Regularized Precision Matrix Estimation via ADMM

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Abstract

`ADMMsigma` is an R package that estimates a penalized precision matrix via the alternating direction method of multipliers (ADMM) algorithm. This report will provide a brief overview of the algorithm and detail how it can be utilized to estimate precision matrices of jointly normal distributions. In addition, examples and simulation results will be provided.

Contents

1 Introduction

Suppose we want to solve the following optimization problem:

$$\begin{aligned} \text{minimize } & f(x) + g(z) \\ \text{subject to } & Ax + Bz = c \end{aligned}$$

where $x \in \mathbb{R}^n, z \in \mathbb{R}^m, A \in \mathbb{R}^{p \times m}, B \in \mathbb{R}^{p \times m}, c \in \mathbb{R}^p$ – though we will later consider cases where x and z are matrices. Further, we will assume f and g are convex. The *augmented lagrangian* is constructed as follows:

$$L_\rho(x, z, y) = f(x) + g(z) + y^T(Ax + Bz - c) + \frac{\rho}{2}\left\| Ax + Bz - c \right\|_2^2$$

where $y \in \mathbb{R}^p$ is the lagrange multiplier. The optimal value is

$$p^* = inf\left\{ f(x) + g(z) | Ax + Bz = c \right\}$$

Clearly, the minimization under the augmented lagrangian is equivalent to that of the usual lagrangian since any feasible point (x, z) satisfies the constraint $\rho \left\| Ax + Bz - c \right\|_2^2 / 2 = 0$.

The alternating direct method of multipliers (ADMM) algorithm consists of the following repeated iterations:

$$x^{k+1} := \arg\min_x L_\rho(x, z^k, y^k) \tag{1}$$

$$z^{k+1} := \arg\min_z L_\rho(z^{k+1}, z, y^k) \tag{2}$$

$$y^{k+1} := y^k + \rho(Ax^{k+1} + Bz^{k+1} - c) \tag{3}$$

A more complete introduction to the algorithm – specifically how it arose out of *dual ascent* and *method of multipliers* – can be found in Boyd et al. (2011).

2 Regularized Precision Matrix Estimation

We now consider the case where $X_1, ..., X_n$ are iid $N_p(\mu, \Sigma)$ and we are tasked with estimating the precision matrix, denoted $\Omega \equiv \Sigma^{-1}$. The maximum likelihood estimator for Ω is

$$\hat{\Omega} = \arg\min_{\Omega \in S_+^p} \left\{ Tr\left(S\Omega\right) - \log\det\left(\Omega\right) \right\}$$

where $S = \sum_{i=1}^n (X_i - \bar{X})(X_i - \bar{X})^T/n$. It is straight forward to show that when the solution exists, $\hat{\Omega} = S^{-1}$.

We can construct a *penalized* likelihood estimator by adding a penalty term, $P\left(\Omega\right)$, to the likelihood:

$$\hat{\Omega}_\lambda = \arg\min_{\Omega \in S_+^p} \left\{ Tr\left(S\Omega\right) - \log\det\left(\Omega\right) + P\left(\Omega\right) \right\}$$

Throughout the rest of this document we will take $P\left(\Omega\right)$ to be $P\left(\Omega\right) = \lambda \left[\frac{1-\alpha}{2} \left\| \Omega \right|_F^2 + \alpha \left\| \Omega \right\|_1 \right]$ so that the full penalized likelihood is as follows:

$$\hat{\Omega}_\lambda = \arg\min_{\Omega \in S_+^p} \left\{ Tr\left(S\Omega\right) - \log\det\left(\Omega\right) + \lambda \left[\frac{1-\alpha}{2} \left\| \Omega \right|_F^2 + \alpha \left\| \Omega \right\|_1 \right] \right\}$$

where $0 \leq \alpha \leq 1$, $\lambda > 0$, $\left\| \cdot \right\|_F^2$ is the Frobenius norm and we define $\left\| A \right\|_1 = \sum_{i,j} \left| A_{ij} \right|$. This *elastic-net* penalty was explored by Hui Zou and Trevor Hastie (Zou and Hastie 2005) and is identical to the penalty used in the popular penalized regression package `glmnet`. Clearly, when $\alpha = 0$ the elastic-net reduces to a ridge-type penalty and when $\alpha = 1$ this reduces to a lasso-type penalty.

