cdot)$ denotes the $\ell$-th greatest eigenvalue. When $M = I$, the masked spectral bound is the diagonal bound: the sum of the logs of the $s$ biggest diagonal components of $C$. The spectral bound was first presented in [KLQ95], and its masked versions in [HLW01, AL04, BL07].

- The (masked) linx bound for $z(C \circ M, s)$ is the optimal value of the following convex-optimization relaxation:
  \[
  \max \frac{1}{2} (\det(\gamma(C \circ M) \text{Diag}(x)(C \circ M) + \text{Diag}(e - x)) - s \log \gamma) \\
  \text{s.t. } e^T x = s, \ 0 \leq x \leq e,
  \]
  where $\gamma > 0$ is a scaling parameter that must be judiciously selected, and $e$ is an all-ones vector. The linx bound was first presented in [Ans20], and its optimal scaling was studied in [Ans20, CFLL21].

Note that $z(C, s)$ is permutation invariant. That is, if $\Pi$ is an $n \times n$ permutation matrix, then $z(C, s) = z(\Pi C \Pi^T, s)$. Moreover the value of most bounds applied to $C$ and $\Pi C \Pi^T$ are identical. But these observations are not at all generally true for $C \circ M$ compared to $(\Pi C \Pi^T) \circ M$ (unless $M$ is permutation invariant, for example $M = I_n$ or $M = J_n$), and so we can try to optimize the bound produced by a bounding method, even for a fixed mask $M$, by varying the permutation matrix $\Pi$. As a first phase, we start with $M$ equal to the $\frac{1}{2}$-mask of order $n$, and we do a local search, using minimization of the spectral bound as a criterion, applied to $(\Pi C \Pi^T) \circ M$. Each permutation matrix $\Pi$ is in one-to-one correspondence with a permutation $\pi$ of $N$ (i.e., each of the $n!$ permutations $\pi$ is an ordered set $(\pi_1, \pi_2, \ldots, \pi_n)^T$ of the $n$ distinct elements of $N = \{1, 2, \ldots, n\}$, so that $\Pi(1, 2, \ldots, n)^T = (\pi_1, \pi_2, \ldots, \pi_n)^T$). Our local moves correspond to choosing an $i, j$ with $1 \leq i < j \leq n$, and then replacing $\pi_i, \pi_{i+1}, \ldots, \pi_{j-1}, \pi_j$ with $\pi_j, \pi_{j-1}, \ldots, \pi_{i+1}, \pi_i$. We do a best-improvement local search: upon convergence, we replace $C$ with $\Pi C \Pi^T$.

Next, we proceed to our second phase. As a general step, we have a blocked tridiagonal mask $M := \text{Diag}(M[S_1, S_1], M[S_2, S_2], \ldots, M[S_p, S_p])$, with $p \geq 1$, where the $S_i$ partition $N$, each $S_i$ is a nonempty ordered contiguous set, each $M[S_i, S_j]$ is a tridiagonal mask (of order $|S_i|$), and for all $1 \leq i < j \leq p$, all elements of $S_i$ are less than all elements of $S_j$. In one-to-one correspondence
with the partitioning is its signature $(|S_1|, |S_2|, \ldots, |S_i|)$, a sequence of positive integers summing to $n$. Let $(s_1, s_2, \ldots, s_p)$ be the current signature. We do local search on the sets underlying the signature. We want to choose a rich set of local moves that we can reasonably search over for a best-improving move.

The moves that we consider are:

- **Merge a pair of adjacent blocks**: If $p > 1$, choose some $1 \leq i < p$, and replace $s_i, s_{i+1}$ with $s_i + s_{i+1}$.

- **Split a block**: If $p < n$, choose some $i$ with $s_i > 1$, choose some $1 \leq t < s_i$, and replace $s_i$ with $t, s_i - t$.

- **Interchange**: If $p > 1$ and not all $s_i$ are equal, choose some $1 \leq i < j \leq p$, with $s_i \neq s_j$, and swap $s_i$ with $s_j$.

The number of available moves at each step of the local search is $O(n^2)$, which we can reasonably search over.

Considering Theorem 11 (and its analogue for $a^*$), for the purpose of our local search, we will restrict our attention to $M[S_i, S_i]$ that are of the form $M(|S_i|, 1, a, |S_i| - 1, b)$. So given an $S_i$, the only flexibility that we will take is in choosing $a$ and $b$, only differing from an order-$|S_i|$ mask in the “end pairs”:

$$
M[S_i, S_i] := \begin{pmatrix}
1 & a & 0 \\
a & 1 & \frac{1}{2} \\
0 & \frac{1}{2} & 1 \\
& \ddots & \ddots & \ddots \\
& & 1 & \frac{1}{2} \\
& & \frac{1}{2} & 1 & b \\
& & \frac{1}{2} & b & 1 \\
0 & b & 1
\end{pmatrix}.
$$

For any new block $M[S_i, S_i] = M(|S_i|, 1, a, |S_i| - 1, b)$ created in the local search over signatures, we consider the following choices of $(a, b)$: $(\frac{1}{2}, b)$ with $b$ maximized and $(a, \frac{1}{2})$ with $a$ maximized. We calculate these maximum values using Theorem 9 (and its analogue for $a^*$).

We take these local search moves, and we perform a best-improvement local search on $f(C \circ M, s)$, where $f$ is the spectral bound. Note that calculation of the spectral bound is quite fast and also easily parallelizes across the blocks. Then, we switch to the linx bound (generally a better bound, but slower to calculate — and not easily parallelized), continuing the local search. Finally, we further continue the local search, using our dynamic-programming recursion to exactly calculate $z(C \circ M, s)$ at each step. We note that linx solves are much faster than dynamic-programming solves (nearly twice as fast in our experiments), justifying the linx phase in our search.

