Abstract

Covariance selection seeks to estimate a covariance matrix by maximum likelihood while restricting the number of nonzero inverse covariance matrix coefficients. A single penalty parameter usually controls the tradeoff between log likelihood and sparsity in the inverse matrix. We describe an efficient algorithm for computing a full regularization path of solutions to this problem.

1 Introduction

We consider the problem of estimating a covariance matrix from sample multivariate data my maximizing its likelihood, while penalizing the inverse covariance so that its graph is sparse. This problem is known as covariance selection and can be traced back at least to [1]. The coefficients of the inverse covariance matrix define the representation of a particular Gaussian distribution as a member of the exponential family, hence sparse maximum likelihood estimates of the inverse covariance yield sparse representations of the model in this class. Furthermore, in a Gaussian model, zeroes in the inverse covariance matrix correspond to conditionally independent variables, so this penalized maximum likelihood procedure simultaneously stabilizes estimation and isolates structure in the underlying graphical model (see [2]).

Given a sample covariance matrix $\Sigma \in \mathbb{S}_n$, the covariance selection problem is written as follows

$$\maximize \log \det X - \text{Tr}(\Sigma X) - \rho \text{Card}(X)$$

in the matrix variable $X \in \mathbb{S}_n$, where $\rho > 0$ is a penalty parameter controlling sparsity and Card$(X)$ is the number of nonzero elements in $X$. This is a combinatorially hard (non-convex) problem and, as in [3, 4, 5, 6], we form the following convex relaxation

$$\maximize \log \det X - \text{Tr}(\Sigma X) - \rho \|X\|_1$$

which is a convex problem in the matrix variable $X \in \mathbb{S}_n$, where $\|X\|_1$ is the sum of absolute values of the coefficients of $X$ here. After scaling, the $\|X\|_1$ penalty can be understood as a convex lower bound on Card$(X)$ and this type of relaxation has been used in variable selection and matrix completion for example [7, 8, 9]. Another completely different approach derived in [10] reconciles the local dependence structure inferred from $n$ distinct $\ell_1$-penalized regressions of a single variable.
against all the others. Both this approach and the convex relaxation (1) have been shown to be consistent in [10] and [11] respectively.

In practice however, both methods are computationally challenging when \( n \) gets large. Various algorithms have been employed to solve (1) with [6] using a custom interior point method and [11] using a block coordinate descent method where each iteration required solving a LASSO-like problem, among others. This last method is efficiently implemented in the GLASSO package by [12] using coordinate descent algorithms from [13] to solve the inner regression problems.

One key issue in all these methods is that there is no a priori obvious choice for the penalty parameter so, in practice, at least a partial regularization path of solutions has to be computed, and this procedure is then repeated many times to get confidence bounds on the graph structure by cross-validation. Pathwise LASSO algorithms such as LARS by [14] can be used to get a full regularization path of solution using the method in [10] but this still requires solving and reconciling \( n \) regularization paths on regression problems of dimension \( n \).

Our contribution here is to formulate a pathwise algorithm for solving problem (1) using numerical continuation methods (see [15] for an application in kernel learning). Each iteration requires solving a large structured linear system (predictor step) then improving precision using a block coordinate descent method (corrector step). Overall, the cost of moving from one solution to problem (1) to another is typically much lower than that of solving two separate instances of (1). We illustrate the performance of our methods on several artificial and realistic data sets.

The paper is organized as follows. Section 2 reviews some basic convex optimization results on the covariance selection problem in (1). Our main pathwise algorithm is described in Section 3. Finally, we present some numerical results in Section 4.

**Notation.** In what follows, we write \( S_n \) the set of symmetric matrices of dimension \( n \). For a matrix \( X \in \mathbb{R}^{m \times n} \), we write \( \|X\|_F \) its Frobenius norm, \( \|X\|_1 = \sum_{ij} |X_{ij}| \) the \( \ell_1 \) norm of its vector of coefficients, and \( \text{Card}(X) \) the number of nonzero coefficient in \( X \).

