# Latent factor models for relational data 

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# Outline 

Introduction

Models based on exchangeability

Homophily and stochastic equivalence

Matrix decomposition models

Multiway data

## Relational data

Relational data consist of

- a set of units or nodes $A$, and
- a set of measurements $Y \equiv\left\{y_{i, j}\right\}$ specific to pairs of nodes $(i, j) \in A \times A$.


## Examples:

International relations

- $A=$ countries,
- $v_{i} i=$ indicator of a dispute initiated by $i$ with target $j$

Needle-sharing network

- $A=$ IV drug users,
- $y_{i, i}=$ needle-sharing activity between $i$ and $j$

Protein-protein interactions

- $A=$ proteins,
- $v_{i, i}=$ the interaction between $i$ and $j$

Not an example:
Dependence graph

- $\mathrm{A}=$ variables,
- $y_{i, i}=$ presence of a high correlation between $i$ and $j$


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## Inferential goals in the regression framework

$y_{i, j}$ measures $i \rightarrow j, \quad \mathbf{x}_{i, j}$ is a vector of explanatory variables.

$$
\mathbf{Y}=\left(\begin{array}{cccccc}
y_{1,1} & y_{1,2} & y_{1,3} & \mathrm{NA} & y_{1,5} & \cdots \\
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Consider a basic (generalized) linear model

$$
y_{i, j} \sim \boldsymbol{\beta}^{T} \mathbf{x}_{i, j}+e_{i, j}
$$

A model can provide

- a measure of the association between $X$ and $Y: \hat{\beta}, \operatorname{se}(\hat{\beta})$
- imputations of missing observations:
- a probabilistic description of network features: $g(\tilde{\mathbf{Y}}), \tilde{\mathbf{Y}} \sim p(\tilde{\mathbf{Y}} \mid \mathbf{Y}, \mathbf{X})$


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## Adolescent health social network



Data on 82 12th graders from a single high school:

54 boys, 28 girls
$\hat{\operatorname{Pr}}\left(y_{i, j}=1 \mid\right.$ same sex $)=0.077$
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Model 0: $\left\{y_{i, j}\right\} \sim$ iid binary $(\theta)$
Model 1: $\left\{y_{i, j}\right\}$ are independent, with

$$
y_{i, j} \sim\left\{\begin{array}{l}
\text { binary }\left(\theta_{A}\right) \text { if } i \text { and } j \text { of same sex } \\
\text { binary }\left(\theta_{B}\right) \text { if } i \text { and } j \text { of opposite sex }
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## Model fit

```
glm(formula = y ~ x, family = binomial(link = "logit"))
```

Coefficients:
Estimate Std. Error z value $\operatorname{Pr}(>|z|)$

| (Intercept) | -2.8332 | 0.1123 | -25.24 | $<2 \mathrm{e}-16{ }^{* * *}$ |
| :--- | ---: | ---: | ---: | :--- |
| x | 0.3471 | 0.1428 | 2.43 | $0.0151^{*}$ |

This result says that a model with preferential association is a better description of the data than an i.i.d. binary model.



Nodal heterogeneity and independence assumptions


## Model lack of fit

Neither of these models do well in terms of representing other features of the data - for example, transitivity:

$$
t(\mathbf{Y})=\sum_{i<j<k} y_{i, j} y_{j, k} y_{k, i}
$$




## Random effects models

Deviations from ordinary regression models can be represented as

$$
y_{i, j} \sim \boldsymbol{\beta}^{T} \mathbf{x}_{i, j}+\gamma_{i, j}
$$

A simple "latent variable" model might include additive node effects:

$$
\gamma_{i, j}=a_{i}+a_{j} \quad \Rightarrow \quad y_{i, j} \sim \boldsymbol{\beta}^{T} \mathbf{x}_{i, j}+a_{i}+a_{j}
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$\left\{a_{1}, \ldots, a_{n}\right\}$ represent nodal heterogeneity, additive on the regressor scale.
Inclusion of these effects in the model can dramatically improve

- within-sample model fit (measured by $R^{2}$, likelihood ratio, BIC, etc.);
- out-of-sample predictive performance (measured by cross-validation).

But this model only captures heterogeneity of outdegree/indegree, and can't represent more complicated structure, such as clustering, transitivity, etc.

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Fit of additive effects model



## Model building goals

Descriptions of local network structure

- identification of important nodes
- identification of groups of nodes
- stochastically equivalent groups
- high density clusters

Descriptions of global network structure

- relationship to explanatory variables
- global measures of density, transitivity, degree distribution

Inference

- prediction and imputation
- confidence intervals for regression effects
- hypothesis testing and model comparison


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## Model building principles

- Statistical inference utilizes probability models
- Networks and relational data are represented by matrices and arrays Social network analysis can utilize probability models of matrices and arrays. We will construct social network models based on these tools:

1. Probability: symmetry considerations (exchangeability) will motivate latent variable models generally.
2. Matrix algebra: matrix decomposition methods will motivate latent factor models specifically.

