Positive Graphical Lasso Estimation of Sparse Inverse Covariance Matrices

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Abstract

We explore the possibility of estimating sparse inverse covariance matrices when for scientific reasons the covariance matrix is restricted to be a non-negative matrix. The process mirrors the graphical lasso process developed by Friedman *and others* (2008) that did not have this additional constraint. Accordingly, the Lasso procedure is done through coordinate descent. To easily add the constraint, we modified the LARS function created by Efron *and others* (2004) to perform positive Lasso (pLasso) estimation. The process is demonstrated on several time series generated datasets to clearly show the effectiveness and limitations.

Introduction

Recent work into mapping gene regulatory networks has led to the use of Fortuin–Kasteleyn–Ginibre (FKG) inequalities to identify unexpected correlations. These correlations can be unexpected for various scientific reasons. However, advancing technology combined with practical/financial constraints gives rise to systems with $n\ (\sim 40) \ll p\ (\sim 10{,}000)$. For example, n could be the number of gene expression samples, and p could be the number of genes for which gene expression is measured. Additionally, most of these genes will be conditionally uncorrelated. The graphical Lasso algorithm developed by Friedman *and others* (2008) was made to deal with this estimation of sparse inverse covariance matrices. However, the desire to eliminate the unexpected correlations from networks results in a simple constraint on this estimation problem. We develop a similar and easy to implement algorithm, utilizing previous work, for performing estimation under these conditions.

Estimation of $\boldsymbol{\Sigma^{-1}}$

Let $\Theta = \Sigma^{-1}$ and S be the sample covariance matrix. The penalized log-likelihood is then

$$\ln|\Theta| - \mathrm{tr}(S\Theta) - \rho\|\Theta\|_1 \qquad (1)$$

where $\|\Theta\|_1 = \sum_{i,j}|\Theta_{ij}|$. We wish to find the positive semi-definite matrix Θ that maximizes this function. Banerjee *and others* (2007) showed that this is convex and instead outlined a method for estimating Σ. It is shown that the problem can be solved in block coordinate descent fashion. If $W = \Theta^{-1}$ is the estimate of Σ, then we can partition W and S.

$$W = \begin{pmatrix} W_{11} & w_{12} \\ w_{12}^T & w_{22} \end{pmatrix}, \qquad S = \begin{pmatrix} S_{11} & s_{12} \\ s_{12}^T & s_{22} \end{pmatrix} \tag{2}$$

Then the solution for each row and column is

$$w_{12} = \text{argmin}_y\{y^T W_{11}^{-1} y : \|y - s_{12}\|_\infty \leq \rho\}\,. \tag{3}$$

By convex duality, this is equivalent to solving

$$\min_{\beta}\left\{\frac{1}{2}\left\|W_{11}^{1/2}\beta - b\right\|^2 + \rho\|\beta\|_1\right\} \tag{4}$$

with $b = W_{11}^{-1/2}s_{12}$. Then, $w_{12} = W_{11}\beta$ is the solution to equation (3), where β is the solution to equation (4).

Equivalence Verification

To maximize the log-likelihood, we take a matrix derivative with respect to Θ and set equal to zero. We get

$$W - S - \rho\Gamma = 0\,, \tag{5}$$

with $\Gamma_{\text{ij}} = sign(\Theta_{ij})$ if $\Theta_{ij} \neq 0$ and $\Gamma_{ij} \in [-1, 1]$ if $\Theta_{ij} = 0$. The upper right component of this equation gives

$$w_{12} - s_{12} - \rho\gamma_{12} = 0\,. \tag{6}$$

To perform the minimization in equation (4), first note that

$$\tfrac{1}{2}\left\|W_{11}^{1/2}\beta - b\right\|^2 + \rho\|\beta\|_1 = \tfrac{1}{2}\beta^T W_{11}\beta - \beta^T W_{11}^{\frac{1}{2}}b + \tfrac{1}{2}b^T b + \rho\textstyle\sum_i|\beta_i| \tag{7}$$