We implemented our algorithm in Matlab, and we carried out some experiments designed to demonstrate the potential of our approach, compared to the
masked linx bound using the $\frac{1}{2}$-mask. Our test instances are described in Appendix 2. In our experiments presented in this section, we took $s \sim n/2$. Our results appear in Table 4, where we tabulated (difference) gaps to a heuristically-generated lower bound on $z(C, s)$ (see [KLQ95, Section 4]). “C” indicates the covariance matrix that we used. “linx($\frac{1}{2}$)” is the gap value of the masked linx bound using the $\frac{1}{2}$-mask. “$\lambda(\frac{1}{2})$” is the spectral-bound gap using the $\frac{1}{2}$-mask. Each remaining column starts from the solution of the previous column. “$\lambda(\Pi)$” is the spectral-bound gap after performing a first-phase (permutation-based local search). “$\lambda(\Sigma)$” is the spectral-bound gap after performing a second phase (signature-based local search). “linx(Σ)” is the linx-bound gap after performing a second phase (signature-based local search). “DP(Σ)” is the DP-bound gap after performing a second phase (signature-based local search). In our exper-

| $C$ | $n$ | $s$ | linx($\frac{1}{2}$) | $\lambda(\frac{1}{2})$ | $\lambda(\Pi)$ | $\lambda(\Sigma)$ | linx(Σ) | DP(Σ) |
|-----|-----|-----|---------------------|-----------------------|----------------|----------------|---------|-------|
| $C_{63}^{-1}$ | 63 | 32 | 3.2512 | 3.2469 | 2.9521 | 2.7197 | 2.4828 | 2.4828 |
| $C_{63}^{-1} + 0.125I$ | 63 | 32 | 3.1841 | 3.1801 | 2.8821 | 2.6584 | 2.4205 | 2.4205 |
| $C_{63}^{-1} + 0.25I$ | 63 | 32 | 3.1182 | 3.1144 | 2.8302 | 2.5994 | 2.3649 | 2.3649 |
| $C_{63}^{-1} + 0.375I$ | 63 | 32 | 3.0523 | 3.0488 | 2.7585 | 2.5404 | 2.3092 | 2.3092 |
| $C_{63}^{-1} + 0.5I$ | 63 | 32 | 2.9891 | 2.9858 | 2.6992 | 2.4838 | 2.2558 | 2.2558 |

| $C_1$ | 100 | 50 | 5.7979 | 5.9629 | 5.4154 | 4.8091 | 4.8091 |
| $C_2$ | 100 | 50 | 5.6529 | 5.8427 | 5.1636 | 4.3299 | 4.3299 |
| $C_3$ | 100 | 50 | 6.0613 | 6.1358 | 5.6738 | 4.8532 | 4.8532 |
| $C_4$ | 100 | 50 | 5.2033 | 5.4311 | 4.8394 | 4.6112 | 4.2871 | 4.2871 |
| $C_5$ | 100 | 50 | 4.835 | 4.8861 | 4.4351 | 4.1941 | 3.8815 | 3.8815 |

| $C_6$ | 100 | 50 | 0.511 | 1.6225 | 0.54995 | 0.4410 | 0.1263 | 0.1263 |
| $C_7$ | 100 | 50 | 0.3905 | 1.3056 | 0.33 | 0.1901 | 0.1332 | 0.1332 |
| $C_8$ | 100 | 50 | 0.3921 | 1.3292 | 0.4362 | 0.3298 | 0.2312 | 0.2312 |
| $C_9$ | 100 | 50 | 0.3477 | 1.598 | 0.3945 | 0.2713 | 0.1984 | 0.1984 |
| $C_{10}$ | 100 | 50 | 0.2422 | 1.4178 | 0.2591 | 0.1735 | 0.133 | 0.133 |

| $C_{11}$ | 100 | 50 | 0.3715 | 1.5703 | 0.382 | 0.2607 | 0.1818 | 0.1818 |
| $C_{12}$ | 100 | 50 | 0.3114 | 1.3027 | 0.3289 | 0.1818 | 0.1289 | 0.1289 |
| $C_{13}$ | 100 | 50 | 0.3859 | 1.3201 | 0.4287 | 0.30696 | 0.215 | 0.215 |
| $C_{14}$ | 100 | 50 | 0.3447 | 1.5994 | 0.3923 | 0.2725 | 0.2182 | 0.2182 |
| $C_{15}$ | 100 | 50 | 0.2579 | 1.4405 | 0.2839 | 0.2072 | 0.1635 | 0.1635 |

| $C_{16}$ | 100 | 50 | 0.7153 | 10.628 | 0.8203 | 0.8202 | 0.8202 | 0.8201 |
| $C_{17}$ | 100 | 50 | 0.7309 | 10.641 | 0.8124 | 0.8123 | 0.8123 | 0.8122 |
| $C_{18}$ | 100 | 50 | 0.8497 | 10.788 | 0.9727 | 0.9727 | 0.9727 | 0.9724 |
| $C_{19}$ | 100 | 50 | 0.9758 | 10.907 | 1.1094 | 1.1093 | 1.1093 | 1.1090 |
| $C_{20}$ | 100 | 50 | 0.7178 | 10.647 | 0.8106 | 0.8105 | 0.8105 | 0.8103 |