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A primer on exchangeability and de Finetti's theorem

Let $Y_{1}, \ldots, Y_{n}$ be an exchangeable sequence for all $n$ :

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\operatorname{Pr}\left(Y_{1}=y_{1}, \ldots, Y_{n}=y_{n}\right)=\operatorname{Pr}\left(Y_{1}=y_{\pi_{1}}, \ldots, Y_{n}=y_{\pi_{n}}\right) \forall n
$$

de Finetti's theorem says

- The parameter $\theta$ represents "global features" of the sequence.
- The $\epsilon_{i}$ 's represent "local features", specific to individual $Y_{i}$ 's.
(This theorem justifies the ubiquitous "conditionally i.i.d." assumption of statistical modeling)

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\operatorname{Pr}\left(Y_{1}=y_{1}, \ldots, Y_{n}=y_{n}\right)=\operatorname{Pr}\left(Y_{1}=y_{\pi_{1}}, \ldots, Y_{n}=y_{\pi_{n}}\right) \forall n
$$

de Finetti's theorem says

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\begin{aligned}
Y_{i} & =g\left(\theta, \epsilon_{i}\right), \text { where } \\
\epsilon_{1}, \ldots, \epsilon_{n} & \stackrel{\text { iid }}{\sim} p_{\epsilon}
\end{aligned}
$$

- The parameter $\theta$ represents "global features" of the sequence.
- The $\epsilon_{i}$ 's represent "local features", specific to individual $Y_{i}$ 's.
(This theorem justifies the ubiquitous "conditionally i.i.d." assumption of statistical modeling)


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## Exchangeability for nested data

Now consider an $m \times n$ data matrix :

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\mathbf{Y}=\left(\begin{array}{cccc}
Y_{1,1} & Y_{1,2} & \cdots & Y_{1, n} \\
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Suppose $\operatorname{Pr}(Y)$ is exchangeable across rows and within rows:


A double application of de Finetti's theorem implies

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## Exchangeability for symmetric relational matrices

Let $\mathbf{Y}$ be a symmetric binary matrix with no explanatory variables. What properties should a probability model $\operatorname{Pr}(\mathbf{Y}=\mathbf{y})$ have?

$$
\mathbf{y}_{A}=\left(\begin{array}{cccc}
. & 0 & 1 & 1 \\
0 & . & 0 & 1 \\
1 & 0 & . & 0 \\
1 & 1 & 0 & .
\end{array}\right) \quad \mathbf{y}_{B}=\left(\begin{array}{cccc}
. & 1 & 0 & 0 \\
1 & . & 1 & 0 \\
0 & 1 & . & 1 \\
0 & 0 & 1 & \cdot
\end{array}\right)
$$

$y_{B}$ is just $y_{A}$ with the nodes relabeled: $y_{B, i, j}=y_{A, \pi_{i}, \pi_{j}}, \pi=(3,1,4,2)$

$$
\operatorname{Pr}\left(\mathbf{Y}=\mathbf{y}_{A}\right) \stackrel{?}{=} \operatorname{Pr}\left(\mathbf{Y}=\mathbf{y}_{B}\right)
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RCE model: $\operatorname{Pr}(\cdot)$ is $\operatorname{RCE}$ if $\operatorname{Pr}(\mathbf{Y}=\mathbf{y})=\operatorname{Pr}\left(\mathbf{Y}=\mathbf{y}_{\pi}\right)$ for all $\mathbf{y}$ and $\pi$.

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(Hoover 1982, Aldous 1983)

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Suppose our model $\operatorname{Pr}()$ for $\mathbf{Y}=\left\{Y_{i, j}, i=1, \ldots, n, j=1, \ldots, n\right\}$ is RCE:
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Then

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\begin{aligned}
Y_{i, j} & =g\left(\theta, a_{i}, b_{j}, \epsilon_{i, j}\right) \\
\left(a_{1}, b_{1}\right), \ldots,\left(a_{n}, b_{n}\right) & \stackrel{i i d}{\sim} p_{a b} \\
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\left(a_{1}, b_{1}\right), \ldots,\left(a_{n}, b_{n}\right) & \stackrel{i i d}{\sim} p_{a b} \\
\left\{\left(\epsilon_{i, j}, \epsilon_{j, i}\right)\right\} & \stackrel{i i d}{\sim} p_{\epsilon}
\end{aligned}
$$

- The parameter $\theta$ represents global features of the matrix.
- The $a_{i}$ 's represent nodal sender features.
- The $b_{j}$ 's represent nodal receiver features.
- The $\left(\epsilon_{i, j}, \epsilon_{j, i}\right)$ 's represent heterogeneity among ordered dyads.

Latent class model: an exchangeable latent variable model (Nowicki and Snijders 2001, Airoldi et al. 2008)

- Each node $i$ is a member of an (unknown) latent class

$$
a_{i} \in\{1, \ldots, K\}
$$

- The probability of a tie between $i$ and $j$ is

$$
\operatorname{Pr}\left(Y_{i, j}=1 \mid a_{i}, a_{j}\right)=\theta_{a_{i}, a_{j}}
$$

- The classes are unknown but exchangeable a priori
$\square$

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$$

- The classes are unknown but exchangeable a priori:

$$
a_{1}, \ldots, a_{n} \stackrel{i d}{\sim} \text { multinomial }\left(p_{1}, \ldots, p_{K}\right)
$$

Nodes in the same class may have a small or high probability of ties: $\theta_{k, k}$ may be small or large
Nodes in the same class are stochastically equivalent