Therefore, taking the derivative of equation (7) with respect to β and setting equal to zero gives

$$W_{11}\beta - s_{12} + \rho\nu = 0\,, \tag{8}$$

with $\nu = sign(\beta)$. Since $W\Theta = I$, we know that $W_{11}\theta_{12} + w_{12}\theta_{22} = 0$, and thus $\theta_{12} = -\theta_{22}W_{11}^{-1}w_{12}$. Then, $\gamma_{12} = sign(\theta_{12}) = -sign(\theta_{22}W_{11}^{-1}w_{12}) = -sign(W_{11}^{-1}w_{12}) = -sign(\beta) = -\nu$, since $\theta_{22} > 0$. Also, we know $w_{12} = W_{11}\beta$, thus equations (6) and (8) are equivalent.

Algorithm

From equation (5) it can be seen that $w_{ii} = s_{ii} + \rho$ since $\theta_{ii} > 0\ \forall\ i$. Equation (4) is effectively Lasso regression with $X = W_{11}^{1/2}$ and $y = b = W_{11}^{-1/2}s_{12}$. Starting with $W = S + \rho I$, recursively solve for and replace each row/column of W, w_{12}, by inputting the rest of W, W_{11}, and the corresponding row/column of S, s_{12}, through Lasso regression until convergence.

FKG Inequality and MTP$_2$

There are many biological contexts, particularly in genetics, where certain types of correlation cannot be physically possible. In these situations, if the data suggests a physically inconsistent correlation, we know it is due to noise. These occurrences are referred to as unexpected correlations. Mathematically, these are any correlations that do not satisfy the Fortuin–Kasteleyn–Ginibre (FKG) inequalities. Fortuin *and others* (1971) state that if the FKG condition, $\mu(x \wedge y)\mu(x \vee y) \geq \mu(x)\mu(y)$, is met for some non-negative function μ and x, y in a finite distributive lattice X, then if f and g are monotonically increasing functions the FKG inequality states

$$[\sum_{x \in X} f(x)g(x)\mu(x)][\sum_{x \in X} \mu(x)] \geq [\sum_{x \in X} f(x)\mu(x)][\sum_{x \in X} g(x)\mu(x)]. \quad (9)$$

If $\mu(x)$ is a probability measure, this simply becomes

$$\mathrm{Cov}\big(f(x), g(x)\big) \geq 0. \quad (10)$$

Rinott and Scarsini (2006) state that a distribution whose probability measure fulfills the FKG condition is equivalently Multivariate Totally Positive of order 2 (MTP$_2$). This is important because Karlin and Rinott (1980) showed that when a density is MTP$_2$, then all off-diagonal elements of $\Theta = \Sigma^{-1}$ are non-positive. This then implies that all elements of W are non-negative.

Estimation of positive Σ

The construction of the previous algorithm does not break down with the additional condition that $w_{12} \geq 0$, since convexity remains. The only change that must be made is that the solution to the Lasso regression must be non-negative, $\beta \geq 0$. Augmentation of the Lasso algorithm into a Positive Lasso (pLasso) regression is not simple. However, both Lasso and pLasso are specific examples of Least Angle Regression (LAR). Efron *and others* (2004) describe the method by which LAR is used to calculate Lasso estimates and list the few changes necessary to instead calculate pLasso estimates.

New Algorithm

The LAR function in R was edited so that the Lasso option instead calculated pLasso estimates. The previous algorithm was then followed with a pLasso solution instead of a Lasso solution for β. To remove bias in particular locations in Σ that may arise from the order in which rows/columns are updated, the order is randomly selected. This new algorithm is named pLarso.

Example 1

$$n = 1000, \quad p = 10, \quad y_t = 0.6y_{t-1} + \epsilon_t, \quad \epsilon_t \sim N\left(0, \frac{1}{4}\right)$$

$$\Sigma^{-1}_{1-2,1-2} = \frac{1}{1-\rho^2}\begin{pmatrix} 1 & -\rho \\ -\rho & 1+\rho^2 \end{pmatrix} = \begin{pmatrix} 1.5625 & -0.9375 \\ -0.9375 & 2.1250 \end{pmatrix}$$

The above AR(1) time series was simulated using `arima.sim`, where n is the number of times series simulated and p is the length of each time series. Estimates of Σ^{-1} are found in Tables 1-3 in the Appendix. While gLasso results in some sparsity, the pLarso algorithm results in the sparsest estimate. The LAR algorithm results in no sparsity, but slightly better (less biased) estimates on the tri-diagonal.