## 2 Covariance Selection

Starting from the convex relaxation defined above

\[
\text{maximize} \quad \log \det X - \text{Tr}(\Sigma X) - \rho \|X\|_1
\]

in the variable \( X \in S_n \), where \( \|X\|_1 \) can be understood as a convex lower bound on the \( \text{Card}(X) \) function whenever \( |X_{ij}| \leq 1 \) (we can always scale \( \rho \) otherwise). Let us write \( X^*(\rho) \) the optimal solution of problem (2). In what follows, we will seek to compute (or approximate) the entire regularization path of solutions \( X^*(\rho) \), for \( \rho \in \mathbb{R}_+ \). To remove the nonsmooth penalty, we can set \( X = L - M \) and rewrite the problem above as

\[
\text{maximize} \quad \log \det (L - M) - \text{Tr}(\Sigma(L - M)) - \rho 1^T(L + M)1
\]

subject to \( L_{ij}, M_{ij} \geq 0, \quad i, j = 1, \ldots, n. \) (3)

in the matrix variables \( L, M \in S_n \).
2.1 Dual & optimality conditions

We can form the following dual to problem (2) as

\[
\begin{align*}
\text{minimize} & \quad -\log \det(U) - n \\
\text{subject to} & \quad U_{ij} \leq \rho + \Sigma_{ij} \\
& \quad U_{ij} \geq \Sigma_{ij} - \rho
\end{align*}
\]

in the variable \( U \in S_n \). The KKT conditions (see [16, §5.9.2]) for problem (3) and (4) are then given by

\[
\begin{align*}
(L - M) &= U^{-1} \\
(\rho + \Sigma_{ij} - U_{ij})L_{ij} &= 0 \\
(\rho - \Sigma_{ij} + U_{ij})M_{ij} &= 0
\end{align*}
\]

in the variable \( U \in S_n \) and \( L, M \in S_n \).

2.2 Regularized reformulation

While problem (4) is a convex optimization problem with \( O(n^2) \) linear constraints. As in [15] for example, in the spirit of barrier methods for interior point algorithms, we form the following (unconstrained) regularized problem

\[
\min_U -\log \det(U) - t \left( \sum_{i,j=1}^{n} \log(\rho + \Sigma_{ij} - U_{ij}) + \sum_{i,j=1}^{n} \log(\rho - \Sigma_{ij} + U_{ij}) \right)
\]

in the variable \( U \in S_n \) and \( t > 0 \) specifies a desired tradeoff level between centrality (smoothness) and optimality. From every solution \( U^*(t) \) corresponding to each \( t > 0 \), the barrier formulation also produces an explicit dual solution \((L^*(t), M^*(t))\) to Problem (4). Indeed we can define matrices \( \lambda, \mu \in S_n \) as follows

\[
\begin{align*}
L_{ij}(U, \rho) &= \frac{t}{\rho + \Sigma_{ij} - U_{ij}} \\
M_{ij}(U, \rho) &= \frac{t}{\rho - \Sigma_{ij} + U_{ij}}
\end{align*}
\]

or alternatively, in the complementarity format

\[
\begin{align*}
L_{ij}(U, \rho)(\rho + \Sigma_{ij} - U_{ij}) &= t \\
M_{ij}(U, \rho)(\rho - \Sigma_{ij} + U_{ij}) &= t.
\end{align*}
\]

First order optimality conditions for problem (6) then imply \((L - M) = U^{-1}\). As \( t \) tends to 0, problem (6) traces a central path towards the optimal solution to problem (4). If we write \( f(U) \) the objective function of problem (4) and call \( p^* \) its optimal value, we get

\[
f(U^*(t)) - p^* \leq 2n^2 t
\]

hence \( t \) can be understood as a surrogate duality gap when solving problem (4).
3 Algorithm

In this section we derive a Predictor-Corrector algorithm to approximate the entire path of solutions \( X^*(\rho) \) when \( \rho \) varies between 0 and \( \max_i \Sigma_{ii} \) (beyond which the solution matrix is diagonal). Define

\[
H(U, \rho) = \lambda(U, \rho) - \mu(U, \rho) - U^{-1}
\]

we trace the curve \( H(U, \rho) = 0 \) (first order optimality conditions for problem (6)).

