Homework 3 - Analysis of High Dimensional Data

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Problem: Consider the Gaussian graphical model as presented in class. In a seminal paper Meinshausen and Buhlmann (Annals of Statistics, 2006) showed that one can estimate the model by using node-wise penalized (lasso) regression, followed by post-processing to obtain a symmetric and positive definite estimate of Ω.

1. Using your code from HW 2, estimate a Gaussian graphical model using the lasso node-wise regression method.

2. Apply your algorithms to a chain network, a nearest neighbor network, and a scale free network of size p = 25 with n = 150 observations. Set the density level of your edge set at 10 (see Section 4 of Guo et al. (Biometrika, 2011)).

3. Replicate the setting in (2) 10 times and provide an estimate of the false positive and false negative rates, as well as the Frobenius norm of the difference between your estimate and the true Ω.

Meinshausen-Buhlmann Method: Suppose $X^1 \sim \mathcal{N}_p(0, \Sigma = \Omega^{-1})$. Then $X_i^1 | X_{-i}^1 \sim \mathcal{N}(-\sum_{j \neq i} \frac{\omega_{ji}}{\omega_{ii}} X_j^1, \frac{1}{\omega_{ii}})$. Now suppose that

$$X^1, ..., X^{150} \overset{iid}{\sim} \mathcal{N}_p(0, \Sigma = \Omega^{-1}).$$

Then define $X^T = [X^1, ..., X^{150}]$ and denote X_i as the 1st column of X. The Meinshausen-Buhlmann method to estimate the partial correlations consists of running the following *lasso* regressions for $i = 1, ..., p$:

$$\min_{\tilde{\beta}_i} \frac{1}{2} \|X_i - \sum_{j \neq i} \beta_{ji} X_j\|_2^2 + \lambda \|\tilde{\beta}_i\|_1 \tag{1}$$

where $\tilde{\beta}_i = (\beta_{ji})_{j \neq i, 1 \leq j \leq p}$ and $\hat{\tilde{\beta}}_i = (\frac{\hat{\omega}_{ji}}{\hat{\omega}_{ii}})_{j \neq i}$. Thus $(\beta_{ji}) = 0 \iff \omega_{ji} = 0$, which allows us to discover the sparsity pattern. However, the Meinshausen-Buhlmann method doesn't produce a positive definite estimate of Ω. As a result, to find the concentration matrices corresponding to chain graphs,

nearest neighbor networks and scale-free networks with edge density of approximately 10%, we use the following method:

$$\max_{\Omega \succcurlyeq 0} \log|\Omega| - tr(\Omega S) \quad \text{subject to } (i,j) \notin E \implies \omega_{ij} = 0. \tag{2}$$

where $|\Omega|$ denotes the determinant of Ω.

Chain Graphs, Nearest Neighbor Networks and Scale-free Networks: To generate Ω corresponding to a chain graph we first construct a 25×25 covariance matrix, Σ where the (i,j)th element of Σ, $\sigma_{i,j}$, is defined as

$$\sigma_{i,j} = e^{-|s_i - s_j|/2} \quad \text{for } s_1 < s_2 < ... < s_p$$
$$\text{and } s_j - s_{j-1} \sim U(0.5, 1) \quad \text{for } j = 2, ..., p.$$

Then we set $\Omega = \Sigma^{-1}$. Our precision matrix thus constructed is a tridiagonal matrix. In the case of the nearest neighbor network, we generate 25 points randomly on the unit square, $(0,1) \times (0,1)$, calculate all $p(p-1)/2$ pairwise distances and find m nearest neighbors of each point in terms of this distance. The nearest neighbor network is then obtained by linking any two points that are m-nearest neighbors of each other. The integer $m = 2$ is chosen for our study as it generates a graph with denisty equal to approximately 0.1. Finally, for the scale-free network we used the *barabasi.game* function in R to generate a graph with density of 0.1. We controlled the final number of edges through the *seq.out* argument and obtained a graph with 30 edges, or equivalently, one with an edge density of 10% (as p = 25), in our scale-free graph. After acquiring the adjacency matrix we generated random uniforms to obtain a symmetric concentration matrix, Ω.

