Mixed Graphical Models via Exponential Families

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Graphical Models : Introduction

- A **multivariate distribution** over a large number of variables can be represented using a graph $G = (V, E)$ (with $|V| = p$)
- Graph Nodes $i \in V$ correspond to **random variables** X_i
- Graph Edges E encode
  - Correlations?
  - Causations?
  - **Markov Independence** Relationships!

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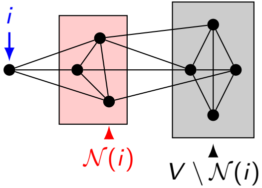
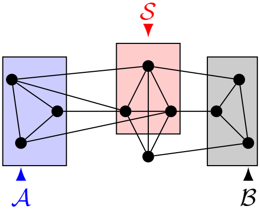


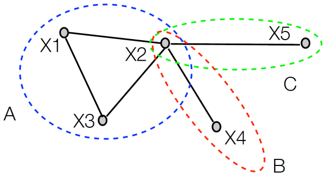


$X_i \perp\!\!\!\perp X_{V \setminus \mathcal{N}(i)} \mid X_{\mathcal{N}(i)}$ $\quad$ $X_{\mathcal{A}} \perp\!\!\!\perp X_{\mathcal{B}} \mid X_{\mathcal{S}}$

Graphical Models: Factorization

- (Hammersley-Clifford theorem) Joint dist. is the product of **local factors**: each of which depends only on a clique

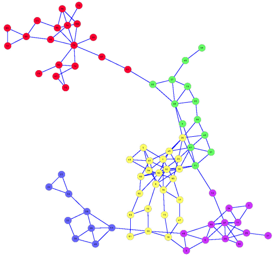
$$P(X) = \frac{1}{Z}\Psi_A(X_A)\Psi_B(X_B)\Psi_C(X_C)$$



MRFs for Categorical Data

- **Categorical data:** $X_s \in \{0, 1, ..., K\}$
- **Potts Model:**

$$\mathbb{P}(X) \propto \exp\left\{ \sum_{(s,t)\in E} \theta_{st} \, \mathbb{I}(X_s = X_t) \right\}$$

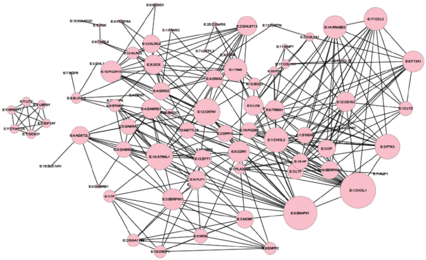


- Other Discrete Data MRFs: Ising MRF, Overcomplete Discrete MRF
- Applications: Internet data, Genomics data, Image processing, Marketing, Statistical physics, ...

MRFs for Thin-tailed Continuous Data

- **(Thin-tailed) Continuous data:** $X_s \in \mathbb{R}$
- **Gaussian MRFs:**

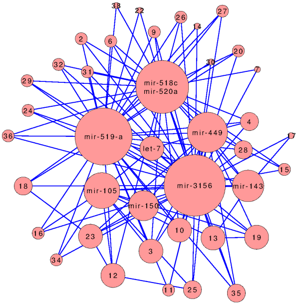
$$\mathbb{P}(X) \propto \exp\left\{ -\frac{1}{2}\langle\langle \Theta, XX^T \rangle\rangle + \langle \theta, X \rangle \right\}$$



MRFs for Count-valued Data

- **Count data:** $X_s \in \{0, 1, \ldots\}$
- **Poisson MRFs:** (Yang et al., 2012,13)

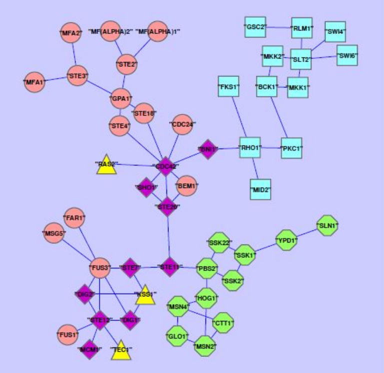
$$\mathbb{P}(X) \propto \exp\left\{ \sum_s \theta_s X_s + \sum_{(s,t)\in E} \theta_{st}\, X_s\, X_t - \sum_s \log(X_s!) \right\}$$



Mixed Data

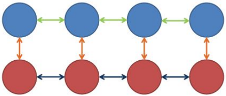
- What if we jointly observe heterogeneous/mixed variables of many **different types?**

  - SNPs: discrete data
  - Gene Expression: continuous data
  - RNA sequencing: count data
  - Genomic Mutations: binary data



- Need multivariate MRFs that permit **dependencies over mixed variables**!

