On the Solution Path of Regularized Covariance Estimators

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Abstract

The recently introduced condition-number-regularized covariance estimation method (CondReg) has been demonstrated to be highly useful for estimating high-dimensional covariance matrices. Unlike $\ell_1$-regularized estimators, this approach has the added advantage that no sparsity assumptions are made. The regularization path of the lasso solution has received much attention in the literature. Despite their importance, the solution paths of covariance estimators however have not been considered in much detail. In this paper, we provide a complete characterization of the entire solution path of the CondReg estimator. Our characterization of the solution path has important applications as it yields fast algorithms that compute the CondReg estimates for all possible values of the regularization parameter at the same cost as that for a single fixed parameter. We present two instances of fast algorithms: the forward and the backward algorithms. These algorithms greatly speed up the cross-validation procedure that selects the optimal regularization parameter. Our new method is efficiently implemented with the R package CondReg.
1 Introduction

The condition-number-regularized covariance estimation (CondReg hereafter) is an efficient way of regularizing the Gaussian likelihood estimate for the covariance matrix via upper-bounding its numerical condition number (Won et al., 2013). This approach yields numerically stable covariance estimators even in low sample high dimensional regimes. Given the practical need to estimate very high dimensional covariance estimators in a computationally tractable manner, this paper analyzes in depth the solution path of the condition-number-regularized covariance estimation method. Given \( n \) samples \( x_1, \ldots, x_n \) from a \( p \)-dimensional zero-mean \( p \)-variate Gaussian distribution, the sample covariance matrix \( S = (1/n)XX^T \), \( X = [x_1, \ldots, x_n]^T \) is the maximum likelihood estimator of the covariance matrix \( \Sigma \), provided \( n \geq p \). It is also well-known that \( S \) is ill-conditioned when \( p/n \) is not small enough (Stein, 1975). Therefore in high-dimensional setting where \( p/n \) is small and often even \( n < p \), stable estimation of \( \Sigma \) has been of great interest. Most approaches regularize \( S \) by inducing sparsity (see Khare et al. (2014) and the references therein). The CondReg method directly targets the ill-conditioning of \( S \), without making sparsity assumptions. It is formulated as an optimization problem

\[
\text{minimize } \text{tr}(\Sigma^{-1}S) - \log \det(\Sigma^{-1}) \text{ subject to } \text{cond}(\Sigma) \leq \kappa, \tag{1}
\]

where \( \text{cond}(\Sigma) = \lambda_{\max}(\Sigma)/\lambda_{\min}(\Sigma) \) denotes the condition number of the positive definite matrix variable \( \Sigma \), with \( \lambda_{\max}(\Sigma) \) and \( \lambda_{\min}(\Sigma) \) being the largest and the smallest eigenvalues of \( \Sigma \), respectively. The upper bound \( \kappa \) for the condition number serves as the regularization parameter. Addressing ill-conditioning directly has significant practical importance because in applications such as mean-variance portfolio optimization, ill-conditioned covariance matrices can lead to large estimation errors (Ledoit and Wolf, 2003; Michaud, 1989). Since its introduction, CondReg has been regarded as a competitive high-dimensional covariance estimation method (Donoho et al., 2013; Chi and Lange, 2013; Tong et al., 2014; Zimmermann, 2015).

Won et al. (2013) show that the solution to (1) shrinks the eigenvalues of \( S \) nonlinearly. More precisely, suppose the spectral decomposition of the sample covariance matrix is \( S = Q \text{diag}(l_1, \ldots, l_p)Q^T \), where \( \text{diag}(l_1, \ldots, l_p) \) is the diagonal matrix with diagonal entries \( l_1 \geq \ldots \geq l_p \), and \( Q \in \mathbb{R}^{p \times p} \) is the orthogonal matrix whose \( i \)-th column is the eigenvector associated with the eigenvalue \( l_i \). Then the solution to (1) is

\[
\hat{\Sigma}(\kappa) = Q \text{diag}(\hat{\lambda}_1(\kappa), \ldots, \hat{\lambda}_p(\kappa))Q^T,
\]

where \( \hat{\lambda}_i^{-1}(\kappa) = \min(\max(u^*, 1/l_i), \kappa u^*) \), \( u^* = u^*(\kappa) \), is adaptively determined by the sample eigenvalues \( l_1, \ldots, l_p \), which in turn depend on the data matrix \( X \). For a given \( \kappa \), the data-dependent threshold \( u^* \) can be determined efficiently by reducing (1) to a univariate convex minimization problem. Specifically, \( u^* \) is the minimizer of the following bivariate function

\[
J(u, v) = \sum_{i=1}^p [l_i \mu_i(u, v) - \log(\mu_i(u, v))], \tag{2}
\]
on a half line \( v = \kappa u, \ u > 0 \). Then the univariate objective \( J_{\kappa_{\text{max}}} (u) \equiv J(u, \kappa_{\text{max}} u) \) can be efficiently minimized, in \( O(p) \) operations on the sample eigenvalues \( l_1, l_2, \ldots, l_p \).

The cited study also shows that for varying \( \kappa \), the solution path can be visualized on the \( uv \)-plane as the trajectory of \((u^*(\kappa), v^*(\kappa))\). Although some properties are studied (Won et al., 2013, Proposition 1), a thorough and complete understanding of the solution path is lacking (despite the importance of the problem for practical reasons).

In this paper, we proceed to provide the complete analytical characterization of the solution path of the CondReg estimator. In particular, we show that 1) the solution path is piecewise linear, and that 2) the entire solution path can be computed at the same cost (namely, in \( O(p) \) operations) as that of finding the solution for a fixed \( \kappa \). These results are used to construct two path algorithms: one that traverses the path in forward direction, the other in backward direction. Both algorithms produce “knots” of the solution path, from which the solution for a specific value of \( \kappa \) is determined exactly by linear interpolation. In this sense, our algorithms are parallel to the lasso regularization path algorithm LARS for regression (Efron et al., 2004). Our algorithms are valid even if \( S \) is singular, i.e. \( n < p \); we provide an explicit treatment for this important special case. Very importantly, our analysis gives new insight into the cross-validation procedure for selecting the regularization parameter, by speeding up the procedure as well as providing a principle for the candidate parameter values; we pay a special attention to leave-one-out cross-validation, for which even further speed-up is achievable. Our methods are implemented in \( R \) and provided as a publicly available package CondReg (Oh et al., 2014).