Table 4: Entropy gaps: $s \sim n/2$
iments, we can see clear and consistent improvements from $\lambda\left(\frac{1}{2}\right)$ to $\lambda(\Pi)$ to $\lambda(\Sigma)$ to linx($\Sigma$). Furthermore, we can see that linx($\Sigma$) improves on linx($\frac{1}{2}$), except for $C_{16}$ to $C_{20}$. Interestingly, for those we can see a small improvement in DP($\Sigma$) compared to linx($\Sigma$) (in contrast to the other test problems). Overall, our method gives a good way to get a better mask for the linx bound than the $\frac{1}{2}$-mask. Considering the final column, DP($\Sigma$), we can see that the masked linx bound using the final mask $M$, consistently gives almost exactly $z(C \circ M, s)$. That is, the dynamic program establishes that the masked linx bound with the final mask $M$ nearly gives the optimal value of $z(C \circ M, s)$.

The plot of Figure 5 shows the average portion of the gap between $\lambda\left(\frac{1}{2}\right)$ and $DP(\Sigma)$ that is bridged by each $\Delta \in \{\lambda\left(\frac{1}{2}\right), \lambda(\Pi), \lambda(\Sigma), \text{linx}(\Sigma), \text{DP}(\Sigma)\}$. That is, we plot averages of $\frac{\lambda(\frac{1}{2}) - \Delta}{\lambda(\frac{1}{2}) - \text{DP}(\Sigma)}$; averaged over each of the five types of instances. In this way, we can understand the improvements obtained by successively adding more bounding effort.
Appendix 1: Deferred proofs

Proof of Lemma 7

Our proof is by induction on $n$, and our base cases are $n = 3$ and $n = 4$. For $n = 3$, we have

$$\det M(3, p, a, q, b) = \det M(3, 1, a, 2, b) = (1 - a^2) - b^2$$

$$= \frac{1}{2^3} (3 - 2 + 1) \left( (1 + 1)(2 - 1 + 1) - 4a^2(2 - 1) \right)$$

$$- \frac{1}{2^3} (3 - 2)(4b^2) \left( (1 + 1)(2 - 1) - 4a^2(2 - 1 - 1) \right).$$

For $n = 4$, we have three combinations of $p$ and $q$ to consider.

Case 1: $p = 1$, $q = 2$.

$$\det M(4, 1, a, 2, b) = \frac{3}{4} (1 - a^2) - b^2$$

$$= \frac{1}{2^4} (4 - 2 + 1) \left( (1 + 1)(2 - 1 + 1) - 4a^2(2 - 1) \right)$$

$$- \frac{1}{2^4} (4 - 2)(4b^2) \left( (1 + 1)(2 - 1) - 4a^2(2 - 1 - 1) \right).$$

Case 2: $p = 1$, $q = 3$.

$$\det M(4, 1, a, 3, b) = (1 - a^2)(1 - b^2) - \frac{1}{4}$$

$$= \frac{1}{2^4} (4 - 3 + 1) \left( (1 + 1)(3 - 1 + 1) - 4a^2(3 - 1) \right)$$

$$- \frac{1}{2^4} (4 - 3)(4b^2) \left( (1 + 1)(3 - 1) - 4a^2(3 - 1 - 1) \right).$$

Case 3: $p = 2$, $q = 3$.

$$\det M(4, 2, a, 3, b) = \frac{3}{4} (1 - b^2) - a^2$$

$$= \frac{1}{2^4} (4 - 3 + 1) \left( (2 + 1)(3 - 2 + 1) - 4a^2(2)(3 - 2) \right)$$

$$- \frac{1}{2^4} (4 - 3)(4b^2) \left( (2 + 1)(3 - 2) - 4a^2(2)(3 - 2 - 1) \right).$$

Next, we suppose that $n > 4$ and that the result holds for matrices of order less than $n$. We apply the recursive determinant formula for tridiagonal matrices (Lemma 1) to $M(n, p, a, q, b)$. Because the recursion has a depth of two, we need to consider six combinations of $p$ and $q$.

Recall our short notation $M(n, p, a) := M(n, p, a, q, 1/2) = M(n, p_1, 1/2, p, a)$.

$$\det M(n, p, a) = \frac{1}{2^n} \left( (p + 1)(n - p) - 4a^2 p(n - p - 1) \right)$$

$$= \frac{1}{2^n} \left( (p + 1)(n - p + 1) - (n - p)4a^2 p \right).$$
Case 1: \( p < q < n - 2 \).

\[
\det M(n, p, a, q, b) = \det M(n - 1, p, a, q, b) - \frac{1}{2^n} \det M(n - 2, p, a, q, b)
\]
\[
= \frac{1}{2^{n-1}} (n - q) \left( (p + 1)(q - p + 1) - 4a^2 p(q - p) \right)
- \frac{1}{2^{n-1}} (n - q - 1) b^2 \left( (p + 1)(q - p + 1) - 4a^2 p(q - p - 1) \right)
- \frac{1}{2^n} (n - q - 1) \left( (p + 1)(q - p + 1) - 4a^2 p(q - p) \right)
+ \frac{1}{2^n} (n - q - 2) b^2 \left( (p + 1)(q - p - 1) - 4a^2 p(q - p - 1) \right)
= \frac{1}{2^n} (n - q + 1) \left( (p + 1)(q - p + 1) - 4a^2 p(q - p) \right)
- \frac{1}{2^n} (n - q) b^2 \left( (p + 1)(q - p) - 4a^2 p(q - p - 1) \right).
\]