Existing Models for Mixed Data Types



- Limited to **Gaussian-Discrete** case: a continuous random vector, conditioned on a discrete random vector, distributed as multivariate Gaussian.
  - Formulated by Lauritzen (1996), where they called these "conditional Gaussian MRFs"
  - Structure can be learnt tractably (Lee and Hastie (2012))
  - Extension to three-way interactions (Cheng, Levina, Zhu (2012))

Extending Heterogenous Univariate Distributions to Multivariate Graphical Models

- Need a general class of mixed graphical models
- **(KEY QUESTION)** Can we go systematically **from heterogenous univariate dist.** to **multivariate mixed MRFs**?

Review: Exponential Families

- Most common **univariate** distributions: Gaussian, Exponential, Bernoulli, Binomial, Poisson, Negative binomial, ...
- A broad class of distributions sharing a certain form:

$$P(X;\theta) = \exp\left\{\sum_{i\in\mathcal{I}} \theta_i B_i(X) + C(X) - A(\theta)\right\}$$

- Ingredients:

$\theta = \{\theta_i\}_{i\in\mathcal{I}}$	Parameters
$B(X) = \{B_i(X)\}_{i\in\mathcal{I}}$	Sufficient statistics
$C(X)$	Base measure
$A(\theta) = \log\left\{\sum_X \exp\langle\theta, B(X)\rangle + C(X)\right\}$	Log-partition function

Heterogeneous Univariate Exponential Families $\rightarrow$ Mixed Graphical Models

- We know
  - Gaussian graphical models: each X_s is Gaussian dist. given all neighbors
  - Ising models: each X_s is Bernoulli dist. given all neighbors
  - Poisson models: each X_s is Poisson dist. given all neighbors
- Introduce a new class of graphical models:
  - Given $X_{V \setminus s}$, each variable X_s follows a **potentially different** univariate exponential family distribution of choice
  - Dependencies between $(X_1, ..., X_p)$ modeled via graphical model structure.

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What form would such a joint distribution take — if any?

Mixed Exponential Family Markov Random Fields

- The most **general** assumptions:
  - Allow **heterogenous** node-conditional distributions:

$P(X_s \mid X_{V\setminus s})$	$=$	$\exp\{E_s(X_{V\setminus s})\, B_s(X_s) + C_s(X_s) - \bar{A}_s(X_{V\setminus s})\}$
$E_s(X_{V\setminus s})$		Parameters
$B_s(X)$		Sufficient statistics
$C_s(X)$		Base measure
$\bar{A}_s(\theta)$		Log-partition function

  - Joint distribution over X given by a graphical model with **factors of size** $\leq k$

$$P(X) \propto \prod_{c \in \mathcal{C}} \Psi_c(X_c).$$

Mixed Exponential Family Markov Random Fields

Theorem

Under the previous general conditions that (a) the node conditional distributions belong to exponential families and (b) the joint is a graphical model with factors of size at most k,

Joint dist. **necessarily** *has the following form:*

$$P(X) = \exp\Bigg\{ \sum_{s} \theta_s B_s(X_s) + \sum_{s\in V} \sum_{t\in N(s)} \theta_{st} \, B_s(X_s) B_t(X_t) + \ldots$$
$$+ \sum_{s\in V} \sum_{t_2,\ldots,t_k \in N(s)} \theta_{s\ldots t_k} \, B_s(X_s) \prod_{j=2}^{k} B_{t_j}(X_{t_j}) + \sum_{s} C_s(X_s) - A(\theta) \Bigg\}$$

Multivariate Graphical Models for Different Types

- Given multiple variables of varied types, only need to specify k, $\{B_s(X)\}_{s \in V}$ and $\{C_s(X)\}_{s \in V}$
- Some could be **time interval** data: time spent on website, networks call time, etc., yet others could be **count** data: incident reports, websites visit counts, next generation genomic data based on RNA fragment counts, etc.), and so on
- The mixed MRF would provide a **joint distribution** over all of these heterogeneous random variables.