By letting f be equal to the non-penalized likelihood and g equal to $P\left(\Omega\right)$, our goal is to minimize the full augmented lagrangian where the constraint is that $\Omega - Z$ is equal to zero:

$$L_\rho(\Omega, Z, \Lambda) = f\left(\Omega\right) + g\left(Z\right) + Tr\left[\Lambda\left(\Omega - Z\right)\right] + \frac{\rho}{2}\left\| \Omega - Z \right\|_F^2$$

The ADMM algorithm for regularized precision matrix estimation is

$$\Omega^{k+1} = \arg\min_\Omega \left\{ Tr\left(\Omega\right) - \log\det\left(\Omega\right) + Tr\left[\Lambda^k\left(\Omega - Z^k\right)\right] + \frac{\rho}{2}\left\| \Omega - Z^k \right\|_F^2 \right\} \tag{4}$$

$$Z^{k+1} = \arg\min_Z \left\{ \lambda \left[\frac{1-\alpha}{2} \left\| Z \right\|_F^2 + \alpha \left\| Z \right\|_1 \right] + Tr\left[\Lambda^k\left(\Omega^{k+1} - Z\right)\right] + \frac{\rho}{2}\left\| \Omega^{k+1} - Z \right\|_F^2 \right\} \tag{5}$$

$$\Lambda^{k+1} = \Lambda^k + \rho\left(\Omega^{k+1} - Z^{k+1}\right) \tag{6}$$

2.1 Condensed-Form ADMM

An alternate form of the ADMM algorithm can constructed by scaling the dual variable. Let us define $R^k = \Omega - Z^k$ and $U^k = \Lambda^k/\rho$. Then

$$\begin{aligned} Tr\left[\Lambda^k\left(\Omega - Z^k\right)\right] + \frac{\rho}{2}\left\|\Omega - Z^k\right\|_F^2 &= Tr\left[\Lambda^k R^k\right] + \frac{\rho}{2}\left\|R^k\right\|_F^2 \\ &= \frac{\rho}{2}\left\|R^k + \Lambda^k/\rho\right\|_F^2 - \frac{\rho}{2}\left\|\Lambda^k/\rho\right\|_F^2 \\ &= \frac{\rho}{2}\left\|R^k + U^k\right\|_F^2 - \frac{\rho}{2}\left\|U^k\right\|_F^2 \end{aligned}$$

The condensed-form can now be written as follows:

$$\Omega^{k+1} = \arg\min_{\Omega}\left\{Tr\left(\Omega\right) - \log\det\left(\Omega\right) + \frac{\rho}{2}\left\|\Omega - Z^k + U^k\right\|_F^2\right\} \tag{7}$$

$$Z^{k+1} = \arg\min_{Z}\left\{\lambda\left[\frac{1-\alpha}{2}\left\|Z\right\|_F^2 + \alpha\left\|Z\right\|_1\right] + \frac{\rho}{2}\left\|\Omega^{k+1} - Z + U^k\right\|_F^2\right\} \tag{8}$$

$$U^{k+1} = U^k + \Omega^{k+1} - Z^{k+1} \tag{9}$$

More generally (in vector form),

$$x^{k+1} := \arg\min_{x}\left\{f(x) + \frac{\rho}{2}\left\|Ax + Bz^k - c + u^k\right\|_2^2\right\} \tag{10}$$

$$z^{k+1} := \arg\min_{z}\left\{g(z) + \frac{\rho}{2}\left\|Ax^{k+1} + Bz - c + u^k\right\|_2^2\right\} \tag{11}$$

$$u^{k+1} := u^k + Ax^{k+1} + Bz^{k+1} - c \tag{12}$$

Note that there are limitations to using this method. For instance, because the dual variable is scaled by ρ (the step size), this form limits one to using a constant step size (without making further adjustments to U^k) – a limitation that could prolong the convergence rate. Because of this, we will only consider the non-condensed form for the remainder of this report.