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$$

## Model characteristics:

Nodes in the same class may have a small or high probability of ties:

$$
\theta_{k, k} \text { may be small or large }
$$

Nodes in the same class are stochastically equivalent:
$\operatorname{Pr}\left(\left\{Y_{i, 1}, \ldots, Y_{i, n}\right\}=\left\{y_{1}, \ldots, y_{n}\right\} \mid a_{i}=k\right)=\operatorname{Pr}\left(\left\{Y_{j, 1}, \ldots, Y_{j, n}\right\}=\left\{y_{1}, \ldots, y_{n}\right\} \mid a_{j}=k\right)$

Latent distance model: an exchangeable latent variable model (Hoff, Raftery and Handcock 2002, Handcock, Raftery and Tantrum 2007)

- Each node $i$ has an (unknown) latent position

$$
a_{i} \in \mathbb{R}^{K}
$$

- The probability of a tie from $i$ to $j$ depends on the distance between them

$$
\text { log odds } \operatorname{Pr}\left(Y_{i, j}=1 \mid a_{i}, a_{j}\right)=\theta-\left|a_{i}-a_{j}\right|
$$

- The positions are unknown but exchangeable a priori

$$
a_{1}, \ldots, a_{n} \stackrel{i i d}{\sim} \operatorname{mvnorm}(0, \Sigma)
$$

will likely have similar ties to others:

$$
a_{i} \approx a_{j} \Leftrightarrow\left\{\begin{array}{l}
\operatorname{Pr}\left(Y_{i, j}=1 \mid a_{i}, a_{j}\right) \approx \theta \\
\operatorname{Pr}\left(Y_{i, k}=1 \mid a_{i}, a_{k}\right) \approx \operatorname{Pr}\left(Y_{j, k}=1 \mid a_{j}, a_{k}\right)
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$$

Model characteristics: Nodes nearby one another are more likely to have a tie, and will likely have similar ties to others:

$$
a_{i} \approx a_{j} \Leftrightarrow\left\{\begin{array}{l}
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## Latent factor model: an exchangeable latent variable model

(Hoff, Raftery and Handcock 2002, Hoff 2005, Hoff 2008)

- Each node $i$ has an (unknown) latent factor

$$
a_{i} \in \mathbb{R}^{K}
$$

- The probability of a tie from $i$ to $j$ depends on their latent factors

- The positions are unknown but exchangeable a priori:

$$
a_{1}, \ldots . a_{n} \stackrel{i i d}{m} \operatorname{mvnorm}(\mu, \Sigma)
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$$
\log \operatorname{odds} \operatorname{Pr}\left(Y_{i, j}=1 \mid a_{i}, a_{j}\right)=\theta+a_{i}^{T} B a_{j}, B=\left(\begin{array}{ccc}
b_{1} & 0 & 0 \\
0 & b_{2} & 0 \\
0 & 0 & b_{3}
\end{array}\right)
$$

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a_{1}, \ldots, a_{n} \stackrel{i i d}{\sim} \operatorname{mvnorm}(\mu, \Sigma)
$$

## Model characteristics:

nodes with similar factors may have a large or small probability of a tie nodes with similar factors are approximately stochastically equivalent

## Incorporation into regression modeling

Consider expanding upon the simple LM or GLM:

$$
Y_{i, j} \sim \boldsymbol{\beta}^{T} \mathbf{x}_{i, j}+\gamma_{i, j}
$$

- The $\left\{\gamma_{i, j}\right\}$ 's represent deviations from the simple regression model - The matrix of deviations is itself a relational (unobserved) data matrix
- The latent variable structure can describe these deviations


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$$
\begin{aligned}
Y_{i, j} & \sim \boldsymbol{\beta}^{T} \mathbf{x}_{i, j}+\gamma_{i, j} & & \\
\gamma_{i, j} & =\theta_{a_{i,}, a_{j}} & & \text { (stochastic blockmodel) } \\
\gamma_{i, j} & =-\left|a_{i}-a_{j}\right| & & \text { (distance model) } \\
\gamma_{i, j} & =a_{i}^{T} \mathbf{B}_{a_{j}} & & \text { (factor model) }
\end{aligned}
$$

High school social network: additive effects fit


$$
Y_{i, j} \sim \boldsymbol{\beta}^{T} \mathbf{x}_{i, j}+a_{i}+a_{j}
$$




## High school social network: Latent factor fit

$$
Y_{i, j} \sim \boldsymbol{\beta}^{T} \mathbf{x}_{i, j}+\mathbf{a}_{i}^{T} \mathbf{B} \mathbf{a}_{j}
$$

Parameters in this model can be fit with the eigenmodel package in R:

```
eigenmodel_mcmc(Y,X,R=3)
```




The latent factors are able to represent the network transitivity.

Underlying structure


Missing variables


## Missing variables

The eigenmodel, without having explicit race information, captures a large degree of the racial homophily in friendship:


eigenmodel log-odds ratio

## Model comparisons

How do the different latent variable models compare?
What structures do they represent?

