NETWORKS 2021

11005. Network Models and Graphical Models: A Survey

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Networks 2021, Session S65. Machine Learning

Scope

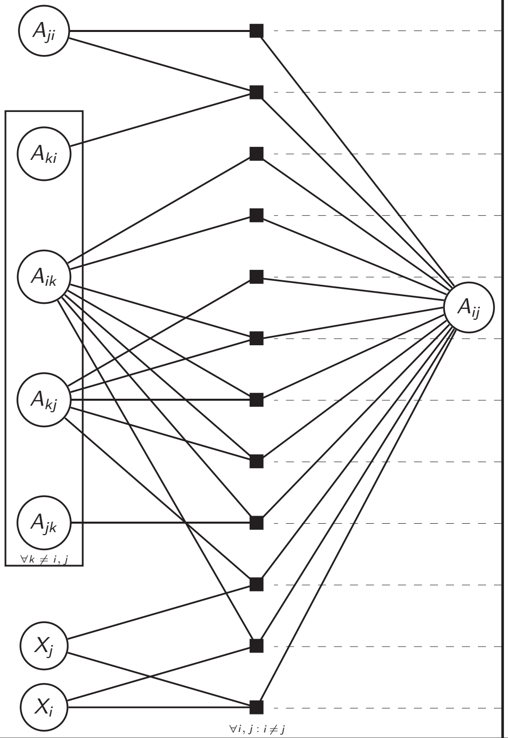
- Network models represent dependencies with graphs; graphical models (one type of which are "Bayesian networks") represent dependencies with graphs. That causes confusion. But they are very different!
- Graphical models haven't done the best job at networks, and networks haven't made use of graphical models
- This talk is primarily to clarify (or create!) a *conceptual* connection between these two types of models
- For examples of *applications* of graphical modeling to networks, see, e.g., Farasat et al. (2015), Maier et al. (2014), and Airoldi et al. (2008)

Key points

- **Graphical models** represent *dependencies* (and causal relationships) *between variables*
- **Networks models** are models of dyads, which represent *dependencies between observations*
  - Dyads can be modeled as random variables (e.g., Bernoulli for unweighted; Poisson for count; etc.)
  - Dyads are themselves dependent! (reciprocity, triadic closure, degree constraints)
  - Graphical models can represent these “dyadic dependencies”!

Key visualization

Terms: Snijders et al. (2006). From (old) joint work with Antonis Manousis and Naji Shajarisales.