Algorithm: The first step is to standardize the data and set the initial value, $\tilde{\beta}_i^0$ (we tried $(\tilde{\beta}_i^0)_j = 0$ and $(\tilde{\beta}_i^0)_j = 1$ for all $j \neq i$ with the same results). Then to find the solutions to the *lasso* regressions in Equation 1 we use a proximal gradient algorithm using a constant step size of 0.0001, denoted by t. The algorithm is as follows:

$$\tilde{\beta}_i^{k+1} = \tilde{\beta}_i^k - t\nabla \frac{1}{2}\|X_i - \sum_{j \neq i} \beta_{ji}^k X_j\|_2^2$$
$$\tilde{\beta}_i^{k+1} = S_{t\lambda}(\tilde{\beta}_i^{k+1})$$

where $S_\lambda(x) \coloneqq \text{sign}(x)(|x| - \lambda)_+$ denotes the soft-thresholding operator.

A disadvantage of the Meinshausen-Buhlmann method is that all the *lasso* regressions are independent, which means that $\hat{\Omega}$ is not necessarily positive definite. To calculate a positive definite estimate for Ω, we used the method outlined in 2. Note that if

$$\Omega = \begin{pmatrix} \Omega_{11} & \Omega_{12} \\ \Omega_{12}^T & \Omega_{22} \end{pmatrix}$$

and

$$S = \begin{pmatrix} S_{11} & S_{12} \\ S_{12}^T & S_{22} \end{pmatrix}$$

where $\Omega_{22}, S_{22} \in \mathbb{R}$ and $\Omega_{11}, S_{11} \in \mathbb{R}^{p-1 \times p-1}$. Now suppose Ω_{11} and Ω_{12} is fixed. The onjective function is maximized with respect to $\gamma_{22} = (\Omega_{22} - \Omega_{12}\Omega_{11}^{-1}\Omega_{12}^T)$ at $\hat{\gamma}_{22} = \frac{1}{S_{22}} > 0$. Then $\hat{\Omega}_{22} = \frac{1}{S_{22}} + \Omega_{12}\Omega_{11}^{-1}\Omega_{12}^T$. In addition, if we hold γ_{22} and Ω_{11} fixed then the objective function is

$$\begin{aligned} &\min_{\Omega_{12}} S_{22}\Omega_{12}\Omega_{11}^{-1}\Omega_{12}^T + 2S_{12}\Omega_{12}^T \\ &\text{subject to } (i,j) \notin E_{12} \implies \omega_{ij} = 0. \end{aligned}$$

Note that this is the *glasso* problem without the ℓ_1 constraint. The solution is

$$(\Omega_{12})_j = \begin{cases} (\frac{1}{S_{22}}\Omega_{11}S_{12})_j & \text{if } (p,j) \in E \\ 0 & \text{otherwise} \end{cases}$$

In addition, regardless of the choice of Ω_{12}, Ω will maintain positive definiteness so long as Ω_{11} is positive definite. Now we swap the last row and column with another, repeat the process desccribed above and iterate for $k = 1, ..., p$.

Results: Let

$$\begin{aligned} F(\hat{\Omega}) &= \frac{\|\Omega - \hat{\Omega}\|_F^2}{\|\Omega\|_F^2} \\ FP(\hat{\Omega}) &= \frac{\sum_{i,j} I(\omega_{ij} = 0, \hat{\omega}_{ij} \neq 0)}{\sum_{i,j} I(\omega_{ij} = 0)} \\ FN(\hat{\Omega}) &= \frac{\sum_{i,j} I(\omega_{ij} \neq 0, \hat{\omega}_{ij} = 0)}{\sum_{i,j} I(\omega_{ij} \neq 0)} \end{aligned}$$