2.2 Algorithm

$$\begin{aligned} \Omega^{k+1} &= \arg\min_{\Omega}\left\{Tr\left(\Omega\right) - \log\det\left(\Omega\right) + Tr\left[\Lambda^k\left(\Omega - Z^k\right)\right] + \frac{\rho}{2}\left\|\Omega - Z^k\right\|_F^2\right\} \\ Z^{k+1} &= \arg\min_{Z}\left\{\lambda\left[\frac{1-\alpha}{2}\left\|Z\right\|_F^2 + \alpha\left\|Z\right\|_1\right] + Tr\left[\Lambda^k\left(\Omega^{k+1} - Z\right)\right] + \frac{\rho}{2}\left\|\Omega^{k+1} - Z\right\|_F^2\right\} \\ \Lambda^{k+1} &= \Lambda^k + \rho\left(\Omega^{k+1} - Z^{k+1}\right) \end{aligned}$$

1. Decompose $S + \Lambda^k - \rho Z^k = VQV^T$.

$$\Omega^{k+1} = \frac{1}{2\rho}V\left[-Q + \left(Q^2 + 4\rho I_p\right)^{1/2}\right]V^T$$

2. Elementwise soft-thresholding for all $i = 1, ..., p$ and $j = 1, ..., p$.

$$
\begin{aligned}
Z_{ij}^{k+1} &= \frac{1}{\lambda(1-\alpha)+\rho} sign\left(\rho\Omega_{ij}^{k+1} + \Lambda_{ij}^{k}\right)\left(\left|\rho\Omega_{ij}^{k+1} + \Lambda_{ij}^{k}\right| - \lambda\alpha\right)_{+} \\
&= \frac{1}{\lambda(1-\alpha)+\rho} Soft\left(\left(\rho\Omega_{ij}^{k+1} + \Lambda_{ij}^{k}\right), \lambda\alpha\right)
\end{aligned}
$$

3. Update Λ.

$$
\Lambda^{k+1} = \Lambda^{k} + \rho\left(\Omega^{k+1} - Z^{k+1}\right)
$$

2.2.1 Proof of (1):

$$
\Omega^{k+1} = \arg\min_{\Omega}\left\{Tr\left(\Omega\right) - \log\det\left(\Omega\right) + Tr\left[\Lambda^{k}\left(\Omega - Z^{k}\right)\right] + \frac{\rho}{2}\left\|\Omega - Z^{k}\right\|_{F}^{2}\right\}
$$

Code snippet:

Note this is not the actual code. The real code is written in c++.

```
# ridge penalized precision matrix
# function
RIDGEsigma = function(S, lam) {

    # dimensions
    p = dim(S)[1]

    # gather eigen values of S (spectral
    # decomposition)
    e.out = eigen(S, symmetric = TRUE)

    # augment eigen values for omega hat
    new.evs = (-e.out$val + sqrt(e.out$val^2 +
        4 * lam))/(2 * lam)

    # compute omega hat for lambda (zero
    # gradient equation)
    omega = tcrossprod(e.out$vec * rep(new.evs,
        each = p), e.out$vec)

    # compute gradient
    grad = S - qr.solve(omega) + lam * omega

    return(list(omega = omega, gradient = grad))
}
```

2.2.2 Proof of (2)

$$Z^{k+1} = \arg\min_{Z} \left\{ \lambda \left[\frac{1-\alpha}{2} \left\| Z \right\|_F^2 + \alpha \left\| Z \right\|_1 \right] + Tr\left[\Lambda^k \left(\Omega^{k+1} - Z \right) \right] + \frac{\rho}{2} \left\| \Omega^{k+1} - Z \right\|_F^2 \right\}$$

Code snippet:

Note this is not the actual code. The real code is written in c++.

```
# ADMMsigma function
ADMMsigma = function(X = NULL, S = NULL,
    lam, alpha = 1, rho = 2, mu = 10, tau1 = 2,
    tau2 = 2, tol1 = 1e-04, tol2 = 1e-04,
    maxit = 1000) {

    # compute sample covariance matrix, if
    # necessary
    if (is.null(S)) {

        # covariance matrix
        n = dim(X)[1]
        S = (n - 1)/n * cov(X)

    }

    # allocate memory
    p = dim(S)[1]
    criterion = TRUE
    iter = lik = s = r = eps1 = eps2 = 0
    new.Z = Y = Omega = matrix(0, nrow = p,
        ncol = p)

    # loop until convergence
    while (criterion && (iter <= maxit)) {

        # ridge equation (1) gather eigen values
        # (spectral decomposition)
        Z = new.Z
        Omega = sigma_ridge(S + Y - rho *
            Z, lam = rho)$omega

        # penalty equation (2) soft-thresholding
        new.Z = soft(Y + rho * Omega, lam *
            alpha)/(lam * (1 - alpha) + rho)

        # update U (3)
        Y = Y + rho * (Omega - new.Z)

        # calculate new rho
        s = sqrt(sum((rho * (new.Z - Z))^2))
        r = sqrt(sum((Omega - new.Z)^2))
```

```r
        rho = rho * (tau1 * (r > mu * s) +
            (s > mu * r)/tau2 + (s/mu <=
            r & r <= mu * s))
        iter = iter + 1

        # stopping criterion
        eps1 = p * tol1 + tol2 * max(sqrt(sum(Omega^2)),
            sqrt(sum(new.Z^2)))
        eps2 = p * tol1 + tol2 * sqrt(sum(Y^2))
        criterion = (r >= eps1 || s >= eps2)

    }
    return(list(Iterations = iter, Omega = Omega))
}
```

3 R Package

3.1 Installation

```r
# The easiest way to install is from the
# development version from GitHub:
# install.packages('devtools')
devtools::install_github("MGallow/ADMMsigma")
```

If there are any issues/bugs, please let me know: github. You can also contact me via my website. Pull requests are welcome!

A (possibly incomplete) list of functions contained in the package can be found below:

- `ADMMsigma()` computes the estimated precision matrix (ridge, lasso, and elastic-net type regularization optional)
- `RIDGEsigma()` computes the estimated ridge penalized precision matrix via closed-form solution
- `plot.ADMMsigma()` produces a heat map for cross validation errors
- `plot.RIDGEsigma()` produces a heat map for cross validation errors

3.2 Usage

```r
library(ADMMsigma)
```

```r
# generate data from a dense matrix first
# compute covariance matrix
S = matrix(0, nrow = 5, ncol = 5)

for (i in 1:5) {
    for (j in 1:5) {
        S[i, j] = 0.9^(i != j)
    }
}

# generate 100 x 5 matrix with rows drawn
# from iid N_p(0, S)
Z = matrix(rnorm(100 * 5), nrow = 100, ncol = 5)
out = eigen(S, symmetric = TRUE)
S.sqrt = out$vectors %*% diag(out$values^0.5) %*%
    t(out$vectors)
X = Z %*% S.sqrt


# elastic-net type penalty (use CV for
# optimal lambda and alpha)
ADMMsigma(X)
```

```
##
## Iterations:
## [1] 35
##
## Tuning parameters:
##       log10(lam)  alpha
## [1,]        -2.5    0.6
##
## Omega:
##          [,1]     [,2]     [,3]     [,4]     [,5]
## [1,]  7.50103 -1.71813 -2.17055 -1.21055 -1.95217
## [2,] -1.71813  6.88957 -2.51084 -1.42759 -1.14920
## [3,] -2.17055 -2.51084  8.17508 -1.79449 -1.38145
## [4,] -1.21055 -1.42759 -1.79449  6.25581 -1.97081
## [5,] -1.95217 -1.14920 -1.38145 -1.97081  6.53472
```

```r
# ridge penalty (use CV for optimal
# lambda)
ADMMsigma(X, alpha = 0)
```

```
##
## Iterations:
## [1] 39
##
## Tuning parameters:
##       log10(lam)  alpha
## [1,]          -3      0
##
## Omega:
##          [,1]     [,2]     [,3]     [,4]     [,5]
## [1,]  7.92134 -1.80920 -2.32991 -1.24122 -2.07704
```

```
## [2,] -1.80920  7.24953 -2.70397 -1.48210 -1.17634
## [3,] -2.32991 -2.70397  8.69320 -1.89807 -1.43455
## [4,] -1.24122 -1.48210 -1.89807  6.54511 -2.08445
## [5,] -2.07704 -1.17634 -1.43455 -2.08445  6.84977
```