Factor graph	Parameter name	Network Motif	Parameterization	Matrix notation
	mutual dyads		$\sum_{i<j} A_{ij}A_{ji}$	$\frac{1}{2}\,\mathrm{tr}\left(\mathbf{AA}^T\right)$
	in-two-stars		$\sum_{(i,j,k)} A_{ji}A_{ki}$	$\mathrm{sum}\left(\mathbf{AA}^T\right) - \mathrm{tr}\left(\mathbf{AA}^T\right)$
	out-two-stars		$\sum_{(i,j,k)} A_{ij}A_{ik}$	$\mathrm{sum}\left(\mathbf{A}^T\mathbf{A}\right) - \mathrm{tr}\left(\mathbf{A}^T\mathbf{A}\right)$
	geom. weighted out-degrees	—	$\sum_i \exp\left\{-\alpha \sum_k A_{ik}\right\}$	$\mathrm{sum}\left(\exp\{-\alpha\ \mathrm{rowsum}\left(\mathbf{A}\right)\}\right)$
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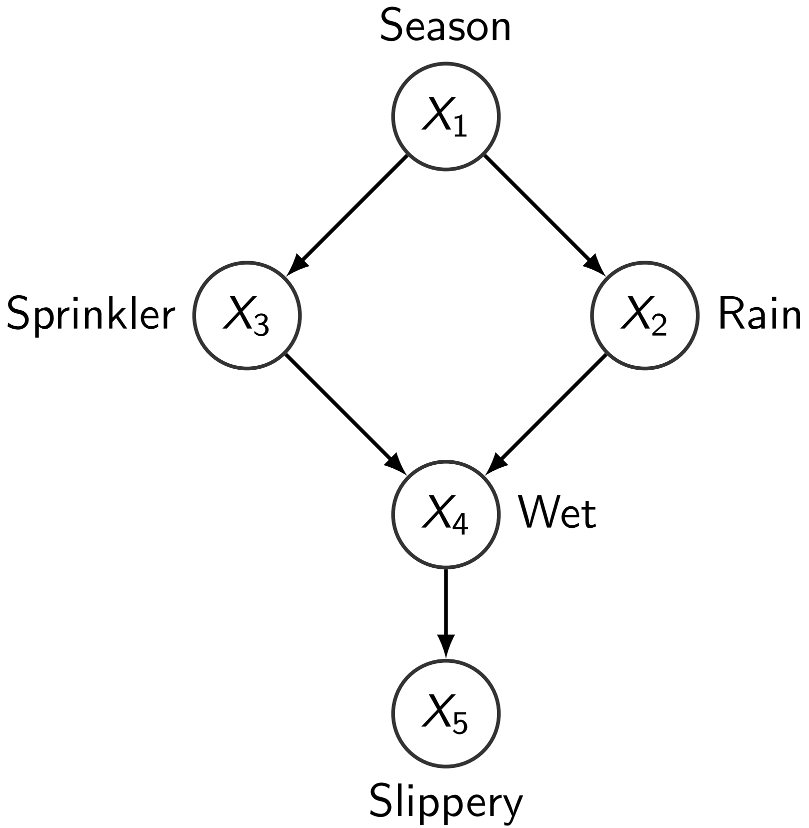
	alternating transitive k-triplets		$\lambda \sum_{i,j} A_{ij} \left\{1-\left(1-\frac{1}{\lambda}\right)^{\sum_{k\neq i,j} A_{ik}A_{kj}}\right\}$	$\lambda\ \mathrm{sum}\left(\mathbf{A}\odot\left(1-\left(1-\frac{1}{\lambda}\right)^{\mathbf{AA}-\mathrm{diag}(\mathbf{AA})}\right)\right)$
	alternating indep. two-paths		$\lambda \sum_{i,j} \left\{1-\left(1-\frac{1}{\lambda}\right)^{\sum_{k\neq i,j} A_{ik}A_{kj}}\right\}$	$\lambda\ \mathrm{sum}\left(1-\left(1-\frac{1}{\lambda}\right)^{\mathbf{AA}-\mathrm{diag}(\mathbf{AA})}\right)$
	two-paths (mixed two-stars)		$\sum_{(i,k,j)} A_{ik}A_{kj}$	$\mathrm{sum}\left(\mathbf{AA}\right) - \mathrm{tr}\left(\mathbf{AA}\right)$
	transitive triads		$\sum_{(i,j,k)} A_{ij}A_{jk}A_{ik}$	$\mathrm{tr}\left(\mathbf{AAA}^T\right)$
	activity effect		$\sum_i X_i \sum_j A_{ij}$	$\mathrm{sum}\left(\mathbf{X}\odot\mathrm{rowsum}\left(\mathbf{A}\right)\right)$
	popularity effect		$\sum_j X_j \sum_i A_{ij}$	$\mathrm{sum}\left(\mathbf{X}\odot\mathrm{colsum}\left(\mathbf{A}\right)\right)$
	similarity effect		$\sum_{i,j} A_{ij}\left(1-\frac{\lvert X_i-X_j\rvert}{\max_{k,l}\lvert X_k-X_l\rvert}\right)$	$\mathrm{sum}\left(\mathbf{A}\odot\mathbf{S}\right)$

What are graphical models?