## Two important types of patterns:

Homophily: Similar nodes link to each other

- "similar" may be in terms of unobserved characteristics
- homophily leads to transitive or clustered social networks
- observed transitivity may be due to exogenous or endogenous factors (See Shalizi and Thomas 2010 for a more careful discussion )



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Stochastic equivalence: Similar nodes have similar relational patterns

- similar nodes may or may not link to each other
- equivalent nodes can be thought of as having the same "role"
- Transitivity (global measure)
- Stochastic equivalence (local measure)


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(See Shalizi and Thomas 2010 for a more careful discussion )
Stochastic equivalence: Similar nodes have similar relational patterns
- similar nodes may or may not link to each other
- equivalent nodes can be thought of as having the same "role"


## Descriptive measures:

- Transitivity (global measure): $\sum_{i, j, k} y_{i, j} y_{j, k} y_{k, i}$
- Stochastic equivalence (local measure): $\rho_{i, j}=\operatorname{cor}\left(\mathbf{y}_{[i,]}, \mathbf{y}_{[j,]}\right)$

Homophily and stochastic equivalence


How well can the distance model represent these networks?
How well can the latent class model represent these networks?

Homophily and stochastic equivalence in real networks


- AddHealth friendships: friendships among 247 12th-graders
- Word neighbors in Genesis: neighboring occurrences among 158 words
- Protein binding interactions: binding patterns among 230 proteins


## Model comparison via cross validation

1. Randomly divide the $\binom{n}{2}$ data values into 5 sets letting $s_{i, j}$ be the set to which pair $\{i, j\}$ is assigned.
```
    2.1 Estimate model parameters with {\mp@subsup{y}{i,j}{}:\mp@subsup{s}{i,j}{}\not=s}\mathrm{ , the data not in set s.}
    2.2 Predict {\mp@subsup{y}{i,j}{}:\mp@subsup{s}{i,j}{}\not=s}\mathrm{ from these estimated parameters}
This generates a sociomatrix }\hat{\mathbf{Y}}\mathrm{ , in which each entry }\mp@subsup{\hat{y}}{i,j}{}\mathrm{ is a predicted value
obtained from using a subset of the data that does not include }\mp@subsup{y}{i,j}{}\mathrm{ .
```


## Model comparison via cross validation

1. Randomly divide the $\binom{n}{2}$ data values into 5 sets letting $s_{i, j}$ be the set to which pair $\{i, j\}$ is assigned.
2. For each $s \in\{1, \ldots, 5\}$ :
2.1 Estimate model parameters with $\left\{y_{i, j}: s_{i, j} \neq s\right\}$, the data not in set $s$.
2.2 Predict $\left\{y_{i, j}: s_{i, j} \neq s\right\}$ from these estimated parameters

This generates a sociomatrix $\hat{\mathbf{Y}}$, in which each entry $\hat{y}_{i, j}$ is a predicted value obtained from using a subset of the data that does not include $y_{i, j}$.

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## AddHealth friendships




## Genesis word neighbors




## Protein bindings




## More cross validation results

| $K$ | Add health |  |  | Genesis |  |  |  | Protein interaction |  |  |
| ---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | dist | class | eigen | dist | class | eigen | dist | class | eigen |  |
| 3 | 0.82 | 0.64 | 0.75 | 0.62 | 0.82 | 0.82 | 0.83 | 0.79 | 0.88 |  |
| 5 | 0.81 | 0.70 | 0.78 | 0.66 | 0.82 | 0.82 | 0.84 | 0.84 | 0.90 |  |
| 10 | 0.76 | 0.69 | 0.80 | 0.74 | 0.82 | 0.82 | 0.85 | 0.86 | 0.90 |  |

 can be made more comparable to the distance model if a diffuse prior is used)

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| 10 | 0.76 | 0.69 | 0.80 | 0.74 | 0.82 | 0.82 | 0.85 | 0.86 | 0.90 |  |

The eigenmodel is generally as good or better than the others in each case (it can be made more comparable to the distance model if a diffuse prior is used).

## Model flexibility

Probit versions of the three latent variable models all have the following form:

$$
\begin{aligned}
y_{i, j} & =\left\{\begin{array}{cc}
1 & \text { if } z_{i, j}>0 \\
0 & \text { if } z_{i, j} \leq 0
\end{array}\right. \\
z_{i, j} & =\mu+\alpha\left(a_{i}, a_{j}\right)+\epsilon_{i, j}
\end{aligned}, \begin{aligned}
& \sim \text { i.i.d. normal }(0,1)
\end{aligned}
$$

where
Latent class model:


Latent factor model:

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\begin{aligned}
& \alpha\left(a_{i}, a_{j}\right)=\theta_{a_{i}, a_{j}} \\
& a_{i} \in\{1, \ldots, K\}, \quad i \in\{1, \ldots, n\} \\
& \Theta \text { a } K \times K \text { symmetric matrix }
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$$

Latent factor model:

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Latent distance model:

$$
\begin{aligned}
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& \left\{\epsilon_{i, j}: 1 \leq i<j \leq n\right\} \quad \sim \text { i.i.d. normal }(0,1) \\
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Latent factor model:

$$
\begin{aligned}
& \alpha\left(a_{i}, a_{j}\right)=a_{i}^{T} \Lambda a_{j} \\
& a_{i} \in \mathbb{R}^{K}, \quad i \in\{1, \ldots, n\} \\
& \Lambda \text { a } K \times K \text { diagonal matrix. }
\end{aligned}
$$

## Model flexibility

Let $\mathcal{S}_{n}$ be the set of symmetric $n \times n$ matrices, and let

$$
\begin{aligned}
\mathcal{C}_{K} & =\left\{C \in \mathcal{S}_{n}: c_{i, j}=\theta_{a_{i}, a_{j}}, a_{i} \in\{1, \ldots, K\}, \Theta \text { a } K \times K \text { symmetric matrix }\right\} ; \\
\mathcal{D}_{K} & =\left\{D \in \mathcal{S}_{n}: d_{i, j}=-\left|a_{i}-a_{j}\right|, a_{i} \in \mathbb{R}^{K}\right\} ; \\
\mathcal{E}_{K} & =\left\{E \in \mathcal{S}_{n}: e_{i, j}=a_{i}^{T} \Lambda a_{j}, a_{i} \in \mathbb{R}^{K}, \Lambda \text { a } K \times K \text { diagonal matrix }\right\} .
\end{aligned}
$$

$\mathcal{C}_{K}, \mathcal{D}_{K}$ and $\mathcal{E}_{K}$ describe the patterns representable by the class, distance and factor models respectively.