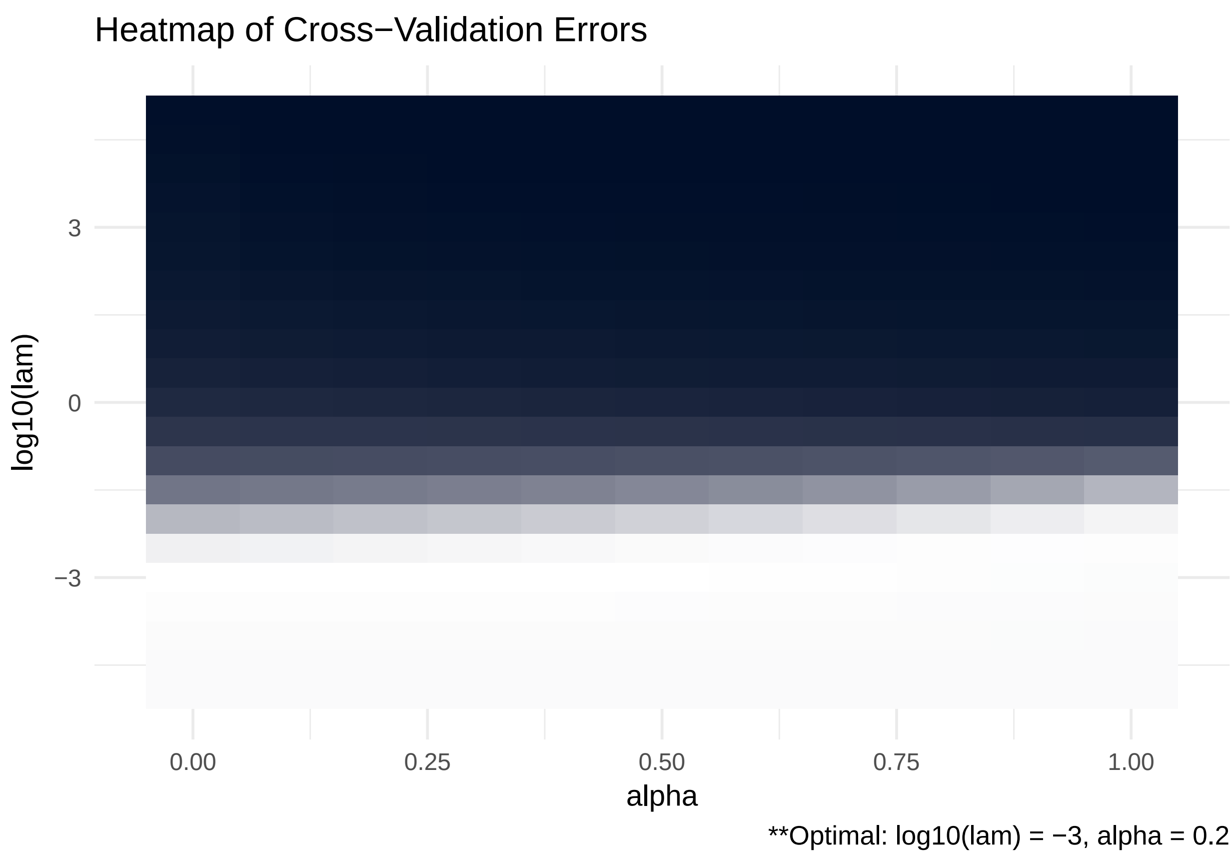
```
# lasso penalty (lam = 0.1)
ADMMsigma(X, lam = 0.1, alpha = 1)
```

```
##
## Iterations:
## [1] 10
##
## Tuning parameters:
##       log10(lam)  alpha
## [1,]          -1      1
##
## Omega:
##           [,1]     [,2]     [,3]     [,4]     [,5]
## [1,]  2.80422 -0.62667 -0.67987 -0.55554 -0.66056
## [2,] -0.62667  2.66766 -0.75422 -0.60328 -0.54369
## [3,] -0.67987 -0.75422  2.88706 -0.65217 -0.57631
## [4,] -0.55554 -0.60328 -0.65217  2.53979 -0.69921
## [5,] -0.66056 -0.54369 -0.57631 -0.69921  2.60963
```