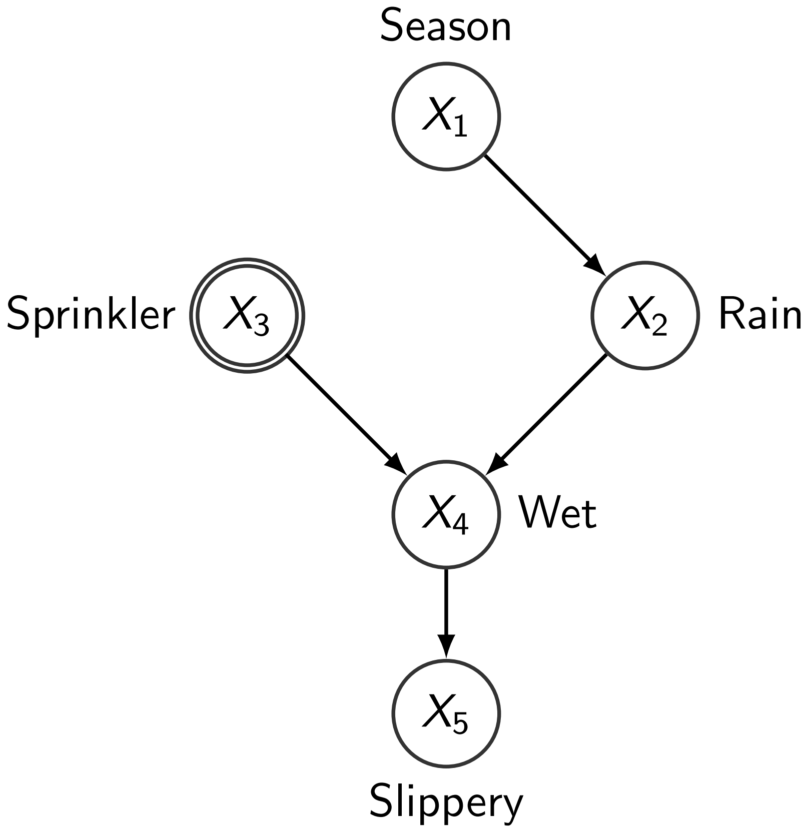
Graphical models = graphs for variables

- Like path diagrams in psych, but more formal. From CS in 90s
- Represent relationships between variables; can reason through dependencies
  - Sprinklers are not directly dependent on Rain, but if we know the grass is wet, we know *either* it rained *or* sprinklers were on (at least one is true)
- With probability distributions on the nodes, they represent *conditional independencies*
  - Equivalent to structural equation modeling (SEMs)!



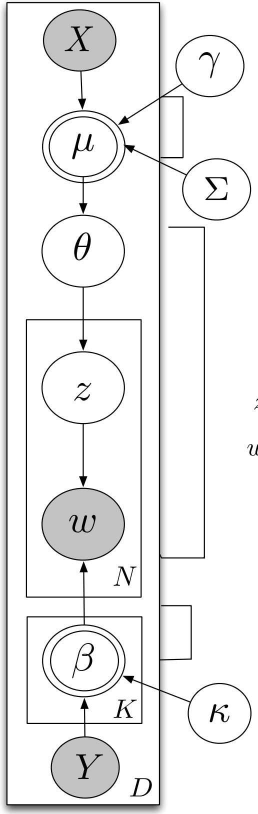
Can represent causality

- Can also reason about *causality*
- Interventions block "paths"
  - Pearl introduced the "do" operator to notate this algebraically
- Are algorithms to determine identifiability of parameters from a given (or assumed) causal structure (Bayes ball)
  - Causal *inference* techniques to estimate a causal graph (e.g., TETRAD algorithm) also exist, but theoretical guarantees for these procedures require strong, untestable, and almost certainly false assumptions



Mostly used for bookkeeping

- Most machine learning applications are effectively "bookkeeping"
- E.g., in structural topic modeling (Roberts et al., 2013), a topic doesn't "cause" a document, but representing it as a directed tie is to help keep track of things for estimation



Topic Prevalence:

$$\mu_{d,k} = X_d \gamma_k$$
$$\gamma_k \sim \mathcal{N}(0, \sigma_k^2)$$
$$\sigma_k^2 \sim \text{Gamma}(s^\gamma, r^\gamma)$$