The next step was to estimate the optimal λ for each graph type. We did this by comparing the Frobenius Norm Loss (F), False Positive Rate (FP) and the False Negative Rate (FN) at various λ between 0 and 114. In general, FP decreased as λ increased while FN increased with λ. In terms of these measures we chose λ so that $FN = FP$. In addition, we want to minimize Frobenius Norm Loss. Thus ideally, we want a λ such that F is minimized and $FN = FP$. In the case of the chain graph $\lambda = 60$ worked well because both the FN and FP were equal to 0 and F was minimized at this value, as Figure 1 illustrates. Also, at this value of λ, we were able to recover the correct sparsity pattern as shown in Figure 2. For the other two types of graphs we picked two λ's - one such that $FN = FP$ and the other to minimize F. For the nearest neighbor network, choosing $\lambda = 15$ implied $FN = FP$ while $\lambda = 15$ implied that F was minimized while for the scale-free network satisfied these criteria were satisfied at $\lambda = 15$ and $\lambda = 7$, respectively. This is illustrated in Figures 3 and 5. However, as Figures 4 and 6 shows, the sparsity pattern predicted by this method is not as good as in the case of the chain graph.

Finally let

$$F_K(\hat{\Omega}) = \frac{1}{K}\sum_{k=1}^{K}\frac{\|\Omega^k - \hat{\Omega^k}\|_F^2}{\|\Omega^k\|_F^2}$$

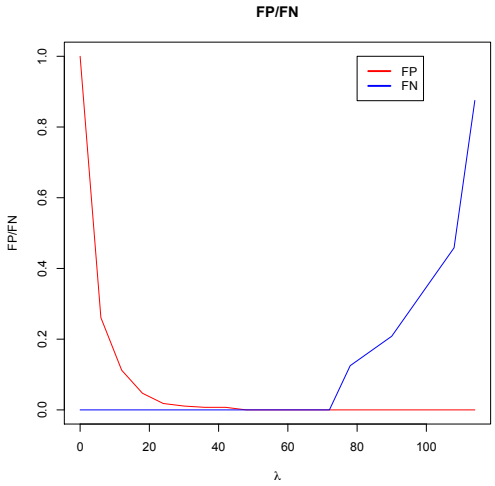
$$FP_K(\hat{\Omega}) = \frac{1}{K}\sum_{k=1}^{K}\frac{\sum_{i,j} I(\omega_{ij}^k = 0, \hat{\omega}_{ij}^k \neq 0)}{\sum_{i,j} I(\omega_{ij}^k = 0)}$$

$$FN_K(\hat{\Omega}) = \frac{1}{K}\sum_{k=1}^{K}\frac{\sum_{i,j} I(\omega_{ij}^k \neq 0, \hat{\omega}_{ij}^k = 0)}{\sum_{i,j} I(\omega_{ij}^k \neq 0)}$$

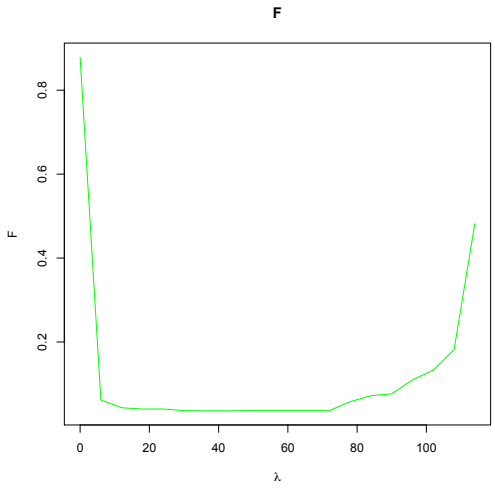
We set $K = 10$ to replicate the numerical experiment ten times and calculated F_K, FP_K and FN_K for our estimates. As Table 1 shows most of the results were consistent with our initial calculations. For the chain graph, the prediction of the sparsity pattern and estimation of the concentration matrix tends to be much more accurate than for other graph types. In the case of the Nearest Neighbor Network and the Scale-Free Network, prediction is worse as is indicated by the higher values for F_K, FP_K and FN_K.