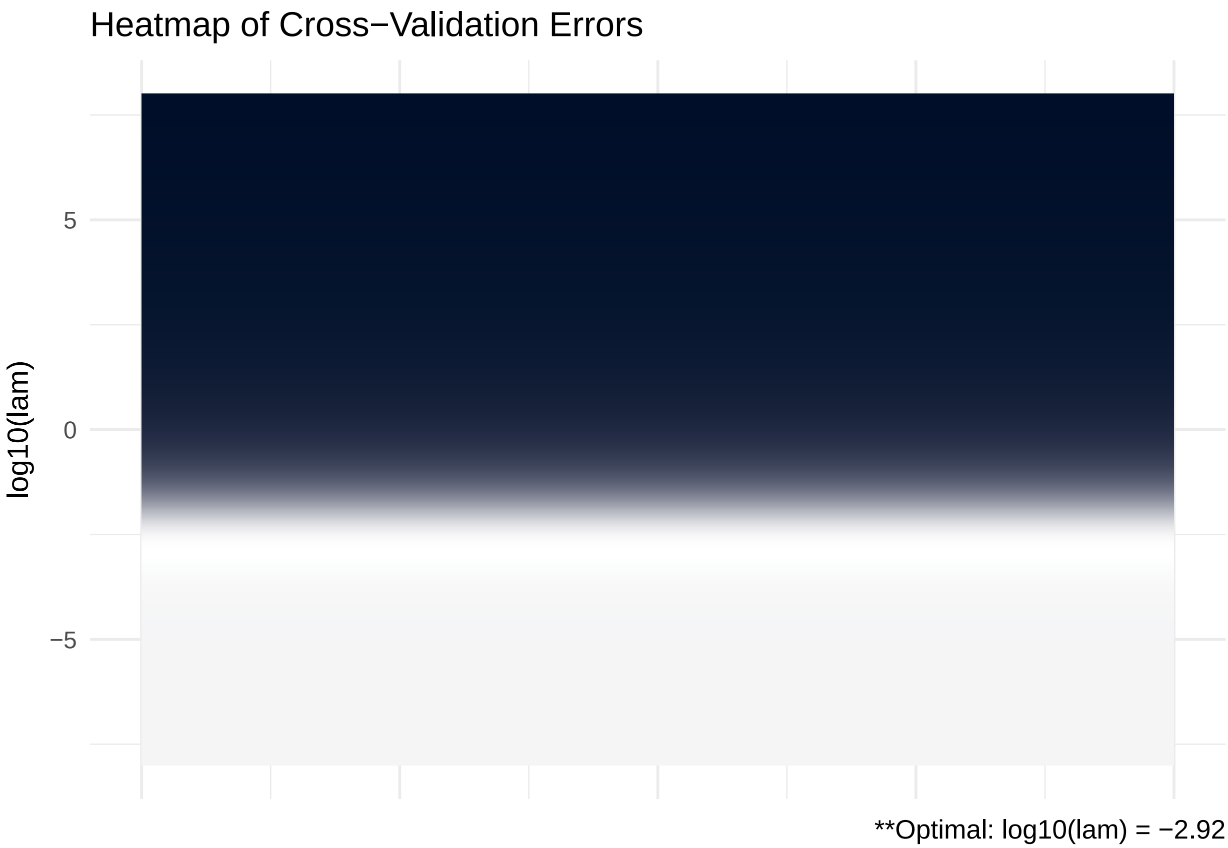
```
# ridge penalty no ADMM
RIDGEsigma(X, lam = 10^seq(-8, 8, 0.01))
```

```
##
## Tuning parameter:
##         lam  log10(lam)
## [1,]  0.001        -3.1
##
## Omega:
##           [,1]     [,2]     [,3]     [,4]     [,5]
## [1,]  8.08365 -1.83697 -2.40822 -1.24051 -2.12903
## [2,] -1.83697  7.38256 -2.79786 -1.49474 -1.17783
## [3,] -2.40822 -2.79786  8.92397 -1.94165 -1.44583
## [4,] -1.24051 -1.49474 -1.94165  6.63854 -2.12649
## [5,] -2.12903 -1.17783 -1.44583 -2.12649  6.95522
```

```
# produce CV heat map for ADMMsigma
ADMMsigma(X) %>% plot
```




```r
# produce CV heat map for RIDGEsigma
RIDGEsigma(X, lam = 10^seq(-8, 8, 0.01)) %>%
    plot
```