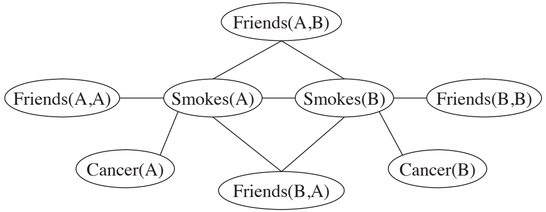
Language Model:

$$\theta_d \sim \text{LogisticNormal}(\mu_d, \Sigma)$$
$$z_{d,n} \sim \text{Mult}(\theta_d)$$
$$w_{d,n} \sim \text{Mult}(\beta_d^{k=z_{d,n}})$$

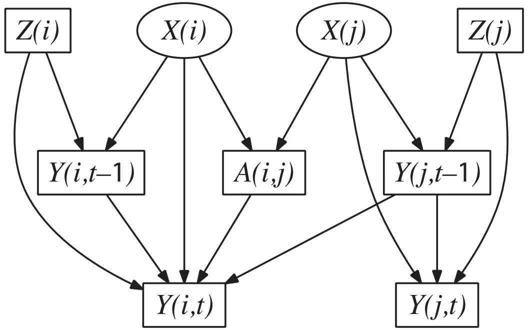
Topical Content:

$$\beta_{d,v}^k \propto \exp(m_v + \kappa_v^{\cdot,k} + \kappa_v^{y,\cdot} + \kappa_v^{y,k})$$
$$\kappa_v^{y,k} \sim \text{Laplace}(0, \tau_v^{y,k})$$
$$\tau_v^{y,k} \sim \text{Gamma}(s^\kappa, r^\kappa)$$

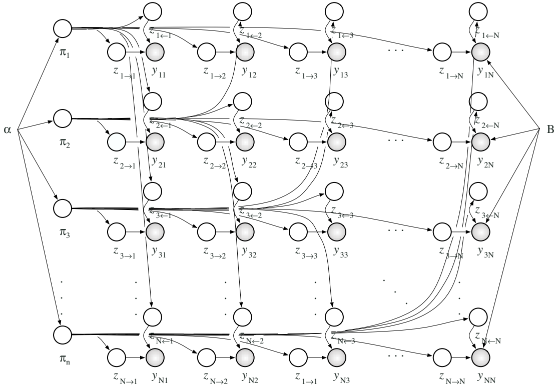
Networks in graphical models



Network edges as graphical model nodes in a "relational Markov network" (Getoor & Taskar, 2007): awkward



Network is only a confounder (Shalizi & Thomas, 2011), no direct dependencies between edges



Full representation, but only of a single type of dependency (block membership) (Airoldi et al., 2008)

Two "directions" of dependencies

- If covariates are independent (trivial graphical model, what we usually assume in linear regression), the joint distribution of a response and a design matrix is:

$$p(Y, \mathbf{X}) = p(Y, X_1, \ldots, X_d) = p(Y | X_1, \ldots, X_d) \prod_{j=1}^{d} p(X_j)$$

- (If we assume fixed $\mathbf{X}$, as we usually do, the probabilities of X_j's go away)
- But a true, complete joint factorization of the conditional distribution would be over *observations* as well:

$$p(Y | \mathbf{X}) = p(y_1, \ldots, y_n | x_{11}, \ldots, x_{1d}, x_{21}, \ldots, x_{2d}, \ldots\ldots, x_{n1}, \ldots, x_{nd})$$

- An iid assumption applies to the *observations*, and are how we even have multiple observations to estimate anything. This looks like:

$$p(Y | \mathbf{X}) = p(y_1, \ldots, y_n | \mathbf{x}_1, \ldots, \mathbf{x}_n) \stackrel{\text{iid}}{=} \prod_{i=1}^{n} p(y_i | \mathbf{x}_i)$$

Parameterizing network models

Networks: Dependencies as observations

Better way of looking at networks: make dyads the observations

- The response is now an edge, or edge attribute
- Transform all node covariates into edge covariates, e.g.,
  - As a difference between continuous node attributes
  - Indicator for if nodes in same category or not (or, make new categories out of possible pairs, e.g., M→M, M→F, F→M, F→F)
  - As "sender" and/or "receiver" attributes

