Mixed Graphical Models

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Outline

- Markov Random Fields
- The Exponential Family
- Mixed Graphical Models
- Learning the Structure of Mixed Graphs
- Simulation Study
- Real World Applications

Historical Background

Define $G = (V, E)$ as the undirected graph over $X = (X_1, \ldots, X_p)$ with node set $V = \{1, \ldots, p\}$ and edge set $E = V \times V$. Note that X is a p-dimensional random vector with each variable taking values in a set $\mathcal{X}_r$.

Besag (1974) showed that a joint distribution can be fully specified in terms of node-neighborhood conditional distributions.

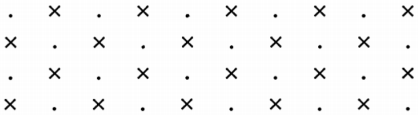


FIG. 1. Coding pattern for a first-order scheme.

$$\prod p_{i,j}(x_{i,j};\, x_{i-1,j}, x_{i+1,j}, x_{i,j-1}, x_{i,j+1}),$$

Exponential MRF's

Theorem (Besag 1974 + Hammersley-Clifford + Yang 2014)

If X has marginal distributions arising from the exponential family and satisfies the Markov independence property then the joint distribution can factorized over the set maximal cliques $\mathcal{C}$ of the graph G.

Let $\phi_c(X_c)$ be a sufficient statistic dependent on the X_c that correspond to the clique $c \in \mathcal{C}$, then the Markov Random Field (MRF) family of distributions has the form:

$$P(X) \propto \exp\left\{ \sum_{c \in \mathcal{C}} \phi_c(X_c) \right\}$$

The Exponential Family

Denote a random variable Z with distribution that is a member of the exponential family as $Z \in \mathcal{F}$. These distributions have the form

$$P(Z) = \exp\left\{\eta^T B(Z) + C(Z) - D(\eta)\right\}$$

with canonical parameter η, sufficient statistics $B(Z)$, base measure $C(Z)$, and log-partition function $D(\eta)$.

- What is the natural parameter space $\mathcal{N} = \{\eta : D(\eta) < \infty\}$?
- Note that in general given a set Θ, we can write $\eta = \eta(\theta)$ where $\eta : \Theta \to \mathcal{N}$ is a bijection.

Mixed Exponential MRF's

Graphical Models via Univariate Exponential Family Distributions (Yang et al. 2012)

For node $r \in V$, consider the distribution of X_r conditioned on the remaining $p-1$ random variables $X_{V\setminus r}$. Note that $\eta_r \equiv \eta_r(X_{V\setminus r}, \theta)$.

$$P(X_r | X_{V\setminus r}) = \exp\left\{\eta_r B_r(X_r) + C_r(X_r) - D_r(\eta_r)\right\}$$

Mixed Graphical Models via Exponential Families (Yang et al. 2014)

- What if each conditional distribution came from a unique distribution in $\mathcal{F}$?
- What restrictions would this impose on $\mathcal{N}$?

Theorem (Mixed Exponential MRF - Yang et al. 2014)

The collection of $P(X_r|X_{V\setminus r}) \in \mathcal{F}$ form a pairwise MRF over the random vector X that is Markov with respect to the graph $G = (V, E)$ if and only if the functions $\{\eta_r(\cdot)\}_{r\in V}$ that specify the conditional distributions have the form:

$$\theta_r + \sum_{(r,t)\in E} \theta_{rt} B_t(X_t)$$

With corresponding joint distribution

$$P(X) = \exp\left\{ \sum_{r\in V} \theta B_r(X_r) + \sum_{(r,t)\in E} \theta_{rt} B_r(X_r) B_t(X_t) + \sum_{r\in V} C_r(X_r) - A(\theta) \right\}$$

with log-partition function

$$A(\theta) = \log \int_X \exp\left\{ \sum_{r\in V} \theta_r B_r(X_r) + \sum_{(r,t)\in E} \theta_{rt} B_r(X_r) B_t(X_t) + \sum_{r\in V} C_r(X_r) \right\} dX$$

Mixed Exponential MRF - Consider the possibilities!