Examples: Mixed MRFs with Two Data Types

- Gaussian - Ising Graphical Models

$$P(Y,Z) \propto \exp\Big\{ \sum_{s \in V_Y} \frac{\theta_s^Y}{\sigma_r} Y_s + \sum_{s' \in V_Z} \theta_{s'}^z Z_{s'} + \sum_{(s,t) \in E_Y} \frac{\theta_{st}^{yy}}{\sigma_r \sigma_t} Y_s Y_t + \sum_{(s',t') \in E_Z} \theta_{s't'}^{zz} Z_{s'} Z_{t'} + \sum_{(s,s') \in E_{YZ}} \frac{\theta_{ss'}^{yz}}{\sigma_r} Y_s Z_{s'} - \sum_{s \in V_Y} \frac{Y_s^2}{2\sigma_r^2} \Big\}.$$

- Poisson - Ising Graphical Models

$$P(Y,Z) \propto \exp\Big\{ \sum_{s \in V_Y} \theta_s^Y Y_s + \sum_{s' \in V_Z} \theta_{s'}^z Z_{s'} + \sum_{(s,t) \in E_Y} \theta_{st}^{yy} Y_s Y_t + \sum_{(s',t') \in E_Z} \theta_{s't'}^{zz} Z_{s'} Z_{t'} + \sum_{(s,s') \in E_{YZ}} \theta_{ss'}^{yz} Y_s Z_{s'} - \sum_{s \in V_Y} \log(Y_s!) \Big\}. \quad (1)$$

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$$+ \sum_{(s',t')\in E_Z} \theta_{s't'}^{zz} Z_{s'} Z_{t'} + \sum_{(s,s')\in E_{YZ}} \frac{\theta_{ss'}^{yz}}{\sigma_r} Y_s Z_{s'} - \sum_{s \in V_Y} \frac{Y_s^2}{2\sigma_r^2} - \sum_{s' \in V_Z} \log(Z_{s'}!) \Bigg\}.$$

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Corollary

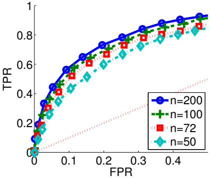
The Gaussian-Poisson distribution is **not normalizable** *unless $\theta_{st} = 0$ for all $(s,t) \in E_{YZ}$.*

Normalizability Conditions for Manichean Graphical Models

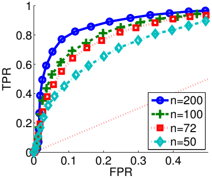
We provide conditions **characterizing normalizability** of general mixed graphical models.

Experiments: Simulated Data

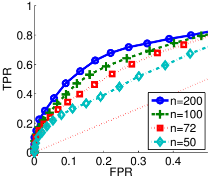
- Lattice graphs, with $p = 72$: $p_Y = 36$ and $p_Z = 36$



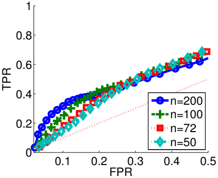
(a) Poisson-Ising



(b) Gaussian-Ising



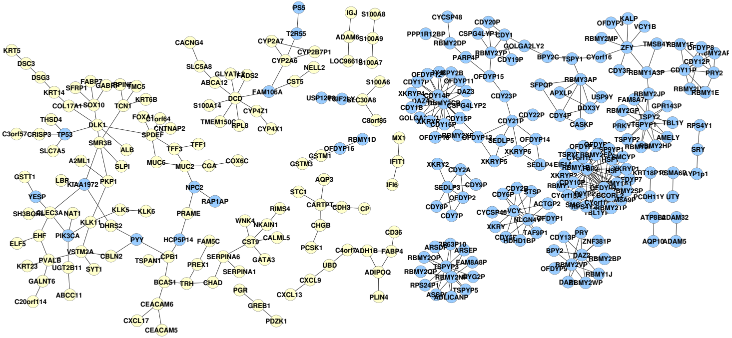
(c) TPGM-Ising



(d) TPGM-Gaussian

Experiments: Cancer Genomic and Transcriptomic Data

- Combine 'Level III RNA-sequencing' data and 'Level II non-silent somatic mutation and level III copy number variation data' for 697 breast cancer patients.



- TPGM - Ising graphical model
- (Yellow) Gene expression via RNA-sequencing, count-valued
- (Blue) Genomic mutation, binary mutation status
- Well known components: (DLK1, THSD4) - (TP53)

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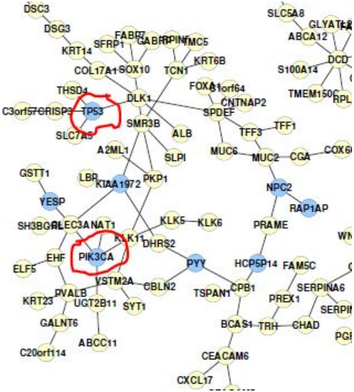

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Summary

- **Broadens the class of off-the-shelf graphical models**, and provides a flexible multivariate modeling toolkit for **mixed data**
  - Univariate exp. family $\rightarrow$ multivariate **Mixed** MRFs
- Allows us to use graphical model machinery to model dependencies for a broader range of data, where each variable may belong to a **potentially different type**
- Can **estimate such graphical models/networks** under standard regularity conditions
- Software (R package) coming soon!

Thank you!

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