## 2 Complete characterization of the solution path

We begin the discussion with the following restatement of Won et al. (2013, Theorem 1).

**Proposition 1.** Given \( 1 \leq \kappa < \text{cond}(S) \), where \( S \) is the sample covariance matrix, the optimization problem (1) is equivalent to the following unconstrained univariate minimization problem

\[
\text{minimize} \quad J_{\kappa}(u) \tag{3}
\]

where \( J_{\kappa}(u) \) is defined in (2). Furthermore, define a set of points \( \{(u_{\alpha,\beta}, v_{\alpha,\beta})\} \) with

\[
u_{\alpha,\beta}(\kappa) = \kappa u_{\alpha,\beta}(\kappa). \tag{5}\n\]

and a set of half-closed rectangles \( \{R_{\alpha,\beta}\} \)

\[
R_{\alpha,\beta} = \{(u, v) : 1/l_\alpha < u \leq 1/l_{\alpha+1}, 1/l_{\beta-1} \leq v < 1/l_\beta\}. \tag{6}\n\]

in the \( uv \)-plane for \( \alpha = \{1, \ldots, p-1\} \) and \( \beta = \{2, \ldots, p\} \). Then (3) has a unique solution \( u^* = u_{\alpha^*, \beta^*}(\kappa) \), where \( \alpha^* \in \{1, \ldots, p-1\} \) and \( \beta^* \in \{2, \ldots, p\} \) satisfy

\[
(u_{\alpha^*, \beta^*}, v_{\alpha^*, \beta^*}) \in R_{\alpha^*, \beta^*}. \tag{6}\n\]
Finding the pair \((\alpha^*, \beta^*)\) takes \(O(p)\) time. If \(\kappa \geq \text{cond}(S)\), the minimizer \(u^*\) may not be unique. However, the solution to (1) is uniquely determined to be \(S\).

This proposition allows \(S\) to be singular, i.e., when \(\text{cond}(S) = \infty\).

To see that the entire solution path is piecewise linear, suppose the optimal point \((u^*_{\alpha^*, \beta^*}(\kappa), v^*_{\alpha^*, \beta^*}(\kappa))\) is in \(\text{int} R_{\alpha^*, \beta^*}\), where \(\text{int} A\) denotes the interior of a set \(A\). Since \(u^*_{\alpha^*, \beta^*}\) and \(v^*_{\alpha^*, \beta^*}\) are both continuous and differentiable functions of \(\kappa\) in this region, a small change in \(\kappa\) will not move the optimal points \((u^*_{\alpha^*, \beta^*}, v^*_{\alpha^*, \beta^*})\) too much, i.e.,

\[
(u^*_{\alpha^*, \beta^*}(\kappa + \Delta \kappa), v^*_{\alpha^*, \beta^*}(\kappa + \Delta \kappa)) \in \text{int} R_{\alpha^*, \beta^*},
\]

for sufficiently small \(\Delta \kappa\). Since (7) satisfies condition (6), it follows that \(u^*_{\alpha^*, \beta^*}(\kappa + \Delta \kappa)\) minimizes \(J_{\kappa + \Delta \kappa}(u)\), which, in turn, characterizes the trajectory of \((u^*_{\alpha^*, \beta^*}(\kappa), v^*_{\alpha^*, \beta^*}(\kappa))\) within the interior of \(R_{\alpha^*, \beta^*}\). Also since

\[
\frac{du^*_{\alpha^*, \beta^*}(\kappa)}{d\kappa} = -\frac{(\alpha^* + p - \beta^* + 1) \sum_{i=1}^{p} l_i}{(\sum_{i=1}^{\alpha^*} l_i + \kappa \sum_{i=\beta}^{p} l_i)^2}, \quad \frac{dv^*_{\alpha^*, \beta^*}(\kappa)}{d\kappa} = \frac{(\alpha^* + p - \beta^* + 1) \sum_{i=1}^{\alpha^*} l_i}{(\sum_{i=1}^{\alpha^*} l_i + \kappa \sum_{i=\beta}^{p} l_i)^2},
\]

it follows

\[
\frac{dv^*_{\alpha^*, \beta^*}}{du^*_{\alpha^*, \beta^*}}(\kappa) = \frac{-\sum_{i=1}^{\alpha^*} l_i}{\sum_{i=\beta}^{p} l_i},
\]

which does not depend on \(\kappa\) as long as \(\alpha^*\) and \(\beta^*\) do not change. Indeed \(\alpha^*\) and \(\beta^*\) do not change within \(\text{int} R_{\alpha^*, \beta^*}\), thus \(dv^*_{\alpha^*, \beta^*}/du^*_{\alpha^*, \beta^*}\) is constant in this region. In other words, the trajectory of \((u^*_{\alpha^*, \beta^*}(\kappa), v^*_{\alpha^*, \beta^*}(\kappa))\) is a straight line inside \(R_{\alpha^*, \beta^*}\).

Will the piecewise linear solution path be continuous as well? The concern is that at the boundary of the rectangle \(R_{\alpha^*, \beta^*}\) where a small change of \(\kappa\) indeed alters \(\alpha^*\) and/or \(\beta^*\), there may be a jump in the path. The following lemma shows that this will not happen.

**Lemma 1.** Suppose for some \(\tilde{\kappa}\) with \((u^*_{\alpha^*, \beta^*}(\tilde{\kappa}), v^*_{\alpha^*, \beta^*}(\tilde{\kappa})) \in \text{int} R_{\alpha^*, \beta^*}\). Let \(\tilde{\kappa} = \sup\{\kappa : (u^*_{\alpha^*, \beta^*}(\kappa), v^*_{\alpha^*, \beta^*}(\kappa)) \in R_{\alpha^*, \beta^*}\}\). Then the point \((u^*_{\alpha^*, \beta^*}(\tilde{\kappa}), v^*_{\alpha^*, \beta^*}(\tilde{\kappa}))\) coincides either with \((u^*_{\alpha^*, \beta^*+1}(\tilde{\kappa}), v^*_{\alpha^*, \beta^*+1}(\tilde{\kappa})) \in R_{\alpha^*, \beta^*+1}\), or \((u^*_{\alpha^*, \beta^*+1}(\tilde{\kappa}), v^*_{\alpha^*, \beta^*+1}(\tilde{\kappa})) \in R_{\alpha^*, \beta^*+1} \) exclusively, depending on the slope (8).