Example 2

$$n = 10, \quad p = 20, \quad y_t = 0.6y_{t-1} + \epsilon_t, \quad \epsilon_t \sim N\left(0, \frac{1}{4}\right)$$

$$\Sigma^{-1}_{1-2,1-2} = \frac{1}{1-\rho^2}\begin{pmatrix} 1 & -\rho \\ -\rho & 1+\rho^2 \end{pmatrix} = \begin{pmatrix} 1.5625 & -0.9375 \\ -0.9375 & 2.1250 \end{pmatrix}$$

The same series is simulated in Example 2, but longer and with fewer replications. In this case S is not full rank and thus not invertible. Left half of estimates of Σ^{-1} are found in Tables 4-6 in the Appendix. In terms of sparsity, the results roughly match Example 1. However, actual estimates are now all inflated. Of course, for model selection (or network mapping) this is not a concern.

Example 3

$$n = 1000, \quad p = 10, \quad y_t = 0.6y_{t-1} - 0.2y_{t-2} + \epsilon_t, \quad \epsilon_t \sim N\left(0, \frac{1}{4}\right)$$

$$\Sigma^{-1}_{1-3,1-3} = \begin{pmatrix} 1.3889 & -0.8333 & 0.2778 \\ -0.8333 & 1.8889 & -1.0000 \\ 0.2778 & -1.0000 & 1.9444 \end{pmatrix}$$

An AR(2) time series was chosen for Example 3 to specifically have positive off-diagonal elements in Σ^{-1}. Estimates of Σ^{-1} are found in Tables 7-9 in the Appendix. Relative sparsity among the methods is similar to Example 1. However, the elements that should be equal to 0.2778 have been suppressed to zero by the pLarso algorithm.

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Appendix

Table 1: Inverse of output (estimate of Σ) of pLarso algorithm from Example 1

1.5056	-0.8674	0	-0.0238	-0.0194	0	-0.0010	0	0	0
-0.8674	2.0031	-0.8454	-0.0349	0	0	0	0	0	0
0	-0.8454	1.9612	-0.8272	0	0	0	0	0	0
-0.0238	-0.0349	-0.8272	1.9850	-0.8460	-0.0091	-0.0115	-0.0215	0	0
-0.0194	0	0	-0.8460	2.0249	-0.9069	0	0	0	0
0	0	0	-0.0091	-0.9069	1.9947	-0.8134	0	0	0
-0.0010	0	0	-0.0115	0	-0.8134	1.9847	-0.8990	0	0
0	0	0	-0.0215	0	0	-0.8990	2.0698	-0.9138	0
0	0	0	0	0	0	0	-0.9138	2.0441	-0.8744
0	0	0	0	0	0	0	0	-0.8744	1.4999

Table 2: Inverse of output (estimate of Σ) of gLasso algorithm from Example 1

1.4809	-0.8397	0	-0.0091	-0.0382	0	-0.0097	0	-0.0024	0.0173
-0.8397	1.9551	-0.8148	-0.0663	0.0412	0	0	0.0313	0	-0.0081
0	-0.8148	1.9154	-0.8007	0	0	0	0.003	0	0.0642
-0.0091	-0.0663	-0.8007	1.9527	-0.8263	-0.0116	-0.0072	-0.0508	0	0.0021
-0.0383	0.0412	0	-0.8263	1.972	-0.8746	0	0	0	0.0117
0	0	0	-0.0115	-0.8746	1.9486	-0.8006	-0.0049	0.02	0.0398
-0.0095	0	0	-0.0072	0	-0.8006	1.9493	-0.8617	-0.0321	0
0	0.0313	0.003	-0.0508	0	-0.0049	-0.8617	2.0168	-0.8829	0
-0.0024	0	0	0	0	0.02	-0.0321	-0.8829	2.0062	-0.8572
0.0173	-0.0081	0.0642	0.0021	0.0117	0.0398	0	0	-0.8572	1.4828