	Y	X_1	X_2	$\cdots$	X_d
1	y_1	x_{11}	x_{12}	$\cdots$	x_{1d}
2	y_2	x_{21}	x_{22}	$\cdots$	x_{2d}
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
n	y_n	x_{n1}	x_{n2}	$\cdots$	x_{nd}

index	*from*	*to*	Y	W_1	W_2	W_3	$\cdots$
e_1	1	2	y_{12}	$\mathbf{1}(x_{11} = x_{21})$	$x_{12} - x_{22}$	x_{13}	$\cdots$
e_2	2	3	y_{23}	$\mathbf{1}(x_{11} = x_{31})$	$x_{12} - x_{32}$	x_{13}	$\cdots$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	
e_{n+1}	2	1	y_{21}	$\mathbf{1}(x_{21} = x_{11})$	$x_{22} - x_{12}$	x_{23}	$\cdots$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	
$e_{2\binom{n}{2}}$	$n-1$	n	$y_{(n-1)n}$	$\mathbf{1}(x_{(n-1)1} = x_{n1})$	$x_{(n-1)2} - x_{n2}$	$x_{(n-1)3}$	$\cdots$

Parameterizing

- Descriptively,

$$a_{ij} = \begin{cases} 1 \text{ if there is a tie } i \to j \\ 0 \text{ otherwise.} \end{cases}$$

- Turn this into a random variable:

$$A_{ij} \overset{\text{iid}}{\sim} \text{Bernoulli}\,(p)$$

As a logistic regression

- Add some covariates and it can become a logistic regression:

$$A_{ij} | x_i, x_j \sim \text{Bernoulli}\left(f(x_i, x_j)^T \boldsymbol{\beta}\right)$$

$$\mathcal{L}(\boldsymbol{\beta}) = \prod_{i=1}^{n} \prod_{j \neq i} f(x_i, x_j)^T \boldsymbol{\beta}^{a_{ij}} \left(f(x_i, x_j)^T \boldsymbol{\beta}\right)^{1-a_{ij}}$$

- The MLE of an intercept-only model is just the density.

$$\widehat{\beta}_{MLE} = \frac{1}{2 \times \binom{n}{2}} \sum_{i \neq j} a_{ij}$$

Problem: Dyads are dependent, too

- In the language of ERGMs, "dyadic dependencies"
  - Social networks: reciprocity makes $A_{ij} \not\perp\!\!\!\perp A_{ji}$
- The p_1 model (Holland & Leinhardt, 1981) deals with reciprocity as a one-off dependency by modeling edges as multinomial, with a cross term:

$$\begin{aligned}\mathbb{P}(A_{ij} = a_{ij}, A_{ji} = a_{ji}) = \frac{1}{k_{ij}} \exp \{\, & a_{ij}(\mu + \alpha_i + \beta_i) \\ & + a_{ji}(\mu + \alpha_j + \beta_j) \\ & + \rho a_{ij} a_{ji} \,\}\end{aligned}$$

Models for dyadic dependencies

- Stochastic blockmodels (Wang & Wong, 1987): alternative to p_1, two-level hierarchical version of Bernoulli model
- Latent space models (Hoff et al., 2002): can be seen as graphical models with observable nodes for edges, produced from hidden nodes representing latent position

Markov property for network edges

- Landmark work: Frank & Strauss (1986)
- Markov dependence assumption: "A graph is said to be a Markov graph if only incident dyads can be conditionally dependent."
- In retrospect, we can clarify this in terms of graphical models
  - The "graph" is the network, and the Markov property is of the graphical model of the network edges as Bernoulli variables

Markov property for network edges

- Remarkably, using Hammersley-Clifford, Frank & Strauss proved that the graphical model of an undirected network is Markov if and only if

$$P_\theta(\mathbf{A}) = \frac{1}{\kappa(\boldsymbol{\theta})} \exp\left\{ \theta_0 L(\mathbf{A}) + \sum_{k=1}^{n-1} \theta_k S_k(\mathbf{A}) + \theta_\tau T(\mathbf{A}) \right\}$$

Normalization constant: need to sum over $2^{2\times\binom{n}{2}}$ possible networks for each candidate $\boldsymbol{\theta}$

Non-maximal k-stars

Number of triangles

- Especially surprising part (Kolaczyk, 2009): how did triangles come out of this as a sufficient statistic??