**Proof.** See Appendix 1. \(\square\)

We have so far seen that the solution path is continuous and piecewise linear, and how the slopes of the line pieces can be traced. The remaining task is to determine where to start and end the path. It is natural to regard \((u_{\alpha, \beta}(1), v_{\alpha, \beta}(1))\) for some \(\alpha\) and \(\beta\) as the initial point, i.e., when \(\kappa = 1\). This point is identified as \((1/\bar{l}, 1/\bar{l})\), where \(\bar{l} = (1/p) \sum_{i=1}^{p} l_i\). To see this, note that for \(\kappa = 1\) the closure of \(R_{\alpha, \beta}\) should intersect with the line \(v = u\) for some \(\alpha\) and \(\beta\), and \((u^*(1), v^*(1))\) must lie inside this rectangle. By construction, \(R_{\alpha, \beta}\) should intersect with the line \(v = u\) if and only if \(\alpha = \beta - 1\). Then, from (4) and (5), it follows

\[
u_{\beta-1, \beta}(1) = v_{\beta-1, \beta}(1) = p/(\sum_{i=1}^{\beta-1} l_i + \sum_{i=\beta}^{p} l_i) = 1/\bar{l}.
\]
Finding the termination point requires some care because when the sample covariance matrix $S$ is singular, the upper bound of $\kappa$, i.e., $\text{cond}(S)$, is indefinite. To make the case of singularity explicit, assume that $S$ is of rank $r \leq p$ so that $p - r$ eigenvalues are zeros:

$$l_1 \geq l_2 \geq \cdots \geq l_r > 0 = l_{r+1} = \cdots = l_p.$$ 

The nonsingular case corresponds to $r = p$. For ease of exposition, write $1/l_{r+1} = \cdots = 1/l_p = +\infty$ and also $l_0 = +\infty$ so that $1/l_0 = 0$. The largest finite ratio $l_1/l_r$ of the sample eigenvalues plays a crucial role in determining the termination point. Suppose we want to evaluate the univariate objective $J_\kappa(u)$ on $R_{0,r}$ for $\kappa \geq l_1/l_r$. Recall from (2) that

$$J(u,v) = \sum_{i=1}^{r} (1 + \log l_i) + \sum_{i=r+1}^{p} (l_i v - \log v)$$

because

$$\mu_i(u,v) = \begin{cases} 
    u, & i \leq \alpha, \\
    1/l_i, & \alpha < i < \beta, \\
    v, & i \geq \beta,
\end{cases}$$

on $R_{\alpha,\beta}$. Since $J(u,v)$ is strictly decreasing in $v$ on $R_{0,r}$, so is $J_\kappa(u) = J(u,\kappa u)$. Moreover, due to convexity, $J_\kappa(u)$ is strictly decreasing for $u \leq 1/l_1$ and its minimum occurs for $u > 1/l_1$. This suggests that we only need to examine $r$ semi-infinite rectangles $R_{\alpha,r+1}$, $\alpha = 1,2,\ldots,r$.

For a fixed value of $\alpha$, $J_\kappa(u) = \left(\sum_{i=1}^{\alpha} l_i\right) u - (\alpha + p - r) \log u - (p - r) \log \kappa$ (9) on $R_{\alpha,r+1}$. The global minimum of the right-hand side is attained at $u_{\alpha,r+1}^* = (\alpha + p - r)/(\sum_{i=1}^{\alpha} l_i)$. However, it is possible that $(u_{\alpha,r+1}^*,\kappa u_{\alpha}^*)$ is outside of $R_{\alpha,r+1}$, in which case $J_\kappa(u)$ is not equal to the right-hand side of (9). To avoid this situation, starting from 1 increase $\alpha$ until $u_{\alpha,r+1}^*$ satisfies $1/l_\alpha < u_{\alpha,r+1}^* \leq 1/l_{\alpha+1}$. This procedure, formally described in Algorithm 1, guarantees that $J_\kappa(u)$ equals the right-hand side of (9) on $R_{\alpha,r+1}$ at its termination. (Algorithm 1 terminates, because for $\alpha = r$, $u_{\alpha,r+1}^* = p/(\sum_{i=1}^{r} l_i) < 1/l_{r+1} = +\infty$ and $p/(\sum_{i=1}^{r} l_i) > 1/l_r$.) Now note that $du_{\alpha,r+1}^*/d\kappa = 0$ at termination. This means that for $\kappa \geq l_1/l_r$, the solution path is the vertical half-line $u = u_{\alpha,r+1}^*$ starting from its intersection with the line $v = (l_1/l_r)u$ and reaches out toward $v = +\infty$. To complete the path inside $R_{\alpha,r+1}$, note that the slope of the path should remain constant inside this (semi-infinite) rectangle. Hence even for $\kappa < l_1/l_r$, the path partially follows the vertical line $u = u_{\alpha,r+1}^*$. It changes the slope at the boundary between $R_{\alpha,r+1}$ and $R_{\alpha,r}$, where $\kappa = 1/(l_r u_{\alpha,r+1}^*)$. In other words, the “termination point” is in fact a set of points lying on the line $u = u_{\alpha}^*$ within $R_{\alpha,r+1}$, where $\alpha$ is found by Algorithm 1.