Table 3: Inverse of output (estimate of Σ) of LAR(Lasso) algorithm from Example 1

1.5122	-0.8854	0.0246	0.0007	-0.0766	0.0246	-0.0218	-0.0191	-0.0205	0.0596
-0.8854	2.0262	-0.8603	-0.0885	0.1069	-0.0544	0.0249	0.0691	-0.0143	-0.0533
0.0246	-0.8603	1.9704	-0.8416	0.0031	0.0340	-0.0358	0.0310	-0.0043	0.0841
0.0007	-0.0885	-0.8416	2.0316	-0.8790	0.0030	-0.0136	-0.0975	0.0309	0.0020
-0.0766	0.1069	0.0031	-0.8790	2.0346	-0.9404	0.0506	0.0249	-0.0373	0.0203
0.0246	-0.0544	0.0340	0.0030	-0.9404	2.0305	-0.8569	-0.0326	0.0745	0.0378
-0.0218	0.0249	-0.0358	-0.0136	0.0506	-0.8569	2.0056	-0.8820	-0.0480	-0.0107
-0.0191	0.0691	0.0310	-0.0975	0.0249	-0.0326	-0.8820	2.0810	-0.9454	0.0413
-0.0205	-0.0143	-0.0043	0.0309	-0.0373	0.0745	-0.0480	-0.9454	2.0916	-0.9110
0.0596	-0.0533	0.0841	0.0020	0.0203	0.0378	-0.0107	0.0413	-0.9110	1.5145

Table 4: Inverse of output (estimate of Σ) of pLarso algorithm from Example 2

3.1462	-1.6959	0	-0.9301	0	0	0	0	0	0
-1.6959	4.3236	-2.3663	0	0	0	0	0	0	0
0	-2.3663	5.6203	-3.0561	0	0	0	0	0	-0.0024
-0.9301	0	-3.0561	7.9218	-3.7612	0	-0.1505	0	0	-0.2735
0	0	0	-3.7612	12.3947	-5.0724	-3.6257	-0.1499	0	0
0	0	0	0	-5.0724	7.9446	-1.9011	-0.6035	0	0
0	0	0	-0.1505	-3.6257	-1.9011	6.1417	0	0	0
0	0	0	0	-0.1499	-0.6035	0	3.4113	-1.1010	-1.5233
0	0	0	0	0	0	0	-1.1010	3.1324	-0.0589
0	0	-0.0024	-0.2735	0	0	0	-1.5233	-0.0589	3.4171
0	0	0	0	0	0	0	0	-1.7624	0
0	0	0	0	0	0	0	-0.0602	0	0
0	0	0	0	0	0	0	0	0	-1.3757
0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0
-0.2797	0	0	0	0	0	-0.1543	0	0	0
-0.0206	0	0	0	0	0	0	-0.0615	0	0
0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	-0.4159	0	0	0	-0.2128