**Algorithm 1** Pathwise Covariance Selection

**Input:** \( \Sigma \in S_n \)

1: Start with \((U_0, \rho_0)\) s.t \( H(U_0, \rho_0) = 0 \)
2: for \( i = 1 \) to \( k \) do
3: \hspace{1em} **Predictor Step.** Let \( \rho_{i+1} = \rho_i + h \). Compute a tangent direction by solving the linear system
\[
\frac{\partial H}{\partial \rho}(U_i, \rho_i) + J(U_i, \rho_i) \frac{\partial U}{\partial \rho} = 0
\]

in \( \partial U/\partial \rho \in S_n \), where \( J(U_i, \rho_i) = \partial H(U, \rho)/\partial U \in S_{n^2} \) is the Jacobian matrix of the function \( H(U, \rho) \).
4: Update \( U_{i+1} = U_i + h \partial U/\partial \rho \).
5: \hspace{1em} **Corrector Step.** Solve problem (6) starting at \( U = U_{i+1} \).
6: end for

**Output:** Sequence of matrices \( U_i, i = 1, \ldots, k \).

Typically here, \( h \) is a small constant, \( \rho_0 = \max_i \Sigma_{ii} \) and \( U_0 \) is computed by solving a single (very sparse) instance of problem (6) for example.

3.1 Predictor: conjugate Gradient method

In the algorithm above, the tangent direction in the predictor step is computed by solving a linear system \( Ax = b \) where \( A = (U^{-1} \otimes U^{-1} + D) \) and \( D \) is a diagonal matrix. This system of equations has dimension \( n^2 \) and we solve it using the conjugate gradient (CG) method.

**CG iterations.** The most expensive operation in the CG iterations is the computation of a matrix vector product \( Ap_k \), with \( p_k \in \mathbb{R}^{n^2} \). Here however, we can exploit problem structure to compute this step very efficiently. Observe that \( (U^{-1} \otimes U^{-1})p_k = \text{vec}(U^{-1}P_k U^{-1}) \) when \( p_k = \text{vec}(P_k) \), so the computation of the matrix vector product \( Ap_k \) needs only \( O(n^3) \) flops instead of \( O(n^4) \). The CG method then needs at most \( O(n^2) \) iterations to converge, leading to a total complexity of \( O(n^5) \) for the predictor step. In practice, we will observe that CG needs considerably fewer iterations.

**Stopping criterion.** To speed up the computation of the predictor step, we can stop the conjugate gradient solver when the norm of the residual falls below the numerical tolerance \( \tau \). In our experiments here, we stopped the solver after the residual decreases by two order of magnitudes.
**Projection** If we are moving backward on the path (i.e. from sparse solutions to dense ones, which is usually faster), there is no guarantee that, after taking a step in the direction given by the predictor, the new matrix $U$ will be in the domain of (6), i.e. will satisfy:

$$U \succeq 0, \quad U_{ij} \leq \rho + \Sigma_{ij}, \quad U_{ij} \geq \Sigma_{ij} - \rho, \quad i, j = 1, \ldots, n.$$ 

However, this domain is the intersection of a box with the semidefinite cone. Projecting on a box has cost $O(n^2)$ and projecting on the p.s.d. cone requires a single eigenvalue decomposition with complexity $O(n^3)$. This means that we can find the closest matrix $U$ using alternating projections (see [17] for details).

### 3.2 Corrector: block coordinate descent

For small-sized problems, we can use Newton’s method to solve the Problem (6). However from a computational perspective, this approach is not practical for large values of $n$. We can simplify iterations using a block coordinate descent algorithm that updates one row/column of the matrix in each iteration ([11]). Let us partition the matrices $U$ and $\Sigma$ as

$$U = \begin{pmatrix} V & u \\ u^T & w \end{pmatrix} \quad \text{and} \quad S = \begin{pmatrix} A & b \\ b^T & c \end{pmatrix}$$

We keep $V$ fixed in each iteration and solve for $u, w$. Without loss of generality, we can always assume that we are updating the last row/column.