Here are some examples, assuming the data is properly transformed

1. Gaussian-Multinomial:
    - Flight delays and weather condition (categorical)
2. Poisson-Bernoulli:
    - Gene expression and mutation state (binary)
3. Exponential-Bernoulli
    - Application use duration and membership status (binary)

Gaussian-Potts Model

Let $\{ Y_r\}$ be a set of univariate Gaussian random variables with domain $\mathcal{Y} = \mathbb{R}$ and known variance σ_r^2. Additionally, let $\{Z_r\}$ be a set of multinomial random variables taking values in the finite set $\mathcal{Z}_r = \{0, 1, 2, \ldots\}$.

$\mathcal{F}$	$B(\cdot)$	$C(\cdot)$
Gaussian	$\frac{Y_r}{\sigma_r}$	$-\frac{Y_r^2}{2\sigma_r^2}$
Multinomial	$\mathbb{I}[\, Z_r = j\,]$	0

Let (V_Y, E_Y), (V_Z, E_Z), and (V_{YZ}, E_{YZ}) be the two homogeneous sub-graphs and the heterogeneous sub-graph respectively.

Marginally we have a Gaussian graphical model and a Potts model!

Gaussian-Potts Model

Prepare your eyes!

Gaussian-Potts Model - A "*Manichean*" MRF

Parameters:

- $\theta \leftrightarrow$ Multinomial node potential
- $\alpha \leftrightarrow$ Gaussian node potential
- $\lambda \leftrightarrow$ Cross type potential

Identity Functions:

- $\mathcal{I}^{j}_{r'} = \mathbb{I}[\, Z_{r'} = j\,]$
- $\mathcal{I}^{jk}_{(r',t')} = \mathbb{I}[\, Z_{r'} = j\,,\; Z_{t'} = k\,]$

Joint density:

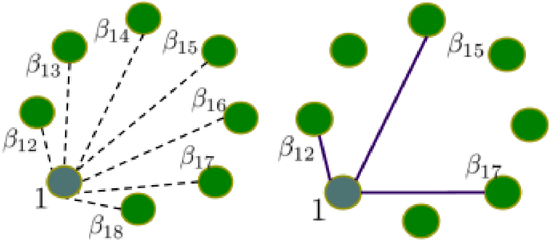
$$P(Y, Z) \propto \exp\left\{ \sum_{\substack{r' \in V_Z \\ j \in \mathcal{Z}}} \theta^{j}_{r'}\, \mathcal{I}^{j}_{r'} + \sum_{\substack{(r',t') \in E_Z \\ j,k \in \mathcal{Z}}} \theta^{jk}_{r't'}\, \mathcal{I}^{jk}_{(r,r')} + \sum_{\substack{(r,r') \in E_{YZ} \\ j \in \mathcal{Z}}} \lambda_{rr'}\, Y_r\, \mathcal{I}^{j}_{r'} \right.$$
$$\left. + \sum_{r \in V_Y} \alpha_r Y_r + \sum_{(r,t) \in E_Y} \frac{\alpha_{rt}}{\sigma_r \sigma_t} Y_r Y_t - \sum_{r \in V_r} \frac{Y_r^2}{2\sigma_r^2} \right\}$$

Parameter Estimation For Homogeneous MRF's

1. Gaussian Graphical Models
    - Node-neighborhood (Meinshausen and Bühlmann 2006)
    - Graphical Lasso (Hastie and Tibshirani 2008), (Friedman et al. 2008)
2. Ising/Potts Models
    - Node-neighborhood (Ravikumar et al. 2010)
    - Group Penalized Lasso (Jalali et al. 2011)

Parameter Estimation: Intuition

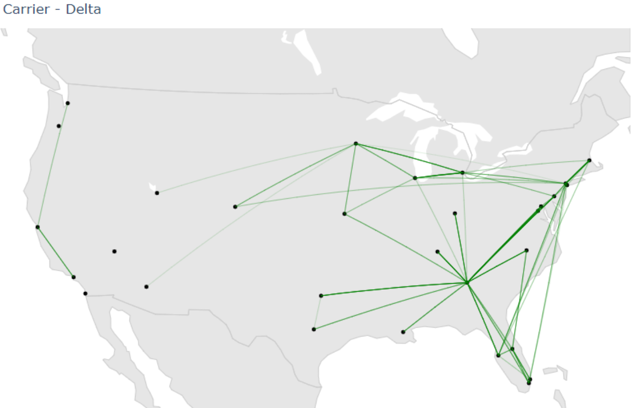
$$\log\det\Theta - \operatorname{tr}(S\Theta) - \rho||\Theta||_1,$$