3.3 Benchmark

3.3.1 Computer Specs:

- MacBook Pro (Late 2016)
- Processor: 2.9 GHz Intel Core i5
- Memory: 8GB 2133 MHz
- Graphics: Intel Iris Graphics 550

```r
# generate data from tri-diagonal
# (sparse) matrix compute covariance
# matrix (can confirm inverse is
# tri-diagonal)
S = matrix(0, nrow = 100, ncol = 100)

for (i in 1:100) {
    for (j in 1:100) {
        S[i, j] = 0.7^(abs(i - j))
    }
}

# generate 1000 x 100 matrix with rows
# drawn from iid N_p(0, S)
```

```r
Z = matrix(rnorm(1000 * 100), nrow = 1000,
    ncol = 100)
out = eigen(S, symmetric = TRUE)
S.sqrt = out$vectors %*% diag(out$values^0.5) %*%
    t(out$vectors)
X = Z %*% S.sqrt


# glasso (for comparison)
microbenchmark(glasso(s = S, rho = 0.1))
```

```
## Unit: milliseconds
##                      expr      min       lq     mean   median       uq
##  glasso(s = S, rho = 0.1) 49.93206 53.11861 57.87519 55.44664 59.30303
##       max neval
##  89.96595   100
```

```r
# benchmark ADMMsigma - default tolerance
microbenchmark(ADMMsigma(S = S, lam = 0.1,
    alpha = 1, tol1 = 1e-04, tol2 = 1e-04))
```

```
## Unit: milliseconds
##                                                                    expr
##  ADMMsigma(S = S, lam = 0.1, alpha = 1, tol1 = 1e-04, tol2 = 1e-04)
##       min       lq     mean   median       uq      max neval
##  39.99944 43.82541 51.62732 46.94982 53.30376 228.9022   100
```

```r
# benchmark ADMMsigma - tolerance 1e-8
microbenchmark(ADMMsigma(S = S, lam = 0.1,
    alpha = 1, tol1 = 1e-08, tol2 = 1e-08))
```

```
## Unit: milliseconds
##                                                                    expr
##  ADMMsigma(S = S, lam = 0.1, alpha = 1, tol1 = 1e-08, tol2 = 1e-08)
##       min       lq     mean   median       uq      max neval
##  189.2626 203.0107 221.2471 211.5412 230.3703 361.4178   100
```

```r
# benchmark ADMMsigma CV - default
# parameter grid
microbenchmark(ADMMsigma(X), times = 5)
```

```
## Unit: seconds
##          expr      min       lq     mean  median       uq      max neval
##  ADMMsigma(X) 55.62628 56.18889 58.61224 56.4466 59.59131 65.20811     5
```

```r
# benchmark ADMMsigma parallel CV
microbenchmark(ADMMsigma(X, parallel = TRUE),
    times = 5)
```

```
## Unit: seconds
##                           expr      min       lq     mean   median
##  ADMMsigma(X, parallel = TRUE) 30.97527 31.30452 31.75878 32.06775
##        uq      max neval
##  32.22213 32.22423     5
```

```r
# benchmark ADMMsigma CV - likelihood
# convergence criteria
```

```r
microbenchmark(ADMMsigma(X, crit = "loglik"),
    times = 5)
```

```
## Unit: seconds
##                           expr      min       lq     mean   median
##  ADMMsigma(X, crit = "loglik") 80.37973 82.30604 83.37748 82.87069
##        uq     max neval
##  85.60625 85.7247     5
```

References

Boyd, Stephen, Neal Parikh, Eric Chu, Borja Peleato, Jonathan Eckstein, and others. 2011. "Distributed Optimization and Statistical Learning via the Alternating Direction Method of Multipliers." *Foundations and Trends in Machine Learning* 3 (1). Now Publishers, Inc.: 1–122.

Zou, Hui, and Trevor Hastie. 2005. "Regularization and Variable Selection via the Elastic Net." *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* 67 (2). Wiley Online Library: 301–20.