**Algorithm.** Problem (6) can be written in block format as:

$$\begin{align*}
\text{minimize} & \quad -\log(w - u^T V^{-1} u) - t(\log(\rho + c - 1) + \log(\rho - c + w)) \\
& \quad -2t \left( \sum_i \log(\rho + b_i - u_i) + \sum_i \log(\rho - b_i + u_i) \right) \\
\end{align*}$$

(11)

in the variables $u \in \mathbb{R}^{(n-1)}$ and $w \in \mathbb{R}$. Here $V \in \mathbb{S}^{(n-1)}$ is kept fixed in each iteration. The above optimization unconstrained problem can be solved for larger values of $n$ using coordinate descent methods for example (as in [13]). We use Newton’s method here because it has explicit complexity bounds and works well on medium scale problems. We summarize the block coordinate algorithm as follows.

**Algorithm 2** Block coordinate descent corrector steps

**Input:** $U_0, \Sigma \in \mathbb{S}_n$

1. for $i = 1$ to $k$ do
2. Pick the row and column to update.
3. Use Newton’s method to solve Problem (11).
4. Update $U^{-1}$.
5. end for

**Output:** A matrix $U_k$ solving (6).

We can use the Sherman-Woodbury-Morrison (SWM) formula (see [16, §C.4.3]) to efficiently update $U^{-1}$ at each iteration, so it suffices to compute the full inverse only once at the beginning of
the path. Assume that the last row/column of the block matrix $U_k$ defined above is being updated and let $(u^*, w^*)$ be the solution to problem (11). If we define the vectors

$$e = (0, 0, \ldots, 1)^T, \quad r = \begin{pmatrix} u^* - u \\ w^* - w \end{pmatrix}, \quad s = \begin{pmatrix} u^* - u \\ 0 \end{pmatrix}$$

the update step in $U$ can be written

$$U_{k+1} = U_k + re^T + e^Ts,$$

which means that $(U_{k+1})^{-1}$ can be computed using the SWM formula on this rank-two update of $U_k$. This step only requires a few matrix vector products, hence can be computed efficiently. It then remains to update $V^{-1}$ using the SWM once again, this time on

$$\begin{pmatrix} V & 0 \\ 0 & 1 \end{pmatrix}^{-1} = \left( \begin{pmatrix} V & u \\ u^T & w \end{pmatrix} - \begin{pmatrix} 0 & u \\ u^T & w - 1 \end{pmatrix} \right)^{-1}$$

which is a rank two update of $(U_{k+1})^{-1}$.

**Dual block problem.** We can derive a dual to problem (11) by rewriting it as a constrained optimization problem to get

$$\begin{align*}
\text{minimize} & \quad -\log x_1 - t(\log x_2 + \log x_3) - 2t \left( \sum_i (\log y_i + \log z_i) \right) \\
\text{subject to} & \quad x_1 \leq w - u^T V^{-1} u \\
& \quad x_2 = \rho + c - w, \ x_3 = \rho - c + w \\
& \quad y_i = \rho + b_i - u_i, \ z_i = \rho - b_i + u_i
\end{align*}$$

(12)

in the variables $u \in \mathbb{R}^{(n-1)}, w \in \mathbb{R}, x \in \mathbb{R}^3, y \in \mathbb{R}^{(n-1)}, z \in \mathbb{R}^{(n-1)}$. We can write the Lagrangian of this problem as

$$L(x, y, z; \alpha, \beta, \eta) = -\log x_1 - t(\log x_2 + \log x_3) - 2t \left( \sum_i (\log y_i + \log z_i) \right) + \alpha_1(x_1 - w + u^T V^{-1} u) + \alpha_2(x_2 - \rho - c + w) + \alpha_3(x_3 - \rho + c - w) + \sum_i (\beta_i(y_i - \rho - b_i + u_i) + \eta_i(z_i - \rho + b_i - u_i))$$

(13)

in the dual variables $\alpha \in \mathbb{R}^3, \beta \in \mathbb{R}^{(n-1)}$ and $\eta \in \mathbb{R}^{(n-1)}$. This Lagrangian is minimized at the following point

$$\begin{align*}
x^* &= (1/\alpha_1, t/\alpha_2, t/\alpha_3), \ u^*_i = \frac{V(\eta_i - \beta_i)}{2x_1} \\
y^*_i &= 2t/\beta_i, \ z^*_i = 2t/\eta_i.
\end{align*}$$

