

Case Study 3: fMRI Prediction

Graphical LASSO

Machine Learning/Statistics for Big Data
CSE599C1/STAT592, University of Washington

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Multivariate Normal Models

- So far, we looked at the univariate multiple regression

- If one has a multivariate response $y^i \in \mathbb{R}^d$
 - Assuming independence between dimensions

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Multivariate Normal Models

- If one has a multivariate response $y^i \in \mathbb{R}^d$
 - Assuming correlation between the output dimensions
- Assume linear (or other mean regression) is removed and focus on the correlation structure
- Matrix valued parameter!

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High-Dimensional Covariance

- What if d is large?
- A few common approaches:
 - Low-rank approximations
 - Sparsity assumptions

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Low-Rank Approximations

- In general, assume some matrix parameter
- Here, Σ must be a symmetric, positive definite matrix

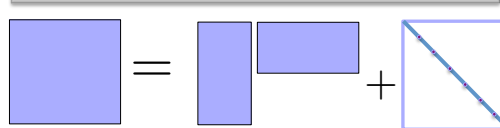
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Low-Rank Approximations

- In pictures...

$$\Sigma_0 = \text{diag}(\sigma_1^2, \dots, \sigma_d^2)$$

$$\Sigma = \Lambda \Lambda' + \Sigma_0$$


- Number of parameters:

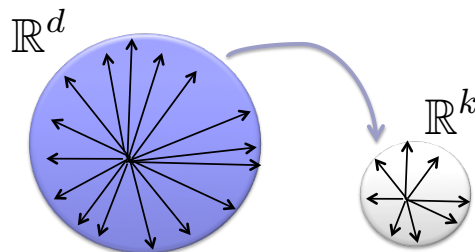
Latent Factor Models

- Low-rank approximation arises from a latent factor model

- Proof:

Lower-dim Embeddings

Sharing information in
low-dim subspace



Sparsity Assumptions

- What if we assume Σ is sparse?
- More often, we can reasonably make statements about *conditional independence*

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Information Form

- Motivations for considering “information form” of multivariate normal
 - Easier to read off conditional densities
 - Has log-linear form in terms of “information parameters”

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Conditional Densities

- Assume a model with

and divide the dimensions into two sets

- Then,

Conditional Densities

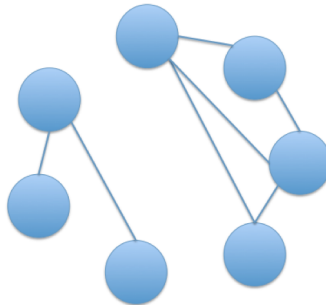
- Let $A = \{s, t\}$

$$p(y_A \mid y_{\bar{A}}) = \mathcal{N}^{-1}(\eta_A - \Omega_{A\bar{A}}y_{\bar{A}}, \Omega_{AA})$$

- Therefore,

Connection with Graphical Models

- Undirected graphical model or Markov random field (MRF)



$$p(y | \eta, \Omega) \propto \prod_t \psi_t(y_t) \prod_{(s,t) \in E} \psi_{st}(y_s, y_t) \quad \psi_t(y_t) \propto e^{\eta_t y_t}$$

$$\psi_{st}(y_s, y_t) \propto e^{-\frac{1}{2} y_s \Omega_{st} y_t}$$

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Sparse Precision vs. Covariance

- For a sparse precision matrix, the covariance need not be

```

MATLAB R2012a
Current Folder: /Users/ebfox/Documents/Research/General_toolboxes/HW

>> Omega
Omega =
    5.0000    0    -1.3731    0    0.7988    0.9681    0    -0.8558    0    0
    0    3.3483    1.5783    -1.6742    0    -0.5654    0    -1.1826    0    0
   -1.3731    1.5783    2.9305    0.9951    0    0    -0.6900    -1.2806    0.7026    0
    0    -1.6742    0.9951    6.0197    0    0    0    0    0    -0.5798
    0.7988    0    0    4.0541    0    0    0    0.8074    0    0
    0.9681    -0.5654    0    0    0    5.0000    0    0    -1.1253    0
   -0.8558    -1.1826    0    0    0.8074    0    5.6526    0.8674    0    0
    0    0    -1.2806    0    0.8074    0    0.8674    5.0000    -1.5453    0
    0    0    0.7026    0    -1.1253    0    -1.5453    5.8288    -1.1129    5.0000
    0    0    0    -0.5798    0    0    0    -1.1129    5.0000

>> Sigma = inv(Omega)
Sigma =
    0.3730    -0.2560    0.4290    -0.1448    -0.0947    -0.1125    0.0360    0.1066    -0.0505    -0.0280
   -0.2560    0.9071    -0.7903    0.3906    0.0453    0.1866    -0.1004    0.0258    0.1533    0.0794
    0.4290    -0.7903    1.2528    -0.4354    -0.1147    -0.2103    0.1297    0.1514    -0.1682    -0.0879
   -0.1448    0.3906    -0.4354    0.3523    0.0319    0.0894    -0.0506    -0.0167    0.0764    0.0578
   -0.0947    0.0453    -0.1147    0.0319    0.2814    0.0229    -0.0016    -0.0808    -0.0026    0.0031
   -0.1125    0.1866    -0.2103    0.0894    0.0229    0.2609    -0.0251    -0.0035    0.0802    0.0282
    0.0360    -0.1004    0.1297    -0.0506    -0.0016    -0.0251    0.1970    -0.0276    -0.0302    -0.0126
   -0.1066    0.0258    0.1514    -0.0167    -0.0808    -0.0035    -0.0276    0.3005    0.0630    0.0121
   -0.0505    0.1533    -0.1682    0.0764    -0.0026    0.0802    -0.0302    0.0630    0.2357    0.0613
   -0.0280    0.0794    -0.0879    0.0578    0.0031    0.0282    -0.0126    0.0121    0.0613    0.2204

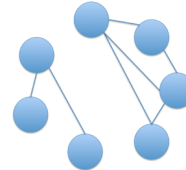
fj >>
  