	Chain	Nearest Neighbor		Scale-free	
		$\lambda = 15$	$\lambda = 30$	$\lambda = 7$	$\lambda = 15$
F_{10}	0.04677425	0.172161	0.0761543	0.7989101	0.826969
FP_{10}	0	0.1805368	0.01344037	0.5114815	0.2085185
FN_{10}	0	0.407647	0.7464521	0.02666667	0.1633333

Table 1: A comparison of the Meinshausen-Buhlmann method for Chain, Nearest Neighbor network and Scale-free network graphs. For the chain graph, the prediction of the sparsity pattern and estimation of the concentration matrix tends to be very accurate than for In tthe Nearest Neighbor Network and the Scale-Free Network as is indicated by the higher values.

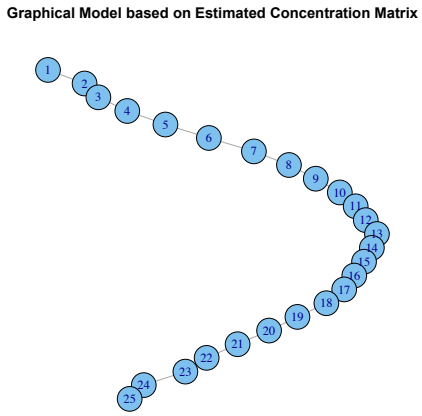


(a) False Positive/False Negative rate vs λ.

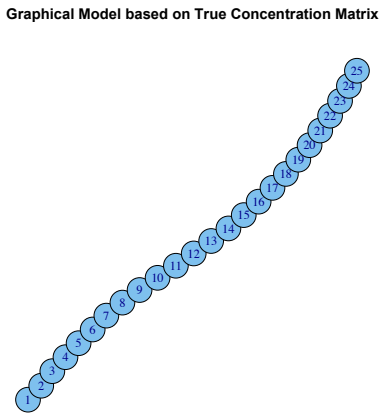


(b) Frobenius Norm Loss vs λ.

Figure 1: Plots for Proximal Gradient Algorithm for Chain Graph. $\lambda \approx 60$ seems to be optimal as both FN and FP are equal to 0 and F seems to be at its minimum point as well.

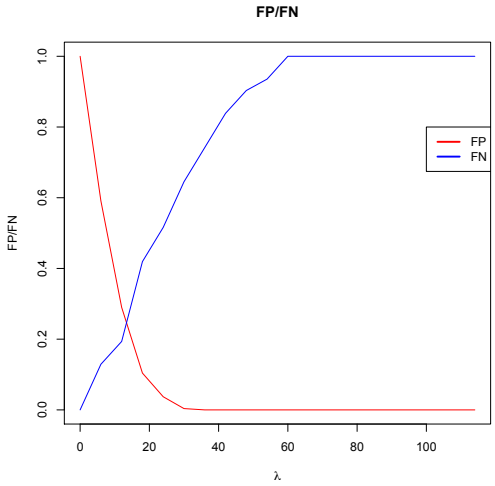


(a) Estimated Chain Graph

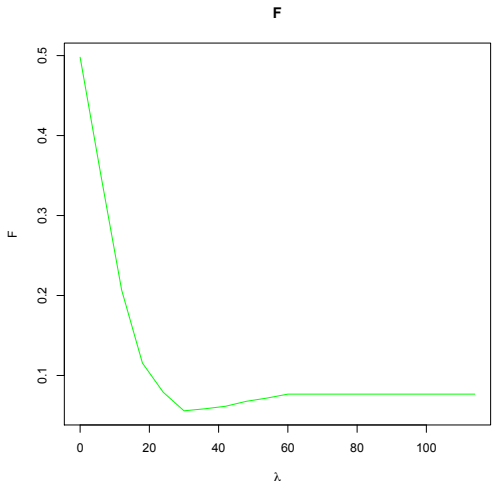


(b) True Chain Graph

Figure 2: As we can see from the graphs, the sparstiy in the case of the chain graphs was predicted exactly.

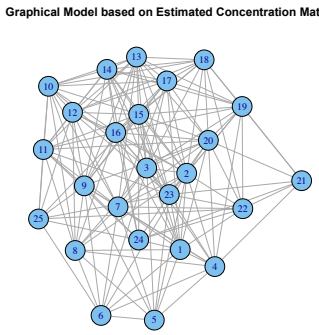


(a) False Positive/False Negative rate vs λ.