From the above discussion, we can regard the point $(u_{\alpha,r+1}^*,1/l_r)$ corresponding to $\kappa = 1/(l_r u_{\alpha,r+1}^*)$ as the effective termination point of the solution path. For all $\kappa$ larger than this critical value, the solution path is a vertical line $u = u_{\alpha,p+1}^*$. Any point on this line
Algorithm 1 Termination point finding algorithm

1: Set $\alpha = 1$
2: While True
3: \quad $u^* \leftarrow (\alpha + p - r)/(\sum_{i=1}^{\alpha} l_i)$
4: \quad If $(1/l_\alpha < u^* \leq 1/l_{\alpha+1})$ break
5: \quad $\alpha \leftarrow \alpha + 1$
6: Return $u^*, \alpha$

results in the same covariance matrix estimate. In particular, if $r = p$, $u^*_{\alpha,p+1} = 1/l_1 \leq 1/l_2$ satisfies the condition sought by Algorithm 1, so the termination point is given by $(1/l_1, 1/l_p)$ corresponding to $\kappa = l_1/l_r = \text{cond}(S)$. Thus for any $\kappa \geq \text{cond}(S)$, the resulting covariance matrix estimate is the sample covariance matrix $S$.

These results can be summarized as the following lemma.

**Lemma 2.** The solution path starts from $(1/\bar{l}, 1/\bar{l})$ corresponding to $\kappa = 1$ and ends with a vertical half-line \{(u,v) : u = u^*_\alpha, v \geq 1/l_r\} corresponding to $\kappa \geq 1/(l_r u^*_\alpha)$, where $l_r$ is the smallest positive sample eigenvalue. The abscissa $u^*_\alpha$ is determined by Algorithm 1.

Combining Lemmas 1 and 2, we are ready to fully describe the entire solution path, as stated in the following theorem.

**Theorem 1.** The optimal truncation range $(u^*(\kappa), v^*(\kappa))$ traces a piecewise linear path on the $u$-$v$ plane as the regularization parameter $\kappa$ varies. The resulting solution path is continuous, and changes its slope only when it intersects the lines $u = 1/l_1, \ldots, 1/l_p$ or $v = 1/l_1, \ldots, 1/l_p$.

One endpoint of this path is $(1/\bar{l}, 1/\bar{l})$, corresponding to $\kappa = 1$, and the other endpoint is a vertical half-line \{(u,v) : u = u^*_\alpha, v \geq 1/l_r\} corresponding to $\kappa \geq 1/(l_r u^*_\alpha)$, where $\alpha$ is determined in $O(p)$ time using Algorithm 1. Furthermore, the entire path can be found in $O(p)$ operations either by starting at $(1/\bar{l}, 1/\bar{l})$ (forward algorithm, Algorithm 2) or by starting at $(u^*_\alpha, 1/l_r)$ (backward algorithm, Algorithm 3).

**Proof.** By inspection it can be seen that the time complexity of Algorithm 1 is $O(p)$. For Algorithm 2, line 2 takes $O(p)$ operations. In the loop, either of the conditions in lines 10 and 11 must be met for each iteration. Thus for each value of $\alpha = 1, 2, \ldots, p$, at most one value of $\beta \in \{1, 2, \ldots, p\}$ is considered. This takes $O(p)$ time. Algorithm 3 is similar to Algorithm 2.

Algorithms 2 and 3 completely describes how to determine the entire solution path. The $O(p)$ complexity of these algorithms is the same as that of determining the solution to (1) for a fixed $\kappa$ (Proposition 1). In fact the forward algorithm does not require the termination point finding algorithm (Algorithm 1) because it terminates if $v^* = 1/l_r$. This makes the forward algorithm slightly simpler than its backward counterpart. However, if the degree of regularization is not too strong, e.g, when $\kappa$ is relatively close to $l_r/l_1$, the backward algorithm may still be advantageous.
**Algorithm 2** Forward path algorithm

1: Set $\kappa_{\text{new}} = 1$, $u_{\text{new}}^\star = v_{\text{new}}^\star = 1/l$, $\kappa = u^* = v^* = \text{empty}$
2: Find $\alpha$ such that $l_{\alpha} > l \geq l_{\alpha+1}$
3: Set $\beta \leftarrow \alpha + 1$
4: While $(\alpha \geq 1$ and $\beta \leq r$)
5: $s \leftarrow -(\sum_{i=1}^{\alpha} l_i)/(\sum_{i=\beta}^{p} l_i)$
6: $\bar{R}_{\alpha,\beta} \leftarrow \{(u, v) : 1/l_{\alpha} \leq u \leq 1/l_{\alpha+1} \text{ and } 1/l_{\beta-1} \leq v \leq 1/l_{\beta}\}$
7: $(u^*, v^*) \leftarrow \text{intersection between line passing }(u_{\text{new}}^\star, v_{\text{new}}^\star) \text{ of slope } s$
   and boundary of $\bar{R}_{\alpha,\beta}$, with $u^* < u_{\text{new}}^\star$
8: $\kappa_{\text{new}} \leftarrow v^*/u^*, u_{\text{new}}^\star \leftarrow u^*, v_{\text{new}}^\star \leftarrow v^*$
9: $\kappa \leftarrow (\kappa, \kappa_{\text{new}})$, $u^* \leftarrow (u^*, u_{\text{new}}^\star)$, $v^* \leftarrow (v^*, v_{\text{new}}^\star)$
10: If $(u^* = 1/l_{\alpha})$ $\alpha \leftarrow \alpha - 1$
11: If $(v^* = 1/l_{\beta})$ $\beta \leftarrow \beta + 1$
12: Return $\kappa, u^*, v^*$