```

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ML Estimation for Given Graph

- Assume a known graph $G = \{V, E\}$
- Rewrite log likelihood:



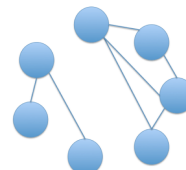
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ML Estimation for Given Graph

$$L(\Omega) = \log |\Omega| - \text{tr}(S\Omega)$$

- Take gradient:



- Many approaches to solving:
 - Barrier method – add penalty if Ω leaves the positive definite cone (Dahl et al. 2008)
 - Coordinate descent method (cf., Hastie et al. 2009)
 - ...

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ML Estimation for Given Graph

- Can show that the optimal solution satisfies

- Example:

$$G = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix} \quad S = \begin{pmatrix} 10 & 1 & 5 & 4 \\ 1 & 10 & 2 & 6 \\ 5 & 2 & 10 & 3 \\ 4 & 6 & 3 & 10 \end{pmatrix}$$

$$\Omega = \begin{pmatrix} & & 0 & \\ & & & 0 \\ 0 & & & \\ & 0 & & \end{pmatrix} \quad \Sigma = \begin{pmatrix} 10 & 1 & & 4 \\ 1 & 10 & 2 & \\ & 2 & 10 & 3 \\ 4 & & 3 & 10 \end{pmatrix}$$

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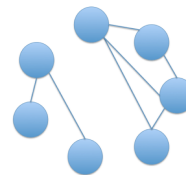
Estimating Graph Structure

- To learn the structure of the Gaussian graphical model, we want to trade off fit and sparsity

- Measure of fit:

- Encouraging sparsity:

- Overall objective = “graphical LASSO” or “Glasso”



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Solving the Graphical LASSO

- Objective is convex, but non-smooth as in LASSO
- Also, positive definite constraint!

- There are many approaches to optimizing the objective
 - Most common = coordinate descent akin to shooting algorithm (Friedman et al. 2008)

- Some issues...
 - Ballpark: several minutes for a 1000-variable problem
 - Algorithms scale as $O(d^3)$

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Faster Computations

From Daniela Witten's talk at JSM 2012:

1. The j th variable is unconnected from all others in the graphical lasso solution if and only if $|S_{ij}| \leq \lambda$ for all $i = 1, \dots, j-1, j+1, \dots, p$.
2. Let \mathbf{A} denote the $p \times p$ matrix whose elements take the form $A_{ij} = 1, A_{ij} = 1_{|S_{ij}| > \lambda}$. Then the connected components of \mathbf{A} are the same as the connected components of the graphical lasso solution.

We can obtain the *exact* right answer by solving the graphical lasso on each connected component separately!

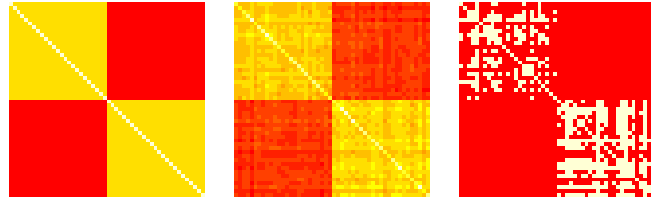
Citations: Witten et al. JCGS 2011, Mazumder and Hastie JMLR 2012

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Covariance Screening for Glasso

From Daniela Witten's talk at JSM 2012:



- ▶ The solution to the graphical lasso problem with $\lambda = 0.7$ has five connected components (why 5?!)
- ▶ Perform graphical lasso on each component separately!
- ▶ **Reduction in computational time:** From $O(50^3)$ to $O(24^3)$.