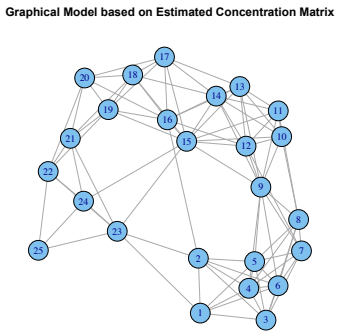


(b) Frobenius Norm Loss vs λ.

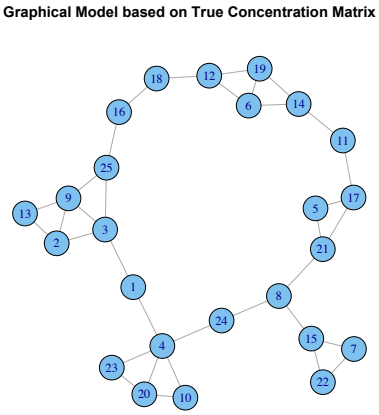
Figure 3: Plots for Proximal Gradient Algorithm for Nearest Neighbor Graph. $\lambda \approx 15$ seems to be optimal to minimize FN/FP while $\lambda \approx 30$ minimizes F.



(a) Estimated Nearest Neighbor Graph at $\lambda = 15$

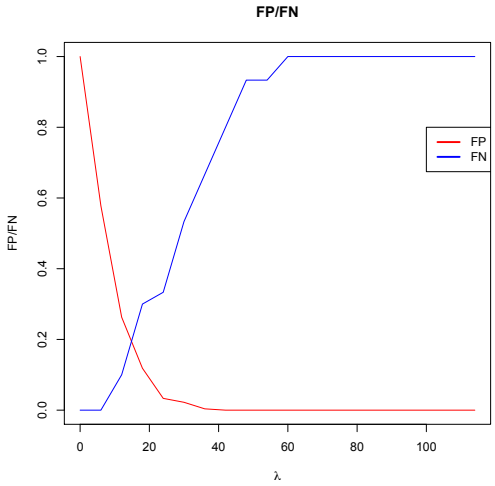


(b) Estimated Nearest Neighbor Graph at $\lambda = 30$

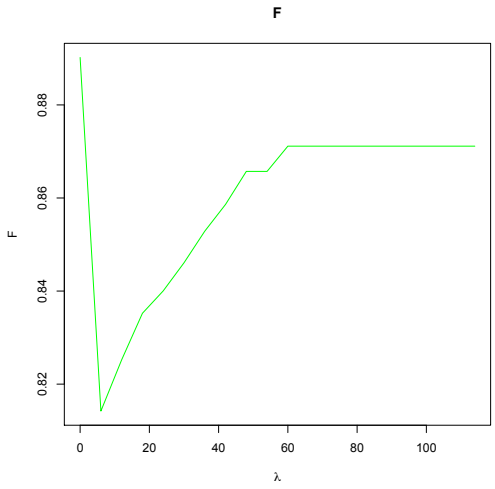


(c) True Nearest Neighbor Graph

Figure 4: The graph shows the sparsity patterns in the estimated and actual graphs in the case of the nearest neighbor network. In this case, we were unable to recover the exact sparsity pattern.

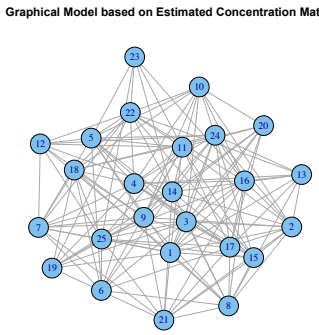


(a) False Positive/False Negative rate vs λ.

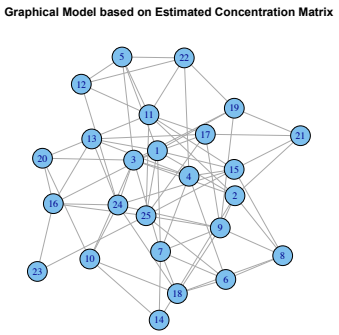


(b) Frobenius Norm Loss vs λ.