- $\mathcal{E}_{K}$ generalizes $\mathcal{C}_{K}$
- EK.. weakly generalizes DK
- $\mathcal{D}_{K}$ does not weakly generalize $\mathcal{E}_{1}$


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$\mathcal{C}_{K}, \mathcal{D}_{K}$ and $\mathcal{E}_{K}$ describe the patterns representable by the class, distance and factor models respectively.

Theoretical results:

- $\mathcal{E}_{K}$ generalizes $\mathcal{C}_{K}$
- $\mathcal{E}_{K+1}$ weakly generalizes $\mathcal{D}_{K}$
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\mathcal{C}_{K} & =\left\{C \in \mathcal{S}_{n}: c_{i, j}=\theta_{a_{i}, a_{j}}, a_{i} \in\{1, \ldots, K\}, \Theta \text { a } K \times K \text { symmetric matrix }\right\} ; \\
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$\mathcal{C}_{K}, \mathcal{D}_{K}$ and $\mathcal{E}_{K}$ describe the patterns representable by the class, distance and factor models respectively.

## Theoretical results:

- $\mathcal{E}_{K}$ generalizes $\mathcal{C}_{K}$
- $\mathcal{E}_{K+1}$ weakly generalizes $\mathcal{D}_{K}$
- $\mathcal{D}_{K}$ does not weakly generalize $\mathcal{E}_{1}$


## Model flexibility

Let $\mathcal{S}_{n}$ be the set of symmetric $n \times n$ matrices, and let

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## Matrix decompositions

Probit version of the latent factor model:

$$
\begin{array}{rlrl}
y_{i, j} & =g\left(z_{i, j}\right), & \text { where } g \text { is a nondecreasing function } \\
z_{i, j} & =\mathbf{u}_{i}^{T} \Lambda \mathbf{u}_{j}+\epsilon_{i, j}, & \text { where } \mathbf{u}_{i} \in \mathbb{R}^{K}, \Lambda=\operatorname{diag}\left(\lambda_{1}, \ldots, \lambda_{K}\right) \\
\left\{\epsilon_{i, j}\right\} & \stackrel{i i d}{\sim} \text { normal }(0,1) & &
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$$

Writing $\left\{z_{i, j}\right\}$ as a matrix,

$$
\mathbf{Z}=\mathbf{U} \wedge \mathbf{U}^{T}+\mathbf{E}
$$

- Every $n \times n$ symmetric matrix $\mathbf{Z}$ can be written

$$
Z=U \wedge U^{\top}
$$

where $\Lambda=\operatorname{diag}\left(\lambda_{1}, \ldots, \lambda_{n}\right)$ and $\mathbf{U}$ is orthonormal.

- If $\mathbf{U} \wedge \mathbf{U}^{T}$ is the eigendecomposition of $\mathbf{Z}$, then

$$
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## Least squares approximations of increasing rank



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## Estimation and Inference

Data: $\mathbf{Y}=\left\{y_{i, j}, 1 \leq i<j \leq n\right\}$

## Model:

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Gibbs sampling: MCMC approximation to $p(\mathbf{Z}, \mu, \mathbf{U}, \Lambda \mid \mathbf{Y})$

1. sample $z_{i, i} \sim p\left(z_{i, j} \mid y_{i, j}, \mu\right)$ for each pair (i,i)
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Posterior inference:

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\begin{aligned}
p(\mathbf{Z}, \mu, \mathbf{U}, \Lambda \mid \mathbf{Y}) & \propto p(\mathbf{Y} \mid \mathbf{Z}, \mu, \mathbf{U}, \Lambda) p(\mathbf{Z}, \mu, \mathbf{U}, \Lambda) \\
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## R-Package eigenmodel

Description:
Construct approximate samples from the posterior distribution of the parameters and latent variables in an eigenmodel for symmetric relational data.

Usage:
eigenmodel_mcmc $(Y, X=N U L L, R=2, S=1000$, seed $=1$, Nss $=\min (S-$ burn, 1000 $)$, burn $=0)$
Arguments:
$\mathrm{Y}:$ an $\mathrm{n} x \mathrm{n}$ symmetric matrix with missing diagonal entries. Off-diagonal missing values are allowed.