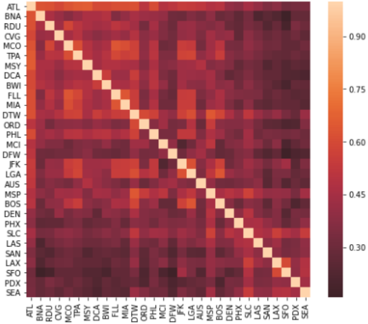


$$\beta^*_{ij} = \max\{\beta_{ij}, \beta_{ji}\}$$

Credit: Hastie and Tibshirani (2008) and CMU Lecture notes: 10-708 PGMs

Parameter Estimation: Intuition





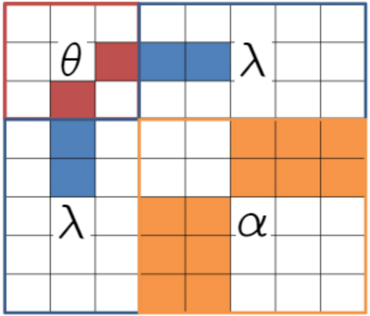
Learning the Structure of Mixed Graphical Models (Lee and Hastie 2014)

- Object of interest $\boldsymbol{\Theta} = \{\theta, \alpha, \lambda\}$
- Maximum likelihood estimation is hard - $D(\eta_r)$

Pseudolikelihood (Besag 1975):

$$\tilde{\ell}(\boldsymbol{\Theta} \mid y, z) = -\sum_{r}^{p} \log p(y_r \mid y_{\setminus r},\ z\,; \boldsymbol{\Theta}) - \sum_{r'}^{q} \log p(z_{r'} \mid z_{\setminus r'},\ y\,; \boldsymbol{\Theta})$$

Estimation: Gaussian-Potts



Symmetric matrix represents the parameters Θ *of the model.*

Credit: Lee and Hastie 2014

Parameter Estimation: Gaussian-Potts

Partition $X = (Y, Z)$ where there are p Gaussian and q Multinomial nodes

1. $\theta_{rt} = 0 \iff X_r \perp X_t \,|\, (X_{V\setminus\{r,t\}},\ Z)$
2. $\lambda_{rr'} = 0$ for all $\mathcal{Z}_{r'} \iff X_r \perp Z_{r'} \,|\, (X_{V\setminus r},\ Z_{V\setminus r'})$
3. $\alpha_{r't'} = 0$ for all values in $\mathcal{Z}_{r'}$ and $\mathcal{Z}_{t'} \iff X_r \perp Z_{r'} \,|\, (Z_{V\setminus\{r',t\}},\ Y)$

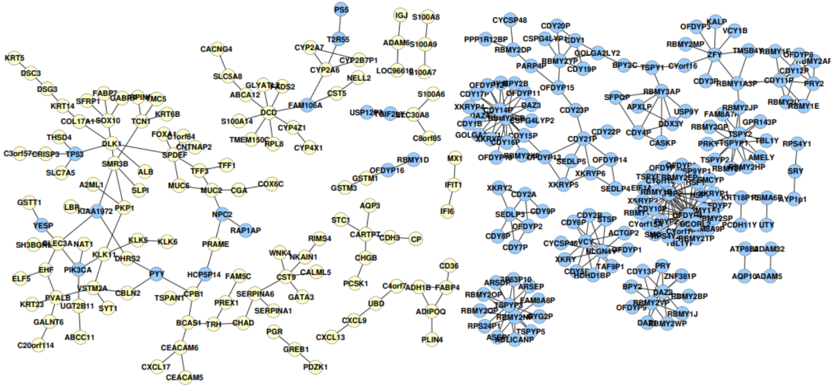
Group-Lasso (Uncalibrated):

$$\min_{\Theta} \ell_\omega(\Theta) = \ell(\Theta) + \omega\left(\sum_{r=1}^{p} \sum_{t=1}^{r-1} |\theta_{rt}| + \sum_{r=1}^{p} \sum_{r'=1}^{q} \|\lambda_{rr'}\|_2 + \sum_{r'=1}^{q} \sum_{t'=1}^{r'-1} \|\alpha_{r't'}\|_F \right)$$

Remaining Work

- Simulation studying comparing the node-neighborhood selection estimation procedure with the group-lasso proposed by Lee and Hastie (2014).
- Test model on real world data
- Spend too much time on network visualization

Questions?



Breast cancer genetic network (Poisson-Ising) Credit: Yang et al. 2014

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