Table 5: Inverse of output (estimate of Σ) of gLasso algorithm from Example 2

12.4188	-2.2936	0	-4.3120	-1.3956	0.3457	0	0	-2.3488	0	-0.4647
-2.2901	21.3005	-9.7546	-4.2540	0	1.1153	0	0	0	-2.6434	0
0	-9.7495	17.1178	-5.4848	0	-2.8118	0.8760	-0.1900	0	-0.0736	0
-4.3185	-4.2598	-5.4758	25.9561	-9.4632	0	-5.2095	0	-1.5316	-2.3697	0
-1.3950	0	0	-9.4680	27.3717	-7.4723	-8.2166	-0.6053	-1.3006	0	0
0.3475	1.1152	-2.8112	0	-7.4735	14.8091	-4.0524	-3.9312	1.7541	1.9021	0
0	0	0.8761	-5.2063	-8.2156	-4.0508	21.0457	-1.0232	-2.2429	-0.5392	5.4366
0	0	-0.1879	0	-0.5995	-3.9325	-1.0232	14.8466	-2.6279	-5.8466	0
-2.3540	0	0	-1.5377	-1.3021	1.7544	-2.2417	-2.6212	15.3517	-4.0624	-10.7217
0	-2.6317	-0.0701	-2.3598	0	1.8989	-0.5435	-5.8612	-4.0648	16.5843	2.2512
-0.4608	0	0	0	0	0	5.4356	0	-10.7223	2.2511	15.4004
5.0436	0	0	2.4875	0	-0.5356	0.1337	-8.6657	0	0	-1.4524
-4.6434	0.6056	0.0274	0	0	1.5573	3.3219	-0.0342	3.0835	-6.4215	0.2777
-0.0822	7.0133	4.1396	-0.5415	-2.1777	0	-3.8107	1.3228	-4.0411	0	-1.4936
4.6626	0	-2.9576	0	2.8172	-3.2526	0	0	0	-0.8269	0
-3.9862	-1.4158	-1.1618	0	2.3633	-1.4629	0	1.3935	2.8937	1.4392	0
-1.4356	0.5976	1.8082	2.7794	0	-2.2560	-2.3517	-5.1910	0.4580	4.2709	2.7320
0	0	-0.3258	0.9714	2.2396	1.6001	0	-1.9013	-0.7353	-3.8471	0
-1.1481	4.5271	-5.9532	0	-0.6741	-1.8757	4.8312	0	0.7229	1.9416	-4.3819
2.2297	3.5357	0	-0.1363	-4.2406	-0.7215	-0.5071	2.4460	1.6405	-4.8341	3.3250

Table 6: Inverse of output (estimate of Σ) of LAR(Lasso) algorithm from Example 2

48.1578	-7.7932	-5.0459	-15.1693	-11.0201	0.9645	0.7606	4.0984	-4.1538	1.4590
-7.7932	67.2252	-26.6232	-13.8947	1.9417	2.8044	-1.3338	-2.3469	-1.7653	-9.9177
-5.0459	-26.6232	58.9937	-14.8519	-3.2736	-13.8538	5.3595	-2.2720	2.6667	-3.0253
-15.1693	-13.8947	-14.8519	78.2234	-17.0745	-8.8387	-15.2151	2.0243	-10.0855	-9.4562
-11.0201	1.9417	-3.2736	-17.0745	74.8705	-20.3087	-20.4840	-5.1971	-5.4564	-1.9678
0.9645	2.8044	-13.8538	-8.8387	-20.3087	59.7051	-16.2666	-16.3593	7.1587	12.8059
0.7606	-1.3338	5.3595	-15.2151	-20.4840	-16.2666	67.1612	-6.5885	-7.2983	-6.6760
4.0984	-2.3469	-2.2720	2.0243	-5.1971	-16.3593	-6.5885	54.9394	-9.2780	-14.5028
-4.1538	-1.7653	2.6667	-10.0855	-5.4564	7.1587	-7.2983	-9.2780	51.3849	-13.4897
1.4590	-9.9177	-3.0253	-9.4562	-1.9678	12.8059	-6.6760	-14.5028	-13.4897	57.0630
-8.0142	3.8772	-5.0645	0.7572	3.4042	3.1238	16.2758	-2.7773	-33.2528	7.8932
18.7914	3.0152	-0.2792	9.7340	2.4974	-10.9708	6.1105	-30.5868	1.4801	-5.8783
-25.3290	4.3730	5.2105	1.5217	1.5109	9.8152	13.4171	-10.3438	12.1243	-23.2735
-3.9013	24.4030	22.2877	-0.7869	-8.5631	-5.3765	-11.8773	5.0786	-15.9954	-0.3308
19.0854	-0.8155	-11.2107	1.5385	7.3093	-10.3446	-0.0212	0.3292	-0.0470	-4.7142
-12.7529	-4.3020	-8.3663	-1.0655	6.3405	-10.1591	1.7865	8.5694	12.4548	9.5291
-11.8628	9.3376	10.3273	8.6901	-2.2537	-13.5452	-5.9670	-19.8709	8.3076	12.8394
2.1157	-2.5330	-3.3761	5.6058	13.5272	7.8011	0.9834	-9.1342	-8.8499	-16.8759
-4.0501	12.5220	-17.1694	2.6200	-4.0855	-12.8830	19.9055	1.0409	2.6759	8.6921
12.0444	13.4060	-2.1185	-5.8498	-12.2300	-4.3127	-5.0086	11.2673	9.2006	-16.6991