Case 2: \( p < n - 3, q = n - 1 \).

\[
\det M(n, p, a, n - 1, b) = \det M(n - 1, p, a) - b^2 \det M(n - 2, p, a)
\]
\[
= \frac{1}{2^{n-1}} \left( (p + 1)(n - p) - (n - p - 1)4a^2 p \right)
- \frac{b^2}{2^{n-2}} \left( (p + 1)(n - p - 1) - (n - p - 2)4a^2 p \right)
= \frac{1}{2^n} \left( (p + 1)(n - p) - (n - p - 1)4a^2 p \right)
- \frac{1}{2^n} b^2 \left( (p + 1)(n - p - 1) - (n - p - 2)4a^2 p \right).
\]

Case 3: \( p = n - 3, q = n - 1 \).

\[
\det M(n, n - 3, a, n - 1, b) = \det M(n - 1, n - 3, a) - b^2 \det M(n - 2, n - 3, a)
\]
\[
= \frac{1}{2^{n-1}} \left( (n - 2)(3) - (2)4a^2(n - 3) \right) - \frac{b^2}{2^{n-2}} \left( (n - 2)(2) - 4a^2(n - 3) \right)
= \frac{1}{2^n} \left( (n - 2)(3) - (2)4a^2(n - 3) \right) - \frac{1}{2^n} b^2 \left( (n - 2)(2) - 4a^2(n - 3) \right).
\]

Case 4: \( p = n - 2, q = n - 1 \).

\[
\det M(n, n - 2, a, n - 1, b) = \det M(n - 1, n - 2, a) - b^2 \det M(n - 2, n - 3, 1/2)
\]
\[
= \frac{1}{2^{n-1}} \left( (n - 1)(2) - 4a^2(n - 2) \right) - \frac{b^2}{2^{n-2}} \left( (n - 2)(2) - (n - 3) \right)
= \frac{1}{2^n} \left( (n - 1)(2) - 4a^2(n - 2) \right) - \frac{1}{2^n} b^2 \left( n - 1 \right).
\]
Case 5: \( p < n - 3, q = n - 2 \).

\[
\det M(n, p, a, n - 2, b) = \det M(n - 1, p, a, n - 2, b) - (1/2)^2 \det M(n - 2, p, a) \\
= \frac{1}{2^{n-1}} 3 \left( (p+1)(n-p-1) - (n-p-2)4a^2p \right) \\
- \frac{b^2}{2^{n-2}} 2 \left( (p+1)(n-p-2) - (n-p-3)4a^2p \right) \\
- \frac{1}{2^n} \left( (p+1)(n-p-1) - (n-p-2)4a^2p \right) \\
= \frac{1}{2^n} 3 \left( (p+1)(n-p-1) - (n-p-2)4a^2p \right) \\
- \frac{1}{2^n} 2 \left( (p+1)(n-p-2) - (n-p-3)4a^2p \right).
\]

Case 6: \( p = n - 3, q = n - 2 \).

\[
\det M(n-3, p, a, n-2, b) = \det M(n - 1, n - 3, a, n - 2, b) - (1/2)^2 \det M(n - 2, n - 3, a) \\
= \frac{1}{2^{n-1}} 2 \left( (n-2)(2) - 4a^2(n-3) \right) - \frac{1}{2^{n-1}} 4b^2(n-2) \\
- \frac{1}{2^n} \left( (n-2)(2) - 4a^2(n-3) \right) \\
= \frac{1}{2^n} (3) \left( (n-2)(2) - 4a^2(n-3) \right) - \frac{1}{2^n} (2) 4b^2(n-2).
\]

\(\square\)

Proof of Theorem 10

First, we note that it is easy to check that \( a^*(n, p) \) is convex and symmetric about \( n/2 \) in \( p \). So \( a^*(n, p) \) is maximized on \([1, n - 2]\) at \( p = 1 \). Therefore, for \( a \in (\frac{1}{2}, a^*(n, p)] \), we also have \( a \in (\frac{1}{2}, a^*(n, 1)] \). Hence, \( b^*(n, 1, a, q) \) is well defined (for \( a \in (\frac{1}{2}, a^*(n, p)] \)).

We begin by investigating where the continuous function \( \beta(p) := (b^*(n, p, a, q))^2 \) is decreasing, for (continuous) \( p \in (1, n - 2) \).

\[
\frac{\partial \beta(p)}{\partial p} = \frac{4a^2 - 1}{4(n-q)} \left( (2a+1)(q+1) + (2a-1)(p-1) \right) \\
\left( (4a^2 - 1) \right) (p-q+1)^2.
\]

It is clear that all factors in the numerator and denominator are positive except for \((2a - 1)p - 1\), which we need to analyze. We can easily see that this is negative, precisely when \( a < \frac{1}{2} \left( 1 + \frac{1}{p} \right) \). So, we only need check that \( a^*(n, p) < \frac{1}{2} \left( 1 + \frac{1}{p} \right) \); that is, we need to check that

\[
\frac{1}{2} \sqrt{\left( 1 + \frac{1}{p} \right) \left( 1 + \frac{1}{n-p} \right)} < \frac{1}{2} \left( 1 + \frac{1}{p} \right).
\]

22
But this easily reduces to $1 + \frac{1}{n - p} < 1 + \frac{1}{p}$, which is true precisely when $p < n/2$.

In particular, $\beta(p)$ is decreasing on $(1, n/2)$ and increasing on $(n/2, n - 2)$. So it is quasiconvex, and has a maximum on $[1, q - 1]$ at an endpoint.