**Algorithm 3** Backward path algorithm

1: Find $\alpha$, $u_{\alpha}$ by Algorithm 1
2: Set $\kappa_{\text{new}} = 1/(l_{\alpha} u_{\alpha}), u_{\text{new}}^\star = u_{\alpha}, v_{\text{new}}^\star = 1/l_{r}$, $\kappa = u^* = v^* = \text{empty}$
3: Set $\beta = r$
4: While True
5: $s \leftarrow -(\sum_{i=1}^{\alpha} l_i)/(\sum_{i=\beta}^{p} l_i)$
6: $\bar{R}_{\alpha,\beta} \leftarrow \{(u, v) : 1/l_{\alpha} \leq u \leq 1/l_{\alpha+1} \text{ and } 1/l_{\beta-1} \leq v \leq 1/l_{\beta}\}$
7: $(u^*, v^*) \leftarrow \text{intersection between the line passing }(u^*(\kappa), v^*(\kappa)) \text{ of slope } s$ and line $v = u$
8: If $((u^*, v^*) \in \bar{R}_{\alpha,\beta})$
9: $\kappa \leftarrow (1, \kappa)$, $u^* \leftarrow (u^*, u^*)$, $v^* \leftarrow (v^*, v^*)$
9: Break
10: $(u^*, v^*) \leftarrow \text{intersection between line passing }(u_{\text{new}}^\star, v_{\text{new}}^\star) \text{ of slope } s$
   and boundary of $\bar{R}_{\alpha,\beta}$, with $u^* > u_{\text{new}}^\star$
11: $\kappa_{\text{new}} \leftarrow v^*/u^*, u_{\text{new}}^\star \leftarrow u^*, v_{\text{new}}^\star \leftarrow v^*$
12: $\kappa \leftarrow (\kappa, \kappa_{\text{new}})$, $u^* \leftarrow (u^*, u_{\text{new}}^\star)$, $v^* \leftarrow (v^*, v_{\text{new}}^\star)$
13: If $(u^* = 1/l_{\alpha})$ $\alpha \leftarrow \alpha + 1$
14: If $(v^* = 1/l_{\beta})$ $\beta \leftarrow \beta - 1$
15: Return $\kappa, u^*, v^*$

**Remark 1.** An interesting question is whether the piecewise solution path is convex. It is plausible since Figure 2a in Won et al. (2013), obtained from $S = \text{diag}(21, 7, 5, 25, 3.5, 3)$, shows a convex solution path; convexity is preserved if we augment $S$ with zero diagonals. However, there is a counterexample: $S = \text{diag}(16, 8, 4, 2, 1)$. Indeed, in (8) both the numerator and the denominator are decreasing with $\kappa$, thus the curvature of the path highly depends on the data. See Section 1 of the supplementary material for an illustration of the cited
3 Fast method for cross-validation

The regularization parameter $\kappa$ for the CondReg estimator is selected by $K$-fold cross-validation that finds $\kappa$ minimizing the sample predictive risk with respect to the negative likelihood loss

$$\hat{PR}(\kappa) = -\left(1/K\right) \sum_{j=1}^{K} l_j(\kappa); \quad l_j(\kappa) = -(n_j/2) \left[ \text{tr}\left(\hat{\Sigma}_{(-j)}^{-1}(\kappa)X_jX_j^T/n_j\right) - \log \det \hat{\Sigma}_{(-j)}^{-1}(\kappa) \right],$$

where $\hat{\Sigma}_{(-j)}^{-1}(\kappa)$ is the CondReg estimator estimated from the samples excluding the $j$th partition $X_j \in \mathbb{R}^{n_j \times p}$ given the regularization parameter $\kappa$. Usually the minimum is sought for a grid of values of $\kappa$. If there are $M$ points in the grid, say $\kappa_1, \ldots, \kappa_M$, $MK$ evaluations of $l_j(\kappa_k)$, $j = 1, \ldots, K$, $k = 1, \ldots, M$, are required.

With a solution path algorithm, these evaluations are greatly sped up because for a fixed $j$, values of $l_j(\kappa)$ on the grid can be computed essentially at the same cost as each value of $l_j(\kappa_k)$. Furthermore, Theorem 1 guides to the choice of the grid points: the knots of the piecewise linear solution path. It appears natural to choose the knots for $\hat{\Sigma}(\kappa)$, the CondReg estimator from the full sample $X \in \mathbb{R}^{n \times p}$.

**Remark 2.** For an important special case of the leave-one-out cross-validation, i.e., when $K = n$, even further reduction of computation is possible because $\hat{\Sigma}_{(-j)}^{-1}(\kappa)$ can be computed directly from the full sample $X$ without extra spectral decompositions; see Section 2 of the supplementary material.

**Supplementary material**

Supplementary material available online includes the illustrative solution paths as discussed in Remark 1, the fast leave-one-out cross-validation method as mentioned in Remark 2, and the description of the user-level functions in the R package CondReg (Oh et al., 2014), which implements both the forward (Algorithm 2) and the backward (Algorithm 3) solution path algorithms as well as the fast leave-one-out cross-validation.

**Appendix 1**

**Proof of Lemma 1.** Increase $\kappa$ from $\bar{\kappa}$. Suppose the line passing the point $(u_{\alpha^*,\beta^*}(\bar{\kappa}), v_{\alpha^*,\beta^*}(\bar{\kappa}))$ with slope $-\sum_{i=1}^{\alpha^*} l_i/\sum_{i=\beta}^{p} l_i$ meets the left side (but not inclusive) $\{(u, v) : v = 1/l_{\beta^*}\}$ of $R_{\alpha^*,\beta^*}$ before it meets the upper side (also not inclusive) $\{(u, v) : u = 1/l_{\alpha^*}\}$. Then, by continuity of $u_{\alpha^*,\beta^*}(\kappa)$ on $\{\kappa : \kappa > 0\}$,

$$u_{\alpha^*,\beta^*}(\lim_{\kappa \uparrow \bar{\kappa}} \kappa) = \frac{\alpha^* + p - \beta^* + 1}{\sum_{i=1}^{\alpha^*} l_i + \bar{\kappa} \sum_{i=\beta}^{p} l_i} = \frac{1}{l_{\alpha^*}} = \lim_{\kappa \uparrow \bar{\kappa}} u_{\alpha^*,\beta^*}(\kappa).$$

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Then,

\[(\alpha^* + p - \beta^*)l_{\alpha^*} = (\alpha^* + p - \beta^* + 1)l_{\alpha^*} - l_{\alpha^*} = \sum_{i=1}^{\alpha^*} l_i + \bar{\kappa} \sum_{i=\beta^*}^{p} l_i - l_{\alpha^*} = \sum_{i=1}^{\alpha^*-1} l_i + \bar{\kappa} \sum_{i=\beta^*}^{p} l_i,\]

or

\[
\frac{1}{l_{\alpha^*}} = \frac{(\alpha^* - 1) + p - \beta^* + 1}{\sum_{i=1}^{\alpha^*-1} l_i + \bar{\kappa} \sum_{i=\beta^*}^{p} l_i} = u_{\alpha^*-1,\beta^*}(\bar{\kappa}).
\]