(14)

We can then write the dual to problem (12) as

$$\begin{align*}
\text{maximize} & \quad 1 + 2t(2n - 1) + \log \alpha_1 - \alpha_2(\rho + c) - \alpha_3(\rho - c) - \sum_i (\beta_i(\rho + b_i) + \eta_i(\rho - b_i)) + t \log(\alpha_2/t) + t \log(\alpha_3/t) + 2t \left( \sum_i (\log(\beta_i/2t) + \log(\eta_i/2t)) \right) \\
\text{subject to} & \quad \alpha_1 = \alpha_2 - \alpha_3 \\
& \quad \alpha_1 \geq 0
\end{align*}$$

(15)

in the variables $\alpha \in \mathbb{R}^3, \beta \in \mathbb{R}^{(n-1)}$ and $\eta \in \mathbb{R}^{(n-1)}$.  

6
Stopping criterion. We can use this last program to bound the suboptimality of the current iterate when solving (11). Let us write \( f_0(x, y, z, u, w) \) and \( g(\alpha, \beta, \eta) \) objective functions of problems (11) and (15) respectively. Starting from the primal point \((x, y, z, u, w)\) we can form a candidate dual solution using (14) as

\[
\begin{align*}
\alpha_2 &= t/x_2, \quad \alpha_3 = t/x_3, \quad \alpha_1 = \alpha_2 - \alpha_3, \\
\beta_i &= 2t/y_i, \quad \eta_i = 2t/z_i
\end{align*}
\]

and the surrogate duality gap \( f_0(x, y, z, u, w) - g(\alpha, \beta, \eta) \) will be an upper bound on the suboptimality of the current point \((u, w)\) in Algorithm (2). This allows us to reliably stop Algorithm (2) when a given target precision is reached.

3.3 Complexity

The complexity of moving from a solution \( X(\rho) \) of (2) to a solution \( X(\rho + h) \) can be summarized as follows. Solving for the predictor step as in §3.1 requires \( O(n^2) \) matrix products, but the number of iterations necessary to get a good estimate of the predictor is typically much lower (cf. experiments in the next section). The corrector steps require solving \( O(n) \) instances of the block problem (11), with each problem having a complexity of \( O(n^{3.5}) \) (both coordinate descent and first-order methods would be much faster here in practice, but explicit complexity bounds are not available for CD). On the other hand, doing a predictor step means that the initial point is very close to the optimal solution of (11), hence the number of iterations required by Newton’s method is typically lower.

4 Numerical Results

In this section, we start by illustrating our problem on a simple example. We then discuss its practical use and performance on larger, more realistic data sets.

4.1 Illustration

To first illustrate our method on an intuitive data set, we solve for a full regularization path of solutions to problem (2) on the covariance matrix of U.S. forward rates for maturities ranging from six months to ten years from 1998 until 2005. Forward rates move as a curve, so we expect their inverse covariance matrix to be close to band diagonal. Figure 1 shows the dependence network obtained from the solution of problem (2) on this matrix along a path, for \( \rho = .02, \rho = .008 \) and \( \rho = .006 \). The graph layout was formed using the yFiles-Organic option in Cytoscape. The string-like dynamics of the rates clearly appear in the last plot.

In Figure 2, we sample from Gaussian model with a given sparse inverse covariance matrix (constructed from the sparse forward rate model inferred in the previous example) and (on the left) plot area under ROC curve versus number of points used in forming the sample covariance matrix, for both covariance selection and a simple thresholding of the inverse matrix coefficients. On the right, we also plot area under ROC curve versus \( \rho \), solving problem (2) with \( \Sigma \) formed using 20 samples. Layout was performed using the yFiles-Organic option in Cytoscape.
Figure 1: Three sample dependence graphs corresponding to the solution of problem (2) on a U.S. forward rates covariance matrix for $\rho = .02$ (left), $\rho = .008$ (center) and $\rho = .006$ (right).

Figure 2: Left: Area under ROC curve versus number of sample points used in forming the covariance matrix $\Sigma$ for covariance selection with fixed $\rho$ (circles) and simple thresholding (squares). Right: Area under ROC curve versus penalty parameter $\rho$ for covariance selection when $\Sigma$ is generated using 20 sample points. The dashed line is the AUROC reached by thresholding the inverse matrix coefficients.