Next, we will demonstrate that $\Delta b^*(q) := b^*(n, 1, a, q) - b^*(n, q - 1, a, q) \geq 0$, which will complete our proof. After some algebraic manipulations, we have that $\Delta b^*(q) \geq 0$ simplifies to

$$\frac{(1 - 2a^2)q + 2a^2}{2((1 - 2a^2)q + (4a^2 - 1))} \geq \frac{(1 - 2a^2)q + 2a^2}{q}. \quad (1)$$

Claim 1: $(1 - 2a^2)q + 2a^2 \geq 0$. To see this, first note that it is clear when $a \leq \sqrt{2}/2$. If $a > \sqrt{2}/2$, then the claim is equivalent to $q \leq \frac{2a^2}{2a^2 - 1}$. The left-hand side of this last expression is trivially increasing in $q$ and the right-hand side is decreasing in $a$, so it suffices to check that

$$n - 1 \leq \frac{(a^*(n, 1))^2}{(a^*(n, 1))^2 - 1/2}.$$

Using Proposition 8, we can check that the right-hand side of this last expression is precisely $n$, and so the claim is verified.

Claim 2: $(1 - 2a^2)q + (4a^2 - 1) > 0$. It is clearly true when $1/2 \leq a \leq \sqrt{2}/2$. For $a > \sqrt{2}/2$, the claim is equivalent to $q \leq \frac{4a^2}{2a^2 - 1}$. Similarly to Claim 1, it suffices to check that

$$n \leq \frac{4(a^*(n, 1))^2 - 1}{2(a^*(n, 1))^2 - 1}.$$

Using Proposition 8, we can check that the right-hand side of this last expression is precisely $n + 1$, and so the claim is verified.

Combining Eq. (1), and the two claims, it remains to show that $2((1 - 2a^2)q + (4a^2 - 1)) \leq q$. But this reduces to showing that $(1 - 4a^2)(q - 2) \leq 0$, which immediately follows from $a \geq 1/2$ and $q \geq 2$.

\[\square\]

**Proof of Theorem 11**

Let $\beta(q) := (b^*(n, 1, a, q))^2$. We first demonstrate that $\beta(q)$ is quasiconvex in $q$. This implies that the maximum is attained a boundary point, that is $q = p + 1$ or $q = n - 1$. First, we calculate the unique stationary point

$$\bar{q}(a) := \frac{n}{2} + 1 + \frac{1}{2(2a^2 - 1)}.$$

Next, we demonstrate that $\bar{q} \notin [\frac{n}{2} + 1, n - 1]$. It is easy to see that $\bar{q}$ is decreasing in $a$. Then, for $a \in [1/2, \sqrt{2}/2]$, $\bar{q}$ is maximized at $a = 1/2$, and we have $\bar{q}(a) \leq \bar{q}(1/2) = n/2$. For $a \in (\sqrt{2}/2, a^*(n, 1)]$, $\bar{q}$ is minimized at $a = a^*(n, 1)$, and we have $\bar{q}(a) \geq \bar{q}(a^*(n, 1)) = n + 1/2$. This implies that for all $a \in [1/2, a^*(n, 1)]$, we have $\bar{q} \notin [\frac{n}{2} + 1, n - 1]$. 

23
Next, we will demonstrate that $\partial \beta / \partial q > 0$ for $q \geq n^2 + 1$. We consider the case of $q = n - 1$, the maximum value for $q$. Then we can calculate $\partial \beta / \partial q$ evaluated at $q = n - 1$:

$$\frac{(2a^2 - 1)(n - 4) - 1}{4((2a^2 - 1)(n - 3) - 1)^2} > 0.$$  

Note that is easy to check that the numerator is positive for $n \geq 4$, and $a \in [1/2, a^*(n, 1)]$. We do this by observing that the two positive roots of the numerator are $\sqrt{\frac{n}{2(n-1)}}$ and $\sqrt{\frac{n-3}{2(n-4)}}$, both of which are greater than or equal to $a^*(n, 1) = \sqrt{n^2(n-1)}$. Then we can plug in any relevant $a$ and observe that both the factors in the numerator are negative. This also implies that if $\bar{q} \in [2, n^2 + 1]$, then $\beta(q)$ is nondecreasing for the interval $[\bar{q}, n - 1]$ and either nonincreasing or nondecreasing for $q \in [2, \bar{q}]$. For $\bar{q} \notin [2, n/2 + 1]$, $\beta(q)$ is strictly increasing. Because $\beta(q)$ has only one stationary point, at $\bar{q}$, we can conclude that $\beta(q)$ (and hence $b^*(n, 1, a, q)$) is quasiconvex in $q$, and therefore the maximum is either at $q = 2$ or $q = n - 1$.

It remains to demonstrate that $b^*(n, 1, n-1, a) \geq b^*(n, 1, 2, a)$, which reduces to demonstrating that

$$\frac{a^2(n - 3)}{2(n - 2)} \frac{(2a^2(n - 1) - n)}{(2a^2(n - 3) - n + 2)} \geq 0.$$  

The positive root of the numerator is $\sqrt{\frac{n}{2(n-1)}}$, which is greater than $a^*(n, 1)$, and then it is easy to check then that the numerator is nonpositive for all $a \in [1/2, a^*(n, 1)]$. Similarly, the positive root of the denominator is $\sqrt{\frac{n-2}{2(n-3)}}$, which is greater than $a^*(n, 1)$, and then it is easy to check then that the numerator is negative for all $a \in [1/2, a^*(n, 1)]$. The result follows.

\[\square\]

Appendix 2: Test instances

Referring to the first column of Table 4, we explain how we built our 20 test instances:

- $C_{63}$ is a well-known benchmark covariance matrix generated from 63 chemical data sensors (see [KLQ95, Ans20], for example). To get some idea of how our results can change when uncorrelated noise is added, we also experimented with adding different positive multiples of the identity matrix. We can see that the behavior is similar, for different multiples, while the gaps are smaller.