From the condition \(1/l_{\beta^*-1} \leq u_{\alpha^*,\beta^*}(\bar{\kappa}) \leq u_{\alpha^*,\beta^*}(\bar{\kappa}) < 1/l_{\beta^*}\), it follows that \((u_{\alpha^*,\beta^*}(\bar{\kappa}), v_{\alpha^*,\beta^*}(\bar{\kappa})) = (u_{\alpha^*,\beta^*}(\bar{\kappa}), v_{\alpha^*,\beta^*}(\bar{\kappa})) \in R_{\alpha^*,\beta^*}\). Similarly it can be shown that \((u_{\alpha^*,\beta^*}(\bar{\kappa}), v_{\alpha^*,\beta^*}(\bar{\kappa})) = (u_{\alpha^*,\beta^*+1}(\bar{\kappa}), v_{\alpha^*,\beta^*+1}(\bar{\kappa})) \in R_{\alpha^*,\beta^*+1}\) if the line meets the upper side before the left side of \(R_{\alpha^*,\beta^*}\). Now suppose the line meets the upper left corner point \((1/l_{\alpha^*}, 1/l_{\beta^*})\) of \(R_{\alpha^*,\beta^*}\). It follows

\[
u_{\alpha^*-1,\beta^*}(\bar{\kappa}) = u_{\alpha^*,\beta^*}(\bar{\kappa}) = 1/l_{\alpha^*}, \quad v_{\alpha^*,\beta^*+1}(\bar{\kappa}) = v_{\alpha^*,\beta^*}(\bar{\kappa}) = 1/l_{\beta^*} = \bar{\kappa}/l_{\alpha^*},
\]

from which we obtain

\[
(\alpha^* + p - \beta^* - 1)\bar{\kappa}l_{\beta^*} = (\alpha^* + p - \beta^*)\bar{\kappa}l_{\beta^*} - \bar{\kappa}l_{\beta^*} = \sum_{i=1}^{\alpha^*} l_i + \bar{\kappa} \sum_{i=\beta^*+1}^{p} l_i - \bar{\kappa}l_{\beta^*} = \sum_{i=1}^{\alpha^*-1} l_i + \bar{\kappa} \sum_{i=\beta^*+1}^{p} l_i - \bar{\kappa}l_{\beta^*} = \sum_{i=1}^{\alpha^*-1} l_i + \bar{\kappa} \sum_{i=\beta^*+1}^{p} l_i - \bar{\kappa}l_{\beta^*} = \sum_{i=1}^{\alpha^*-1} l_i + \bar{\kappa} \sum_{i=\beta^*+1}^{p} l_i - \bar{\kappa}l_{\beta^*}.
\]

Hence

\[
\frac{1}{l_{\beta^*}} = \frac{(\alpha^* - 1) + p - (\beta^* + 1) + 1)\bar{\kappa}}{\sum_{i=1}^{\alpha^*-1} l_i + \bar{\kappa} \sum_{i=\beta^*+1}^{p} l_i} = v_{\alpha^*-1,\beta^*+1}(\bar{\kappa}),
\]

\[
\frac{1}{l_{\alpha^*}} = \frac{1}{\bar{\kappa}l_{\beta^*}} = \frac{(\alpha^* - 1) + p - (\beta^* + 1) + 1}{\sum_{i=1}^{\alpha^*-1} l_i + \bar{\kappa} \sum_{i=\beta^*+1}^{p} l_i} = u_{\alpha^*-1,\beta^*+1}(\bar{\kappa}).
\]

and \((1/l_{\alpha^*}, 1/l_{\beta^*}) \in R_{\alpha^*-1,\beta^*+1}\). □

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1 Illustrative solution paths

Figure S1 shows four illustrative solution paths that the algorithms of the main text generate. In panel (a), sample covariance matrices $S = \text{diag}(21, 7, 21/4, 7/2, 3)$ (outer path) and its zero-padded counterpart $S = \text{diag}(21, 7, 21/4, 7/2, 3, 0, 0)$ (inner path) are considered. The grid consists of the finite reciprocals of the eigenvalues of $S$, i.e., the diagonals. A solution paths starts from a point on the line $v = u$, corresponding to the inverse of the mean eigenvalue (0.126 for the outer path, 0.176 for the inner path), and changes its slope whenever it meet a grid line (“knots”, solid circles). Upon the point the path meets the grid line for the smallest positive eigenvalue (intersection with the line $v = 7u$ for the outer path; $v = (7/3)u$ for the inner path), the solution path becomes a vertical line, on which the resulting regularized covariance matrix estimate does not vary.

The solution paths shown in panel (a) are both convex; in panel (b) a non-convex path is exhibited. The non-convex outer path corresponds to $S = \text{diag}(16, 8, 4, 2, 1)$, whereas the inner path is drawn for $S = \text{diag}(16, 8, 4, 2, 1, 0, 0)$. The latter is shown to illustrate that the vertical part of the path does not necessarily coincide with a grid line. (The $u$-axis is stretched to emphasize non-convexity of the outer path.)

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2 Fast leave-one-out cross-validation

While the path algorithm greatly facilitates the cross-validation procedure as described in §3 of the main text, for large problems it may be still computationally demanding because a spectral decomposition has to be conducted for each fold, i.e., each of $j = 1, \ldots, K$ to obtain $\Sigma_{(-j)}(\kappa)$. Surprisingly, for leave-one-out cross-validation (LOOCV), i.e., when $K = n$ and $n_j = 1$, the computational burden can be dramatically reduced using the special structure of LOOCV.