Table 7: Inverse of output (estimate of Σ) of pLarso algorithm from Example 3									
1.3069	-0.6289	0	0	0	0	0	0	0	-0.1058
-0.6289	1.6542	-0.6954	0	0	0	0	0	0	0
0	-0.6954	1.7141	-0.7035	0	0	0	0	0	0
0	0	-0.7035	1.6551	-0.6216	0	0	0	0	0
0	0	0	-0.6216	1.6447	-0.6907	0	0	0	0
0	0	0	0	-0.6907	1.6807	-0.6671	0	0	0
0	0	0	0	0	-0.6671	1.5809	-0.5633	0	0
0	0	0	0	0	0	-0.5633	1.5764	-0.6615	0
0	0	0	0	0	0	0	-0.6615	1.6329	-0.6367
-0.1058	0	0	0	0	0	0	0	-0.6367	1.3130

Table 8: Inverse of output (estimate of Σ) of gLasso algorithm from Example 3									
1.3273	-0.7062	0.1331	0.0902	0.0217	0.0300	-0.0160	0	0	-0.1052
-0.7062	1.7510	-0.8903	0.1947	-0.0225	0	-0.0189	-0.0069	0	0.0181
0.1331	-0.8903	1.8632	-0.9085	0.1769	0	0.0323	-0.0061	-0.0091	0
0.0902	0.1947	-0.9085	1.8301	-0.8590	0.2338	0.0858	0	0.0180	0
0.0217	-0.0225	0.1768	-0.8590	1.8217	-0.9312	0.1624	0.0282	-0.0227	0.0112
0.0300	0	0	0.2338	-0.9312	1.8389	-0.8254	0.1019	0.0757	-0.0680
-0.0160	-0.0189	0.0323	0.0858	0.1624	-0.8254	1.6862	-0.7145	0.1710	-0.0050
0	-0.0069	-0.0061	0	0.0282	0.1019	-0.7145	1.6929	-0.8663	0.2367
0	0	-0.0091	0.0180	-0.0227	0.0757	0.1710	-0.8663	1.7584	-0.7511
-0.1052	0.0181	0	0	0.0112	-0.0680	-0.0050	0.2367	-0.7511	1.3351

Table 9: Inverse of output (estimate of Σ) of LAR(Lasso) algorithm from Example 3									
1.3636	-0.7635	0.1868	0.0677	0.0363	0.0577	-0.0341	-0.0036	0.0380	-0.1480
-0.7635	1.8423	-0.9974	0.2908	-0.1062	0.0257	-0.0422	0.0045	-0.0236	0.0593
0.1868	-0.9974	1.9848	-1.0347	0.3037	-0.0890	0.0920	-0.0317	-0.0312	0.0014
0.0677	0.2908	-1.0347	1.9597	-0.9895	0.3457	0.0388	-0.0067	0.0996	-0.0621
0.0363	-0.1062	0.3037	-0.9895	1.9463	-1.0503	0.2236	0.0500	-0.1194	0.0899
0.0577	0.0257	-0.0890	0.3457	-1.0503	1.9554	-0.9082	0.1290	0.1201	-0.1183
-0.0341	-0.0422	0.0920	0.0388	0.2236	-0.9082	1.7738	-0.7969	0.2346	-0.0417
-0.0036	0.0045	-0.0317	-0.0067	0.0500	0.1290	-0.7969	1.7886	-0.9662	0.3093
0.0380	-0.0236	-0.0312	0.0996	-0.1194	0.1201	0.2346	-0.9662	1.8596	-0.8259
-0.1480	0.0593	0.0014	-0.0621	0.0899	-0.1183	-0.0417	0.3093	-0.8259	1.3825