X : an $\mathrm{n} \times \mathrm{n} \times \mathrm{p}$ array of regressors
$R$ : the rank of the approximating factor matrix
S: number of samples from the Markov chain
seed: a random seed

Nss: number of samples to be saved
burn: number of initial scans of the Markov chain to be dropped
Value: a list with the following components:

Z_postmean: posterior mean of the latent variable in the probit specification

ULU_postmean: posterior mean of the reduced-rank approximating matrix

Y_postmean: the original data matrix with missing values replaced by posterior means
L_postsamp: samples of the eigenvalues
b_postsamp: samples of the regression coefficients

## Friendship example

> library(eigenmodel)
> data(YX_Friend)
> fit<-eigenmodel_mcmc (Y=YX_Friend\$Y,X=YX_Friend\$X,R=2,S=100000,burn=5000)


## Protein interaction example

> library(eigenmodel)
> data(Y_Pro)
> fit<-eigenmodel_mcmc(Y=Y_Pro,R=2,S=100000,burn=5000)



## R-Software svdmodel

The same idea, except for asymmetric data...
Recall from linear algebra:

- Every $m \times n$ symmetric matrix $\mathbf{Z}$ can be written

$$
\mathbf{Z}=\mathbf{U D V}^{T}
$$

where $\mathbf{D}=\operatorname{diag}\left(d_{1}, \ldots, d_{n}\right), \mathbf{U}$ and $\mathbf{V}$ are orthonormal.

- If UDV ${ }^{T}$ is the svd of $\mathbf{Z}$, then

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\hat{\mathbf{Z}}_{k} \equiv \mathbf{U}_{[, 1: k]} \mathbf{D}_{[1: k, 1: k]} \mathbf{V}_{[, 1: k]}^{\top}
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## Multiway relational arrays

$y_{i, j, k}=$

- $j$ th measurement on ith subject under condition $k$ (psychometrics)
- type-k relationship between $i$ and $J$ (relational data/network)
- relationship between $i$ and $i$ at time $t$ (longitudinal relational data)



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## Longitudinal network example

Cold war cooperation and conflict

- 66 countries
- 8 years $(1950,1955, \ldots, 1980,1985)$
- $y_{i, j, t}=$ relation between $i, j$ in year $t$
- also have data on odp and polity



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## Reduced rank models

## $\mathbf{Y}=\boldsymbol{\Theta}+\mathbf{E}$

- $\Theta$ contains the "main features" we hope to recover,
- $\mathbf{E}$ is "patternless."

Matrix decomposition: If $\Theta$ is a rank- $R$ matrix, then

$$
\theta_{i, j}=\left\langle\mathbf{u}_{i}, \mathbf{v}_{j}\right\rangle=\sum_{r=1}^{R} u_{i, r} v_{j, r} \quad \Theta=\sum_{r=1}^{R} \mathbf{u}_{r} \mathbf{v}_{r}^{T}=\sum_{r=1}^{R} \mathbf{u}_{r} \circ \mathbf{v}_{r}
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Array decomposition: If $\Theta$ is a rank- $R$ array, then

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(Harshman[1970], Kruskal[1976,1977], Harshman and Lundy[1984], Kruskal[1989] )

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(Harshman[1970], Kruskal[1976,1977], Harshman and Lundy[1984], Kruskal[1989] )

## Some things you should know

1. Computing the rank

- matrix: easy to do
- array: no known algorithm

2. Possible rank

- matrix: $R_{\max }=\min \left(m_{1}, m_{2}\right)$
- array: $\max \left(m_{1}, m_{2}, m_{3}\right) \leq R_{\max } \leq \min \left(m_{1} m_{2}, m_{1} m_{3}, m_{2} m_{3}\right)$

3. Probable rank

- matrix: "almost all" matrices have full rank.
- array: a nonzero fraction (w.r.t. Lebesgue measure) have less than full rank.

4. Least squares approximation

- matrix: SVD of $\mathbf{Y}$ provides the rank $R$ least-squares approximation to $\boldsymbol{\Theta}$.
- array: iterative "least squares" methods, but solution may not exist (de Silva and Lim[2008] )

5. Uniqueness

- matrix: The representation $\boldsymbol{\Theta}=\langle\mathbf{U}, \mathbf{V}\rangle=\mathbf{U} \mathbf{V}^{\top}$ is not unique.
- array: The representation $\boldsymbol{\Theta}=\langle\mathbf{U}, \mathbf{V}, \mathbf{W}\rangle$ is essentially unique.


## A model-based approach

For a $K$-way array $\mathbf{Y}$,

$$
\begin{aligned}
& \mathbf{Y}=\boldsymbol{\Theta}+\mathbf{E} \\
& \boldsymbol{\Theta}=\sum_{r=1}^{R} \mathbf{u}_{r}^{(1)} \circ \cdots \circ \mathbf{u}_{r}^{(K)} \equiv\left\langle\mathbf{U}^{(1)}, \ldots, \mathbf{U}^{(K)}\right\rangle \\
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## Some motivation:

- shrinkage: $\Theta$ contains lots of parameters.
- hierarchical: covariance among columns of $\boldsymbol{U}^{(k)}$ is identifiable.
- estimation: $p\left(Y \mid U^{(1)}, \ldots, v U^{(K)}\right)$ multimodal, MCMC "stochastic search"
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& \mathbf{u}_{1}^{(k)}, \ldots, \mathbf{u}_{m_{k}}^{(k)} \stackrel{\text { iid }}{\sim} \text { multivariate normal }\left(\boldsymbol{\mu}_{k}, \boldsymbol{\Psi}_{k}\right), \\
& \text { with }\left\{\boldsymbol{\mu}_{k}, \boldsymbol{\Psi}_{k}, k=1, \ldots, K\right\} \text { to be estimated. }
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Some motivation:

- shrinkage: $\boldsymbol{\Theta}$ contains lots of parameters.
- hierarchical: covariance among columns of $\mathbf{U}^{(k)}$ is identifiable.
- estimation: $p\left(\mathbf{Y} \mid \mathbf{U}^{(1)}, \ldots, v U^{(K)}\right)$ multimodal, MCMC "stochastic search"
- adaptability: incorporate reduced rank arrays as a model component
- multilinear predictor in a GLM
- multilinear effects for regression parameters


## A model-based approach

For a K-way array Y,

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## Longitudinal network example

- $y_{i, j, t} \in\{-5,-4, \ldots,+1,+2\}$, the level of military conflict/cooperation

- $x_{i, j, t, 2}=\left(\log g \mathrm{dp}_{i}\right) \times\left(\log g \mathrm{gp}_{j}\right)$, the product of the $\log \mathrm{gdps} ;$
- $x_{i, j, t, 3}=$ polity $_{i} \times$ polity $_{j}$, where polity ${ }_{i} \in\{-1,0,+1\}$;
- $x_{i, j, t, 4}=\left(\right.$ polity $\left._{i}>0\right) \times\left(\right.$ polity $\left._{j}>0\right)$.


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- $y_{i, j, t} \in\{-5,-4, \ldots,+1,+2\}$, the level of military conflict/cooperation
- $x_{i, j, t, 1}=\log g d p_{i}+\log g d p_{j}$, the sum of the $\log g d p s$ of the two countries;
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## Model:

$$
\begin{aligned}
y_{i, j, t} & =\max \left\{y: z_{i, j, t}>c_{y}\right\} \\
z_{i, j, t} & =\boldsymbol{\beta}^{T} \mathbf{x}_{i, j, t}+\left\langle\mathbf{u}_{i}, \mathbf{u}_{j}, \boldsymbol{\lambda}_{t}\right\rangle+\epsilon_{i, j, t} \\
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"Interpretation":

$$
\mathbf{Z}_{t}=\mathbf{U} \Lambda_{t} \mathbf{U}^{T}+\mathbf{E}_{t}
$$

## Longitudinal network example


$\mathrm{u}_{1}$



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## Covariance structure of multiple relational arrays

Yearly change in log exports (2000 dollars) : $\mathbf{Y}=\left\{y_{i, j, k, l}\right\} \in \mathbb{R}^{30 \times 30 \times 6 \times 10}$

- $i \in\{1, \ldots, 30\}$ indexes exporting nation
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"Replications" over time: $\mathbf{Y}=\left\{\mathbf{Y}_{1}, \ldots, \boldsymbol{Y}_{10}\right\}$

$$
\mathbf{Y}_{t}=\mathbf{M}+\mathbf{E}_{t}
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- $\mathbf{M} \in \mathbb{R}^{30 \times 30 \times 6}$, constant over time;
- $\mathbf{F}_{t} \in \mathbb{R}^{30 \times 30 \times 6}$, changing over time

How should the covariance among $\left\{\mathrm{E}_{1}, \ldots, \mathrm{E}_{10}\right\}$ be described?

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## The Tucker product

$$
\mathbf{Y}=\boldsymbol{\Theta}+\mathbf{E}
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Decompose $\boldsymbol{\Theta}$ using the Tucker decomposition (Tucker 1964,1966):

$$
\begin{aligned}
\theta_{i, j, k} & =\sum_{r=1}^{R} \sum_{s=1}^{S} \sum_{t=1}^{T} z_{r, s, t} a_{i, r} b_{j, r} c_{k, r} \\
\boldsymbol{\Theta} & =\mathbf{Z} \times\{\mathbf{A}, \mathbf{B}, \mathbf{C}\}
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- $\mathbf{Z}$ is the $R \times S \times T$ core array
- $R, S$ and $T$ are the 1-rank, 2-rank and 3 -rank of $\Theta$
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## Separable covariance via Tucker products

Multivariate normal model:

$$
\begin{aligned}
\mathbf{z}=\left\{z_{j}: j=1, \ldots, m\right\} & \stackrel{\text { iid }}{\sim} \quad \text { normal }(\mathbf{0}, 1) \\
\mathbf{y}=\boldsymbol{\mu}+\mathbf{A z} & \sim \text { multivariate normal }\left(\boldsymbol{\mu}, \boldsymbol{\Sigma}=\mathbf{A A}^{T}\right)
\end{aligned}
$$

$$
\mathbf{Z}=\left\{z_{i, j}\right\}_{i=1, j=1}^{m_{1}, m_{2}} \stackrel{i i d}{\sim} \operatorname{normal}(\mathbf{0}, 1)
$$

$$
\mathbf{Y}=\mathbf{M}+\mathbf{A Z B} \mathbf{B}^{T} \sim \text { matrix normal }\left(\mathbf{M}, \boldsymbol{\Sigma}_{1}=\mathbf{A A}^{T}, \Sigma_{2}=\mathbf{B B}^{T}\right)
$$

$$
\text { NOTE: } \mathbf{A Z B} \mathbf{B}^{T}=\mathbf{Z} \times\{\mathbf{A}, \mathbf{B}\}
$$

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$$
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Matrix normal model:

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Array normal model:

$$
\begin{aligned}
\mathbf{Z} & =\left\{\boldsymbol{z}_{i, j, k}\right\}_{i=1,1, j=1, k=1}^{m_{1}, m_{2}, m_{3}} \\
\mathbf{i i d} & \operatorname{normal}(\mathbf{0}, 1) \\
\mathbf{Y}=\mathbf{M}+\mathbf{Z} \times\{\mathbf{A}, \mathbf{B}, \mathbf{C}\} & \sim \operatorname{array} \operatorname{normal}\left(\mathbf{M}, \boldsymbol{\Sigma}_{1}=\mathbf{A A}^{T}, \boldsymbol{\Sigma}_{2}=\mathbf{B B}^{T}, \boldsymbol{\Sigma}_{3}=\mathbf{C C}^{T}\right)
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## Separable covariance structure

For the matrix normal model:

$$
\begin{aligned}
\operatorname{Cov}[\mathbf{Y}] & =\boldsymbol{\Sigma}_{1} \circ \boldsymbol{\Sigma}_{2} \\
\operatorname{Cov}[\operatorname{vec}(\mathbf{Y})] & =\boldsymbol{\Sigma}_{2} \otimes \boldsymbol{\Sigma}_{1} \\
\mathrm{E}\left[\mathbf{Y} \mathbf{Y}^{T}\right] & =\boldsymbol{\Sigma}_{1} \times \operatorname{tr}\left(\boldsymbol{\Sigma}_{2}\right) \\
\mathrm{E}\left[\mathbf{Y}^{T} \mathbf{Y}\right] & =\boldsymbol{\Sigma}_{2} \times \operatorname{tr}\left(\boldsymbol{\Sigma}_{1}\right)
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For the array normal model:

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\operatorname{Cov}[\mathbf{Y}] & =\boldsymbol{\Sigma}_{1} \circ \boldsymbol{\Sigma}_{2} \circ \boldsymbol{\Sigma}_{3} \\
\operatorname{Cov}[\operatorname{vec}(\mathbf{Y})] & =\boldsymbol{\Sigma}_{k} \otimes \cdots \otimes \boldsymbol{\Sigma}_{1} \\
\mathrm{E}\left[\mathbf{Y}_{(k)} \mathbf{Y}_{(k)}^{T}\right] & =\boldsymbol{\Sigma}_{k} \times \prod_{j \neq k} \operatorname{tr}\left(\boldsymbol{\Sigma}_{j}\right)
\end{aligned}
$$

## International trade example

Yearly change in log exports (2000 dollars) : $\mathbf{Y}=\left\{y_{i, j, k, l}\right\} \in \mathbb{R}^{30 \times 30 \times 6 \times 7}$

- $i \in\{1, \ldots, 30\}$ indexes exporting nation
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Full "cell means" model:

$$
y_{i, j, k, l}=\mu_{i, j, k}+e_{i, j, k, l}
$$

Let $\mathbf{E}=\left\{e_{i, j, k, l}\right\}$

- iid error model:

$$
\mathbf{E} \sim \operatorname{array} \operatorname{normal}\left(0, \mathbf{I}, \mathbf{I}, \mathbf{I}, \sigma^{2} \mathbf{I}\right)
$$

- vector normal error model:
- matrix normal error model: $\mathbf{E} \sim$ array normal $\left(0, \mathbf{I}, \mathbf{I}, \boldsymbol{\Sigma}_{3}, \boldsymbol{\Sigma}_{4}\right)$
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- $k \in\{1, \ldots, 6\}$ indexes commodity
- $I \in\{1, \ldots, 10\}$ indexes year

Full "cell means" model:

$$
y_{i, j, k, l}=\mu_{i, j, k}+e_{i, j, k, l}
$$

Let $\mathbf{E}=\left\{e_{i, j, k, l}\right\}$

- iid error model:

$$
\mathbf{E} \sim \operatorname{array} \operatorname{normal}\left(0, \mathbf{I}, \mathbf{I}, \mathbf{I}, \sigma^{2} \mathbf{I}\right)
$$

- vector normal error model: $\mathbf{E} \sim$ array normal $\left(0, \mathbf{I}, \mathbf{I}, \boldsymbol{\Sigma}_{3}, \mathbf{I}\right)$
- matrix normal error model: $\mathbf{E} \sim$ array normal $\left(0, \mathbf{I}, \mathbf{I}, \boldsymbol{\Sigma}_{3}, \boldsymbol{\Sigma}_{4}\right)$
- array normal model:
$\mathbf{E} \sim$ array normal $\left(\mathbf{0}, \boldsymbol{\Sigma}_{1}, \boldsymbol{\Sigma}_{2}, \boldsymbol{\Sigma}_{3}, \boldsymbol{\Sigma}_{4}\right\}$


## International trade example

Model comparison:
reduced: array normal $\left(0, \mathbf{I}, \mathbf{I}, \boldsymbol{\Sigma}_{3}, \boldsymbol{\Sigma}_{4}\right)$
full: array normal $\left(0, \boldsymbol{\Sigma}_{1}, \boldsymbol{\Sigma}_{2}, \boldsymbol{\Sigma}_{3}, \boldsymbol{\Sigma}_{4}\right)$




## International trade example








## Summary

- Exchangeability implies a latent variable representation
- Matrix and array decompositions provide latent variable representations
- Lots of work to be done

1. Theoretical: asymptotics, sampling frame, MDL
2. Methodological: Rank selection, regularization
3. Computational: MCMC, VB, other approximate solutions.

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