Graphical models for networks

General modeling of dyadic dependencies

- This eventually led to Exponential-family Random Graph Models, which can model generic dependencies between edges
- Can add any sufficient statistic, although they can be collinear. E.g., two-paths are collinear with in-degrees, out-degrees, and mutual dyads (Snijders et al., 2006)

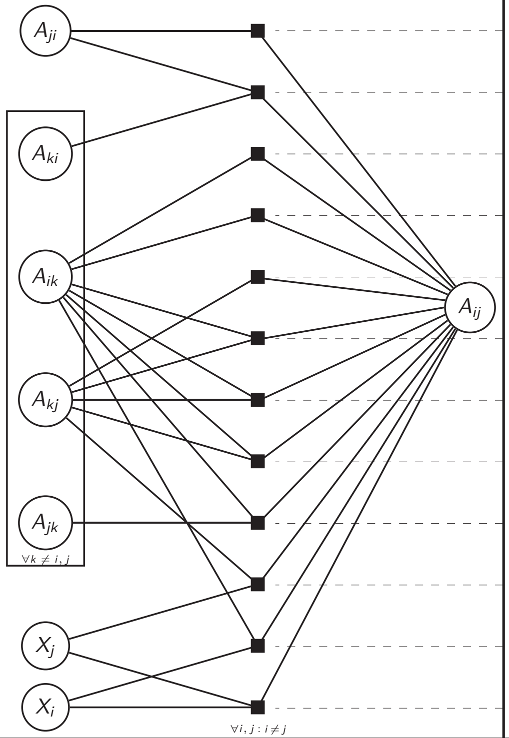
$$\sum_{i,j,k:k\neq i} A_{ij}A_{jk} = \sum_{j=1}^{n}\sum_{i,k:k\neq i} A_{ij}A_{jk} = \sum_{j=1}^{n}\left(A_{+j}A_{j+} - \sum_{i=1}^{n} A_{ij}A_{ji}\right)$$

- But: bad theoretical properties, tricky to estimate, and tricky to specify

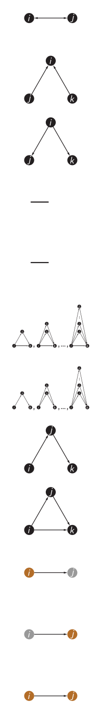
Dyadic dependencies in a graph

Terms: Snijders et al. (2006). From (old) joint work with Antonis Manousis and Naji Shajarisales.

Factor graph



Network Motif



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Conclusions

Key points, redux

- **Graphical models** represent *dependencies* (and causal relationships) *between variables*
- **Networks models** are models of dyads, which represent *dependencies between observations*
- They are not the same thing, but we can represent dyadic dependencies (dependencies between edges of a network, in processes like reciprocity and transitivity) as graphical models

Why should we care?

- Graphical models are network models are both powerful for representing, reasoning through, and modeling dependencies
  - But graphical models haven't done the best job at networks, and networks haven't made use of graphical models
  - Maybe because they are used by different communities, and the same words ("networks", "dependencies") mean subtly different things
- Clarifying the relationship of these two types of models helps head off confusion, as well as deepen our appreciation of the idea of "dependencies"
  - As well as helping to train students
- Practically: Can graphical models help create, and estimate, new statistical network models, and unify existing ones? Almost certainly, although in many cases the estimation will still be MCMC (maybe variational inference; Celisse et al., 2012)

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Scope

Key points

What are graphical models?

Parameterizing network models

Graphical models for networks

Conclusions

References

References

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