Recall that the full sample data matrix is given by $X = [x_1, \ldots, x_n]^T$ with $x_j \in \mathbb{R}^p$, and the sample covariance matrix by $S = (1/n)X^TX$. The empirical predictive risk for LOOCV is

$$\hat{PR}(\kappa) = -(1/n) \sum_{j=1}^{n} l_j(\kappa),$$

where

$$l_j(\kappa) = -(1/2) [\text{tr}(\Sigma_{(-j)}^{-1}(\kappa)x_jx_j^T - \log \det \Sigma_{(-j)}^{-1}(\kappa))].$$

The CondReg estimator $\hat{\Sigma}_{(-j)}(\kappa)$ is computed from the spectral decomposition of the $(n-1)$-sample covariance matrix $S_{(-j)} = \frac{1}{n-1}X_{(-j)}^TX_{(-j)}$, where $X_{(-j)} \in \mathbb{R}^{(n-1) \times p}$ is the data matrix with the $j$-th sample $x_j$ left out. Observe that

$$X_{(-j)}^TX_{(-j)} = X^TX - x_jx_j^T,$$

where the matrix $x_jx_j^T$ is of rank 1. Because the LOOCV is conducted for the full-sample CondReg estimator $\hat{\Sigma}(\kappa)$ obtained from $S$, the spectral decomposition of the matrix $X^TX$ is readily available. Then (1) suggests that the eigenvalues and the eigenvectors of $X_{(-j)}^TX_{(-j)}$ will not be “too far” from those of $X^TX$. This conjecture is indeed true, and the procedure for downdating the eigenvalues and the eigenvectors has been extensively studied in the numerical linear algebra literature (Bunch et al., 1978; DeGroat and Roberts, 1990; Gu and Eisenstat, 1994).

We give a brief review here. The discussion closely follows Demmel (1997). A similar approach is used for cross-validating principal component regression (Mertens et al., 1995).

**Eigenvalues** As the spectral decomposition of $S = Q\text{diag}(l_1, \ldots, l_p)Q^T$ is given, we write that of $X^TX$ as $QDQ^T$, where $D = \text{diag}(d_1, \ldots, d_p)$, $d_k = nk$, $k = 1, \ldots, p$. Then,

$$X_{(-j)}^TX_{(-j)} = QDQ^T - x_jx_j^T = Q(D - Q^Tx_jx_j^TQ)Q^T = Q(D + \rho zz^T)Q^T,$$

where $z = Q^Tx_j/||Q^Tx_j|| = (z_1, \ldots, z_p)^T$ and $\rho = -||Q^Tx_j||^2$. Therefore the problem reduces to that of finding the spectral decomposition of $D + \rho zz^T$, a rank-1 perturbation of a diagonal matrix. Assuming that $d_i$ are distinct, the characteristic equation of this matrix is

$$0 = \det(D + \rho zz^T - \lambda I) = \det(D - \lambda I) \det(I + \rho(D - \lambda I)^{-1}zz^T).$$

The right hand side equals zero whenever $\det(I + \rho(D - \lambda I)^{-1}zz^T)$ is. In other words, the eigenvalues of $D + \rho zz^T$ (hence those of $X_{(-j)}^TX_{(-j)}$) are the zeros of the following rational function

$$\det(I + \rho(D - \lambda I)^{-1}zz^T) = 1 + \rho z^T(D - \lambda I)^{-1}z = 1 + \rho \sum_{k=1}^{p} \frac{z_k^2}{d_k - \lambda} \equiv f(\lambda).$$

The equation $f(\lambda) = 0$ is called the secular equation. It is monotone decreasing and has a root on $(d_{k-1}, d_k)$, $k = 1, \ldots, p$ ($d_0 \equiv -\infty$). Hence each eigenvalue can be found by applying the Newton algorithm on $(d_{k-1}, d_k)$. 

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This text is an excerpt from a larger document that focuses on the application of spectral decomposition and cross-validation techniques in statistical computing, particularly in the context of principal component regression. The section highlights the computational challenges and the mathematical techniques employed to efficiently handle leave-one-out cross-validation procedures, especially for large datasets. The approach described leverages the special structure of leave-one-out cross-validation to significantly reduce computational costs, making it feasible for large-scale problems. The text further delves into the details of calculating the empirical predictive risk and discusses the eigenvalues and eigenvectors of the covariance matrix, which are crucial for understanding the behavior of the cross-validation procedure.
Eigenvectors  If \( \lambda_k \) is an eigenvalue of \( D + \rho zz^T \), then \((D - \lambda_k I)^{-1}z\) is the corresponding eigenvector because

\[
(D + \rho zz^T)(D - \lambda_k I)^{-1}z = (D - \lambda_k I + \lambda_k I + \rho zz^T)(D - \lambda_k I)^{-1}z \\
= z + \lambda_k(D - \lambda_k I)^{-1}z + (\rho z^T(D - \lambda_k I)^{-1}z)z \\
= z + \lambda_k(D - \lambda_k I)^{-1}z - z = \lambda_k(D - \lambda_k I)^{-1}z,
\]

where the third equation is due to \( f(\lambda_k) = 0 \). However, when two eigenvalues \( \lambda_k \) and \( \lambda_{k+1} \) are close, they are also close to the \( d_k \) since \( \lambda_k \in (d_{k-1}, d_k) \) and \( \lambda_{k+1} \in (d_k, d_{k+1}) \). Hence the computation of \((D - \lambda_k I)^{-1}z\) and \((D - \lambda_{k+1} I)^{-1}z\) that involves \( 1/(d_k - \lambda_k) \) and \( 1/(d_k - \lambda_{k+1}) \) may result in large numerical error. In particular, the computed eigenvectors can be far from orthogonal to each other. This numerical difficulty can be resolved by replacing \( z \) with \( \hat{u} = (\hat{u}_1, \ldots, \hat{u}_p)^T \), where

\[
\hat{u}_m^2 = \frac{\prod_{l=1}^p(\lambda_l - d_k)}{\prod_{l \neq k}(d_l - d_k)}, \quad m = 1, \ldots, p,
\]

using the fact that the computed eigenvalues of \( D + \rho zz^T \) are the exact eigenvalues of \( D + \hat{u}\hat{u}^T \).