- $C_1$ through $C_5$ were generated using the Matlab sprandsym function. This function can take eigenvalues as input; for each randomly generated positive-definite matrix we set $\lambda_i := 4^{\frac{n-1}{n-3}} i$, for each $i \in \mathbb{N}$. This
gives a nice concave decreasing sequence of eigenvalues that is preserved under matrix inversion (see [CFLL21]).

- Each of $C_6$ through $C_{10}$ were generated as follows. First, we randomly generated a diagonally dominant tridiagonal matrix $\bar{C}$ with:
  
  \[ \bar{C}_{i,i} \sim U[2, 5], \quad \text{for } i = 1, \ldots, n; \]
  
  \[ \bar{C}_{i,i+1} = \bar{C}_{i+1,i} \sim U[-1, 1], \quad \text{for } i = 1, \ldots, n - 1, \]

independently generated. Next, we made $m = 100,000$ independent samples from the multivariate normal distribution $N(\mathbf{0}, \bar{C})$. From these $m$ samples, we calculated the sample covariance matrix $C$. In this way, we get $C$ as a dense noisy version of the tridiagonal $\bar{C}$.

- $C_{11}$ through $C_{15}$ are generated in a similar way to $C_6, \ldots, C_{10}$ but with a different $\bar{C}$. In this case tridiagonal $\bar{C}$ is made up $n/2$ blocks of $J_2 = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$ plus independent random samples from $U[0, 0.05]$ added to each diagonal element. Here we have samples from $n/2$ pairs of bivariate normals, with no correlation between pairs and high correlation within a pair. Again, we made $m = 100,000$ independent samples from the multivariate normal distribution $N(\mathbf{0}, \bar{C})$, and from these $m$ samples, we calculated the sample covariance matrix $C$.

- For $C_{16}$ through $C_{20}$, we randomly and independently generated
  
  \[ R_i \sim N(0, 0.2), \quad \text{for } i = 1, \ldots, n; \]
  
  \[ E_i \sim N(0, 1), \quad \text{for } i = 0, \ldots, n + 1. \]

Then, with $d = 0.2$, let

\[ Y_i := R_i + E_i + d \times (E_{i-1} + E_{i+1}), \quad \text{for } i = 1, \ldots, n. \]

In this way, we have significant correlation between “neighbors”. We made $m = 100,000$ independent samples from this distribution, we calculated the sample covariance matrix, and we used this as $C$.

In Table 6, we summarize some statistics for our test matrices. The ratios $\lambda_1/\lambda_n$ clearly indicate that all of our matrices are not nearly diagonal. The column ‘abs sum’ tabulates $\Sigma_{i,j} |C[i,j]|$. The column ‘abs sum tridiag’ tabulates $\Sigma_{i,j \leq 1} |C[i,j]|$. Hence, the ratios between these two, the tri-ratio’ values, measures how far from tridiagonal these matrices are. We can see that the the first five have only a very modest degree of tridiagonality. $C_1-C_5$ are not tridiagonal at all. Finally, $C_6-C_{20}$ are decidedly not tridiagonal, but not extremely far from being tridiagonal, as desired.
\begin{table}[h!]
\centering
\begin{tabular}{c|c|c|c|c|c|c}
\textbf{$C$} & \textbf{$n$} & $\lambda_n(C)$ & $\lambda_1(C)$ & $\lambda_1/\lambda_n$ & abs sum & abs sum diag & tri ratio \\
\hline
$C_{63}^{-1}$ & 63 & 0.65 & 31.50 & 48.42 & 1780.66 & 920.04 & 1.94 \\
$C_{63}^{-1} + 0.125I$ & 63 & 0.78 & 31.63 & 40.78 & 1788.54 & 927.92 & 1.93 \\
$C_{63}^{-1} + 0.25I$ & 63 & 0.90 & 31.75 & 35.26 & 1796.41 & 935.79 & 1.92 \\
$C_{63}^{-1} + 0.375I$ & 63 & 1.03 & 31.98 & 31.18 & 1804.29 & 943.67 & 1.91 \\
$C_{63}^{-1} + 0.5I$ & 63 & 1.15 & 32.00 & 27.81 & 1812.16 & 951.54 & 1.90 \\
\hline
$C_1$ & 100 & 0.25 & 4.00 & 16.00 & 582.96 & 146.62 & 3.98 \\
$C_2$ & 100 & 0.25 & 4.00 & 16.00 & 620.53 & 143.78 & 4.32 \\
$C_3$ & 100 & 0.25 & 4.00 & 16.00 & 543.63 & 146.14 & 3.72 \\
$C_4$ & 100 & 0.25 & 4.00 & 16.00 & 580.94 & 144.61 & 4.02 \\
$C_5$ & 100 & 0.25 & 4.00 & 16.00 & 574.24 & 143.15 & 4.01 \\
\hline
$C_6$ & 100 & 1.16 & 5.74 & 4.97 & 546 & 459.67 & 1.19 \\
$C_7$ & 100 & 1.41 & 5.74 & 4.07 & 520.34 & 435.59 & 1.19 \\
$C_8$ & 100 & 1.38 & 5.91 & 4.27 & 544.32 & 459.57 & 1.18 \\
$C_9$ & 100 & 1.17 & 5.78 & 4.94 & 537.27 & 451.79 & 1.19 \\
$C_{10}$ & 100 & 1.58 & 5.47 & 3.45 & 534.84 & 451.56 & 1.18 \\
\hline
$C_{11}$ & 100 & 1.11 & 5.88 & 5.31 & 524.93 & 442.32 & 1.19 \\
$C_{12}$ & 100 & 1.42 & 5.83 & 4.09 & 518.17 & 435.43 & 1.19 \\
$C_{13}$ & 100 & 1.38 & 5.90 & 4.29 & 546.19 & 459.26 & 1.19 \\
$C_{14}$ & 100 & 1.16 & 5.74 & 4.93 & 535.49 & 452.04 & 1.18 \\
$C_{15}$ & 100 & 1.59 & 5.45 & 3.43 & 536.84 & 450.93 & 1.19 \\
\hline
$C_{16}$ & 100 & 0.49 & 2.51 & 5.12 & 274.69 & 212.78 & 1.29 \\
$C_{17}$ & 100 & 0.49 & 2.53 & 5.14 & 276.40 & 213.01 & 1.30 \\
$C_{18}$ & 100 & 0.49 & 2.52 & 5.13 & 275.30 & 213.04 & 1.29 \\
$C_{19}$ & 100 & 0.49 & 2.52 & 5.11 & 275.19 & 212.97 & 1.29 \\
$C_{20}$ & 100 & 0.49 & 2.51 & 5.09 & 275.68 & 212.94 & 1.29 \\
\end{tabular}
\caption{Test-matrix statistics}
\end{table}