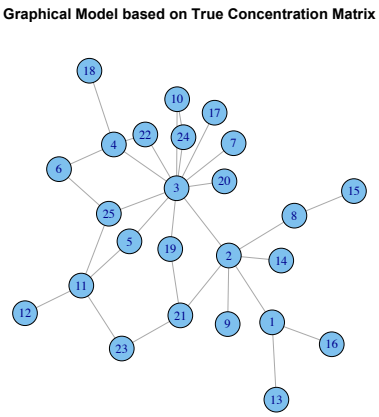
Figure 5: Plots for Proximal Gradient Algorithm for Scale-free Network. $\lambda \approx 15$ minimizes FN/FP while $\lambda \approx 7$ seems to minimize F .



(a) Estimated Scale-free network Graph at $\lambda = 7$



(b) Estimated Scale-free network Graph at $\lambda = 15$



(c) True Scale-free network Graph

Figure 6: The graph shows the sparsity patterns in the estimated and actual graphs in the case of the Scale-free network. In this case also, we were unable to recover the exact sparsity pattern.

Appendix: R Code for Proximal Gradient Algorithm

```
                                        #replications
(pdfrobeniusnorm = 0)
(frobeniusnorm = 0)
(fp = 0)
(fn = 0)
for (K in 1:10){
Omega1 = chain(p)
Sigma1 = solve(Omega1)

Y = mvrnorm(n, mu, Sigma1, tol = 1e-6, empirical = FALSE, EISPACK = FALSE)
Y = scale(Y, center = TRUE, scale = TRUE)

(omegahat = diag(p))
(allnodes = seq(1:p))
for(node in 1:p){
    (y = Y[,node])
    (allothernodes = setdiff(allnodes,node))
    (X = Y[,allothernodes])
    (betaold = matrix(0,dim(X)[2],1))

    stepsize = 0.0001
    lambda = 60
    iter = 1
    maxIter = 10000
    delta = 10^(-5)
    eps = 1
    while(iter<maxIter && eps>delta){
        (betanew = betaold - stepsize*grad(y,X,betaold,lambda))
        (betanew = softthresh(betanew,stepsize*lambda))
        (eps = norm(betanew - betaold))
        (betaold = betanew)
        (iter = iter + 1)
        ###(stepsize = stepsize/sqrt(iter))  #using diminishing stepsize
        ###(stepsize = stepsize) #using fixed stepsize
    }
    omegahat[node,allothernodes] = betanew
```

```
}
(adjmatrixhat = (abs(omegahat)>10^(-5)))
(adjmatrix = (abs(Omega1)>10^(-5)))
pdomegahat = makesymmetric(omegahat)
while(min(eigen(pdomegahat)$value)<0){
    pdomegahat = boostdiagonal(pdomegahat)}
(adjmatrixhat = (abs(pdomegahat)>10^(-5)))
(zero = medgeset(adjmatrixhat))
if(dim(zero)[1]>0){
    (omegahat = glasso(S,0,zero=zero)$wi)}
else{glasso(S,0)$wi}
(adjmatrixhat = (abs(omegahat)>10^(-5)))
(pdfrobeniusnorm[K] = (norm((pdomegahat-Omega1), type = c("F"))^2)
/(norm((Omega1), type = c("F"))^2))
(frobeniusnorm[K] = (norm((omegahat-Omega1), type = c("F"))^2)
/(norm((Omega1), type = c("F"))^2))
(fp[K] = (sum((upper.tri(adjmatrixhat,diag=FALSE)*adjmatrixhat
-upper.tri(adjmatrix,diag=FALSE)*adjmatrix)>0))
/(sum(upper.tri(adjmatrix,diag=FALSE)*adjmatrix==0)-(1/2)*(p)*(p+1)))
(fn[K] = (sum(upper.tri(adjmatrix,diag=FALSE)*adjmatrix-
upper.tri(adjmatrixhat,diag=FALSE)*adjmatrixhat>0))
/(sum(upper.tri(adjmatrix,diag=FALSE)*adjmatrix>0)))
}
```