4.2 Experiments

Here, we first discuss how thresholding is used to bring exact zeros in approximate solutions on the regularization path. We also describe how to produce a confidence measure on graph edges. We conclude by applying the techniques to a topic model of the journal *Science*, produced by [18].

**Thresholding** Because we only produce a path of approximate solutions to problem (2), with relative duality gap typically of the order $10^{-2}$, it is then necessary to threshold the coefficients of $X^{-1}$. Once simple heuristic is to prune out all the coefficients of $X^{-1}$ that are smaller than $\max_{ij} X^{-1}_{ij}$ by at least an order of magnitude. Standard matrix perturbation results (see [19] for example) then ensure that the effect on the spectrum of $X$ is negligible.
Cross validation  Leave-one-out cross-validation to get a confidence measure on the graph edges: we can remove one variable at random from the data set, compute the dependence graph corresponding to the remaining variables and repeat this experiment a number of times. Confidence in a graph edge is then measured by the frequency with which it appeared in the random subgraphs. Perhaps more importantly, this same technique can be used to select the penalty parameter ρ in (2), by simply picking the value of ρ for which overall graph stability is maximum.

Performance  To generate test matrices here, we sample sparse random matrices and add multiples of the identity to make them positive semidefinite, then use the inverse matrix as our sample matrix Σ. In Figure 3, we plot the number of nonzero coefficients (cardinality) in the inverse covariance versus penalty parameter ρ, along a path of solutions to problem (2). We then plot the number of conjugate gradient iterations required to compute the predictor in §3.1 versus number of nonzero coefficients in the inverse covariance matrix. We notice that the number of CG iterations decreases significantly for sparse matrices, which makes the algorithm faster at the sparse (i.e. interesting) end of the regularization path.

We also compare numerical performance of three methods for computing a full regularization path of solutions to problem (2). We first compute a full path of solutions solving separate instances of problem (2) using the block coordinate code in [4], we then compute the same path of solutions using the methods detailed here and finally repeat this experiment using the Glasso path code [12] which restarts the covariance selection problem at ρ + ε at the current solution of (2) obtained at ρ. Both COVSEL and our (prototype) code here are written in MATLAB (excepts for a few steps in C), while Glasso is compiled from Fortran and interfaced with R (hence much faster). We report CPU time (in seconds) versus problem dimension in Table 1. Note that the predictor step in §3.1 could also be used to speed up Glasso, but interfacing issues make this option slower at this point. Unfortunately, Glasso does not use the duality gap as a stopping criterion but rather lack of progress (average absolute parameter change less than 10^{-4}), it also performs some thresholding before returning a solution, so these direct comparisons are somewhat noisy.

| Dimension | Covsel | Covsel path | Glasso path |
|-----------|--------|-------------|-------------|
| 50        | 235    | 11          | 8           |
| 100       | 843    | 78          | 25          |

Table 1: CPU time (in seconds) versus problem dimension for computing a regularization path for 200 values of the penalty ρ, solving separate covariance selection problems using block coordinate descent (Covsel), the path following method detailed here (Covsel path) and the Glasso code (Glasso path).

Application  To illustrate our results on a more realistic data set, we applied our algorithm to the covariance matrix extracted from the Correlated Topic Model calibrated in [18] on 10 years of articles from the journal Science, targeting a graph density low enough to reveal some structure. The corresponding network is detailed in Figure 4. Graph edge color is related to the sign of the conditional correlation (green for positive, red for negative) while edge thickness is proportional to the correlation magnitude. The five most important words are listed for each topic.
Figure 3: *Left:* We plot the number of nonzero coefficients in the inverse covariance versus penalty parameter $\rho$, along a path of solutions to problem (2). *Right:* Number of conjugate gradient iterations required to compute the predictor step versus number of nonzero coefficients in the inverse covariance matrix.

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Figure 4: Topic network for the Science Correlated Topic Model in [18]. Network layout using cytoscape. Graph edge color is related to the sign of the conditional correlation (green for positive, red for negative) while edge thickness is proportional to the correlation magnitude.

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