**Appendix 3: Further experiments**

Figure 7 is of the same type as Figure 5, but now with $s \sim n/4$ and $s \sim 3n/4$. A more detailed view of these experiments, following what we presented in Table 4, is in Tables 8 and 9. While the general trends seen for $s \sim n/2$ persist, we do see now several instances where DP($\Sigma$) improves upon linx($\Sigma$).
Figure 7: Average fraction of gap closed by each masking phase

| \( C \)          | \( n \) | \( s \) | \( \ln(x(\frac{1}{2})) \) | \( \lambda(\frac{1}{2}) \) | \( \lambda(\Pi) \) | \( \lambda(\Sigma) \) | \( \ln(x(\Sigma)) \) | \( \text{DP}(\Sigma) \) |
|------------------|--------|-------|-----------------|-----------------|----------------|----------------|----------------|----------------|
| \( C_{63}^{-1} \) | 63     | 15    | 0.9839          | 0.9880          | 0.8745         | 0.8150         | 0.6880         | 0.6880         |
| \( C_{63}^{-1} + 0.125I \) | 63   | 15    | 0.9696          | 0.9739          | 0.8616         | 0.8027         | 0.6772         | 0.6772         |
| \( C_{63}^{-1} + 0.25I \) | 63    | 15    | 0.9558          | 0.9601          | 0.8490         | 0.7908         | 0.6677         | 0.2334         |
| \( C_{63}^{-1} + 0.375I \) | 63    | 15    | 0.9423          | 0.9467          | 0.8368         | 0.7791         | 0.6565         | 0.2262         |
| \( C_{63}^{-1} + 0.5I \) | 63    | 15    | 0.9292          | 0.9336          | 0.8248         | 0.7678         | 0.6466         | 0.2192         |
| \( C_{1} \)      | 100    | 25    | 1.0899          | 1.2264          | 0.9922         | 0.9616         | 0.8183         | 0.8183         |
| \( C_{2} \)      | 100    | 25    | 1.0936          | 1.1161          | 0.9034         | 0.7943         | 0.5885         | 0.5885         |
| \( C_{3} \)      | 100    | 25    | 0.8229          | 0.8743          | 0.7404         | 0.7144         | 0.6201         | 0.6201         |
| \( C_{4} \)      | 100    | 25    | 0.9130          | 0.9969          | 0.7969         | 0.7766         | 0.5616         | 0.5616         |
| \( C_{5} \)      | 100    | 25    | 0.8480          | 0.8997          | 0.7065         | 0.6521         | 0.4981         | 0.4981         |
| \( C_{6} \)      | 100    | 25    | 0.0592          | 0.9574          | 0.0775         | 0.0763         | 0.0366         | 0.0566         |
| \( C_{7} \)      | 100    | 25    | 0.0277          | 0.6608          | 0.0193         | 0.0147         | 0.0026         | 0.0026         |
| \( C_{8} \)      | 100    | 25    | 0.1028          | 0.9697          | 0.1175         | 0.1168         | 0.0752         | 0.0752         |
| \( C_{9} \)      | 100    | 25    | 0.0424          | 0.7216          | 0.0509         | 0.0426         | 0.0426         | 0.0426         |
| \( C_{10} \)     | 100    | 25    | 0.0447          | 0.6762          | 0.0435         | 0.0236         | 0.0236         | 0.0236         |
| \( C_{11} \)     | 100    | 25    | 0.0574          | 0.6121          | 0.0505         | 0.0092         | 0.0057         | 0.0057         |
| \( C_{12} \)     | 100    | 25    | 0.0298          | 0.6763          | 0.0195         | 0.0137         | 0.0026         | 0.0026         |
| \( C_{13} \)     | 100    | 25    | 0.0853          | 0.9386          | 0.0955         | 0.0930         | 0.0514         | 0.0514         |
| \( C_{14} \)     | 100    | 25    | 0.0443          | 0.7356          | 0.0463         | 0.0375         | 0.0146         | 0.0139         |
| \( C_{15} \)     | 100    | 25    | 0.0534          | 0.6781          | 0.0541         | 0.0341         | 0.0341         | 0.0341         |
| \( C_{16} \)     | 100    | 25    | 0.3970          | 7.2480          | 0.0462         | 0.0461         | 0.0461         | 0.0461         |
| \( C_{17} \)     | 100    | 25    | 0.3929          | 7.2532          | 0.0499         | 0.0498         | 0.0498         | 0.0498         |
| \( C_{18} \)     | 100    | 25    | 0.3823          | 7.2506          | 0.0590         | 0.0590         | 0.0588         | 0.0588         |
| \( C_{19} \)     | 100    | 25    | 0.3769          | 7.2391          | 0.0497         | 0.0497         | 0.0497         | 0.0496         |
| \( C_{20} \)     | 100    | 25    | 0.3949          | 7.2591          | 0.0439         | 0.0438         | 0.0438         | 0.0438         |