Deflation  The assumption that \( d_i \) are distinct can be lifted as follows. If \( z \) has zero at its \( k \)-th component, then \( d_k \) is the eigenvalue of \( D + \rho zz^T \) and \( e_k \), the \( k \)-th elementary unit vector is the associated eigenvector. In other words, the \( k \)-th eigenvalue and eigenvector are unchanged from \( X^TX \) in \( X_{(\cdot \setminus j)}^TX_{(\cdot \setminus j)} \). Now suppose \( d_k = d_l \) for some \( k < l \). Then we can find a Givens rotation \( G_{kl} \) such that \( \hat{z}_l = 0 \) for \( \hat{z} = G_{kl}z \). Since \( G_{kl}(D + \rho zz^T)G_{kl}^T = D + \hat{u}\hat{u}^T \), applying the rotation does not change the \( k \)-th and the \( l \)-th eigenvalues; only the eigenvectors associated with these eigenvalues are rotated. Proceeding in this manner, we see that there exists an orthogonal matrix \( U \) such that

\[
UDU^T = \begin{bmatrix} D_1 & 0 \\ D_2 & 0 \end{bmatrix}, \quad D_1 = \text{diag}(d_{\pi_1}, \ldots, d_{\pi_\tau}), \quad d_{\pi_1} > \cdots > d_{\pi_\tau} > 0, \quad D_2 = \text{diag}(d_{\pi_{\tau+1}}, \ldots, d_{\pi_p}),
\]

and

\[
Uz = \begin{bmatrix} w \\ 0 \end{bmatrix}, \quad w = (w_1, \ldots, w_p)^T,
\]

where \( \pi = (\pi_1, \ldots, \pi_p) \) is a suitable permutation of the sequence \( 1, \ldots, p \). Then

\[
X_{(\cdot \setminus j)}^TX_{(\cdot \setminus j)} = Q(D + \rho zz^T)Q^T = QU \begin{bmatrix} D_1 + \rho w^T w & 0 \\ 0 & D_2 \end{bmatrix} U^T Q^T
\]

\[
= QU \begin{bmatrix} Q_1 A_1 Q_1^T & 0 \\ 0 & Q_2 D_2 \end{bmatrix} \begin{bmatrix} A_1 & 0 \\ 0 & D_2 \end{bmatrix} \begin{bmatrix} Q_1^T & 0 \\ 0 & I \end{bmatrix} U^T Q^T
\]

where \( Q_1 A_1 Q_1^T \) is the spectral decomposition of the rank-1 perturbed diagonal matrix \( D_1 + \rho w^T w \) obtained by using the above procedure. Thus the spectral decomposition of \( X_{(\cdot \setminus j)}^TX_{(\cdot \setminus j)} \) is given by

\[
D_{(\cdot \setminus j)} = \begin{bmatrix} A_1 & 0 \\ 0 & D_2 \end{bmatrix}, \quad Q_{(\cdot \setminus j)} = QU \begin{bmatrix} Q_1 & 0 \\ 0 & I \end{bmatrix}.
\]

Note that \( D_2 \) is constructed from the deflated eigenvalues of \( X^TX \). The \( \hat{\Sigma}_{(\cdot \setminus j)}(\kappa) \) shares \( Q_{(\cdot \setminus j)} \) with \( X_{(\cdot \setminus j)}^TX_{(\cdot \setminus j)} \), and modifies \( D_{(\cdot \setminus j)} \).

While the theory is sound, its implementation is tricky due to numerical difficulties, e.g., in solving secular equations. LAPACK (Anderson et al., 1999) subroutines DLAED4 and DLAED3, provided by R natively, stably implement the computation of eigenvalues and the eigenvectors, respectively. While written for DLAED1 that computes the spectral decomposition of symmetric tridiagonal matrices, the implementation in R is general and applies to any symmetric matrix. Deflation is implemented by DLAED2, which needs some modification to be used with general symmetric matrices. Package CondReg makes use of these subroutines.
3 Package CondReg

This section describes the user-level functions in the CondReg package, which implements Algorithms 2 and 3 of the main text at the core. Table S1 summarizes these functions. In the subsections that follow, we discuss each user-level functions in context. These user-level functions in the CondReg package are sufficient in most application settings.

| Function name      | Description                                                                 |
|--------------------|-----------------------------------------------------------------------------|
| condreg()          | Computes the CondReg estimator for a given value of $\kappa$                |
| kgrid()            | Generates gridpoints of penalty parameters                                   |
| select_kmax()      | Computes $\kappa$ by cross-validation                                         |
| select_condreg()   | Computes the CondReg estimator with $\kappa_{\text{max}}$ selected with select_kmax() |

Table S1: User-level functions in CondReg

Selection of regularization parameter: select_kmax and kgrid

The CondReg package supports general $K$-fold cross-validation for selecting $\kappa$ through the function select_kmax; for $K = n$, the LOOCV procedure described in the previous section is conducted. This function performs the cross-validation procedure minimizing the empirical predictive risk, and returns the optimal regularization parameter $\widehat{\kappa}$ from a search over a set of possible values of $\kappa$. If otherwise specified, the knots of the solution path, as computed using Algorithm 2 or 3, are used. The user may pass in a vector of values of $\kappa$. The function kgrid can be used for this purpose. The function kgrid returns $\{\kappa \in \text{kgrid}(a,b)\}$ in the complete search space $\{\kappa \geq 1 : \kappa \in \mathbb{R}\}$. The user chooses the maximum possible value $\{a \geq 1 : a \in \mathbb{R}\}$ and $b \in \mathbb{N}$, the number of possible values.

Regularized covariance estimation: condreg and select_condreg

As described, functions kgrid and select_kmax can be used to approximate the optimal value of regularization parameter that minimizes the predictive risk. These regularization parameters can be used as inputs to the function condreg. Given a value of $\kappa$ and the data, the condreg function returns the CondReg estimator $\widehat{\Sigma}(\kappa)$. The user can determine whether to use the forward algorithm (Algorithm 1) or the backward algorithm (Algorithm 2). The CondReg package provides a convenience function select_condreg that automates the selection of $\widehat{\kappa}$ and returns $\Sigma(\widehat{\kappa})$ with a single call.

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