Table 8: Entropy gaps: \( s \sim n/4 \)
Table 9: Entropy gaps: $s \sim 3n/4$

| $C$           | $n$ | $s$ | linx$(\frac{1}{2})$ | $\lambda(\frac{1}{2})$ | $\lambda(\Pi)$ | $\lambda(\Sigma)$ | linx$(\Sigma)$ | DP$(\Sigma)$ |
|---------------|-----|-----|----------------------|------------------------|----------------|-------------------|----------------|--------------|
| $C_{63}^{-1}$ | 63  | 47  | 5.1504               | 5.1546                 | 4.7257         | 4.1712           | 4.0911         | 4.0582       |
| $C_{63}^{-1} + 0.125I$ | 63  | 47  | 5.0078               | 5.0120                 | 4.5895         | 4.0436           | 3.9649         | 3.9323       |
| $C_{63}^{-1} + 0.25I$ | 63  | 47  | 4.8736               | 4.8777                 | 4.4614         | 3.9239           | 3.8467         | 3.8142       |
| $C_{63}^{-1} + 0.375I$ | 63  | 47  | 4.7471               | 4.7512                 | 4.3409         | 3.8115           | 3.7358         | 3.7035       |
| $C_{63}^{-1} + 0.5I$  | 63  | 47  | 4.6268               | 4.6308                 | 4.2265         | 3.7050           | 3.6307         | 3.6040       |
| $C_1$         | 100 | 75  | 14.1800              | 14.2440                | 12.9740        | 11.7390          | 11.2780        | 11.2780      |
| $C_2$         | 100 | 75  | 12.8690              | 12.9300                | 11.8830        | 11.0540          | 10.4730        | 10.4730      |
| $C_3$         | 100 | 75  | 12.0690              | 12.1220                | 10.8660        | 9.6651           | 8.9006         | 8.9006       |
| $C_4$         | 100 | 75  | 13.5630              | 13.5810                | 12.2950        | 11.1710          | 10.2000        | 10.2000      |
| $C_5$         | 100 | 75  | 12.9400              | 13.0260                | 11.7660        | 10.6340          | 9.6674         | 9.6674       |
| $C_6$         | 100 | 75  | 1.1464               | 2.2101                 | 1.2271         | 0.7309           | 0.6028         | 0.6028       |
| $C_7$         | 100 | 75  | 0.8360               | 1.6736                 | 0.8169         | 0.4710           | 0.3384         | 0.3384       |
| $C_8$         | 100 | 75  | 0.9222               | 1.9064                 | 0.9357         | 0.5663           | 0.4240         | 0.4240       |
| $C_9$         | 100 | 75  | 1.1488               | 2.1226                 | 1.1956         | 0.8275           | 0.4835         | 0.4835       |
| $C_{10}$      | 100 | 75  | 1.0013               | 1.8240                 | 1.0901         | 0.7925           | 0.4964         | 0.4964       |
| $C_{11}$      | 100 | 75  | 0.9316               | 2.3084                 | 0.9966         | 0.6492           | 0.4991         | 0.0584       |
| $C_{12}$      | 100 | 75  | 0.8318               | 1.6619                 | 0.8143         | 0.4657           | 0.3406         | 0.3406       |
| $C_{13}$      | 100 | 75  | 0.9199               | 1.9245                 | 0.9319         | 0.5658           | 0.4228         | 0.4228       |
| $C_{14}$      | 100 | 75  | 1.1488               | 2.1226                 | 1.2121         | 0.8175           | 0.5496         | 0.5496       |
| $C_{15}$      | 100 | 75  | 0.9909               | 1.8258                 | 1.0688         | 0.7949           | 0.4852         | 0.4852       |
| $C_{16}$      | 100 | 75  | 6.8324               | 14.6930                | 8.4079         | 8.4078           | 8.4072         | 8.4072       |
| $C_{17}$      | 100 | 75  | 6.8630               | 14.7360                | 8.4535         | 8.4533           | 8.4526         | 8.4526       |
| $C_{18}$      | 100 | 75  | 6.8601               | 14.7380                | 8.4570         | 8.4570           | 8.4567         | 8.4567       |
| $C_{19}$      | 100 | 75  | 6.8393               | 14.7240                | 8.4577         | 8.4573           | 8.4567         | 8.4567       |
| $C_{20}$      | 100 | 75  | 6.8605               | 14.7390                | 8.4501         | 8.4500           | 8.4493         | 8.4493       |
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