Generative Models for Complex Network Structure

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- **what is structure?**

- generative models for complex networks
  - general form
  - types models
  - opportunities and challenges

- weighted stochastic block models
  - a parable about thresholding
  - checking our models
  - learning from data (approximately)

what is structure?

- makes data different from noise
  - makes a network different from a random graph

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- helps us compress the data
  - describe the network succinctly
  - capture most relevant patterns

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- helps us compress the data
  - describe the network succinctly
  - capture most relevant patterns
- helps us generalize,
  from data we've seen to data we haven't seen:
  i. from one part of network to another
  ii. from one network to others of same type
  iii. from small scale to large scale (coarse-grained structure)
  iv. from past to future (dynamics)

statistical inference

- imagine graph G is drawn from an ensemble or **generative model**: a probability distribution $P(G \mid \theta)$ with parameters θ
- θ can be continuous or discrete; represents structure of graph

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- if θ is partly known, constrain inference and determine the rest
- if G is partly known, infer θ and use $P(G \mid \theta)$ to generate the rest
- if model is good fit (application dependent), we can generate synthetic graphs structurally similar to G
- if part of G has low probability under model, flag as possible anomaly

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generative models for complex networks

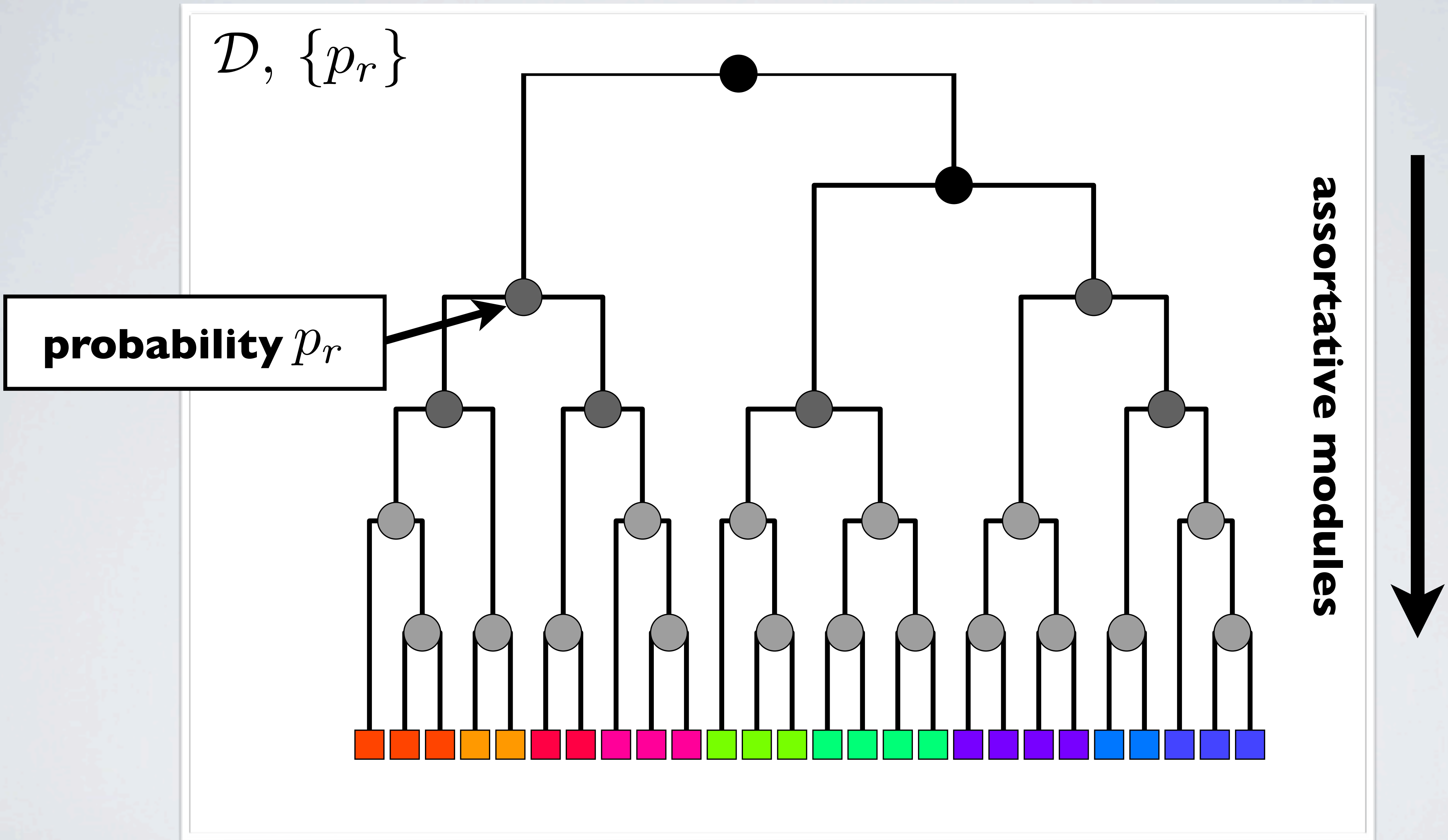
general form

$$P(G \,|\, \theta) = \prod_{i<j} P(A_{ij} \,|\, \theta)$$

assumptions about "structure" go into $P(A_{ij} \,|\, \theta)$

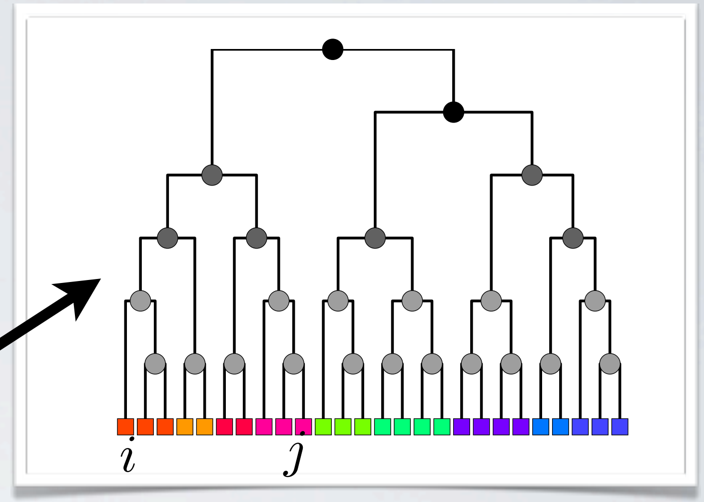
consistency $\lim_{n\to\infty} \Pr\left(\hat{\theta} \neq \theta\right) = 0$

requires that edges be conditionally independent [Shalizi, Rinaldo 2011]

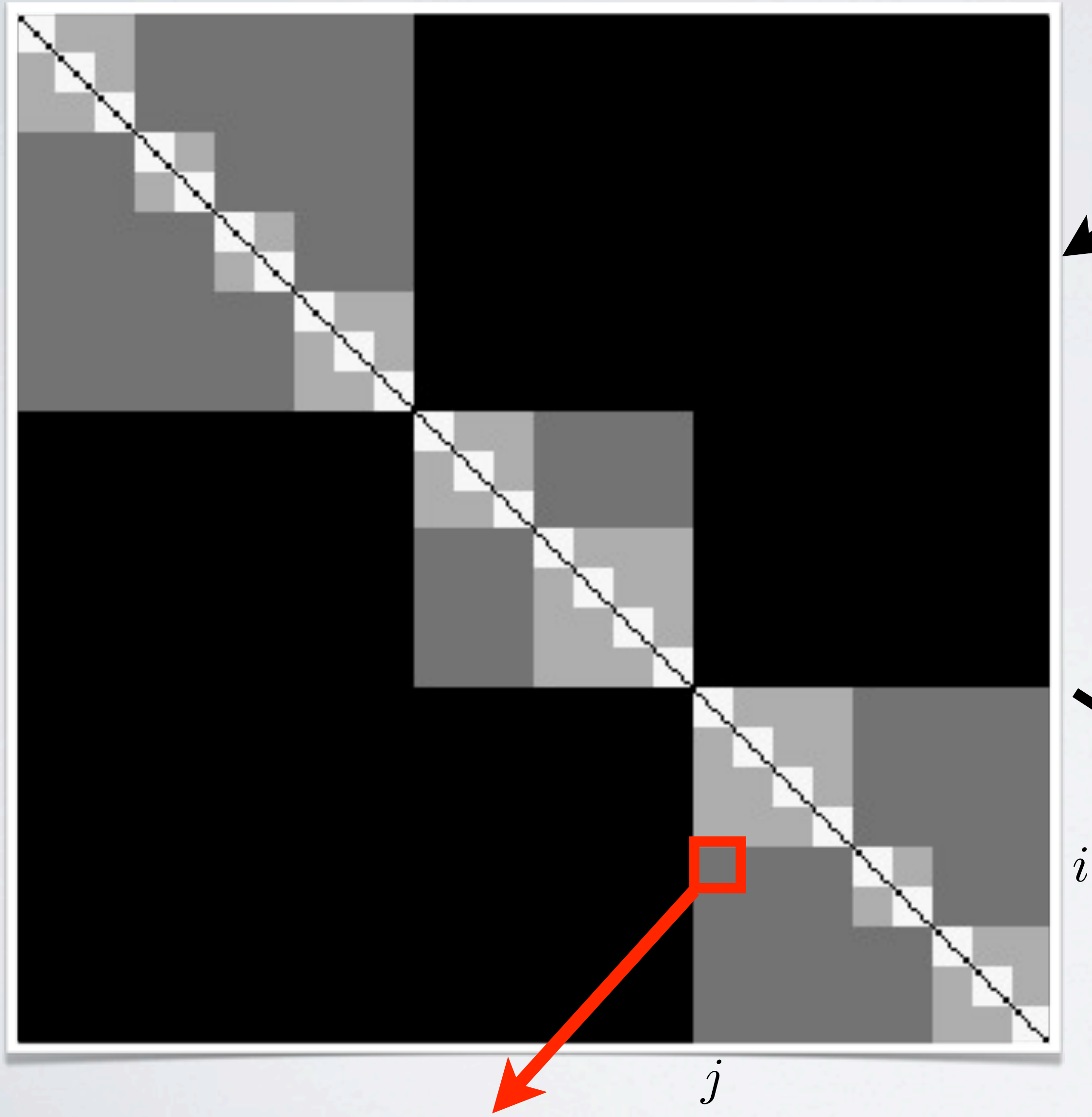


$\mathcal{D},\ \{p_r\}$
probability p_r
assortative modules

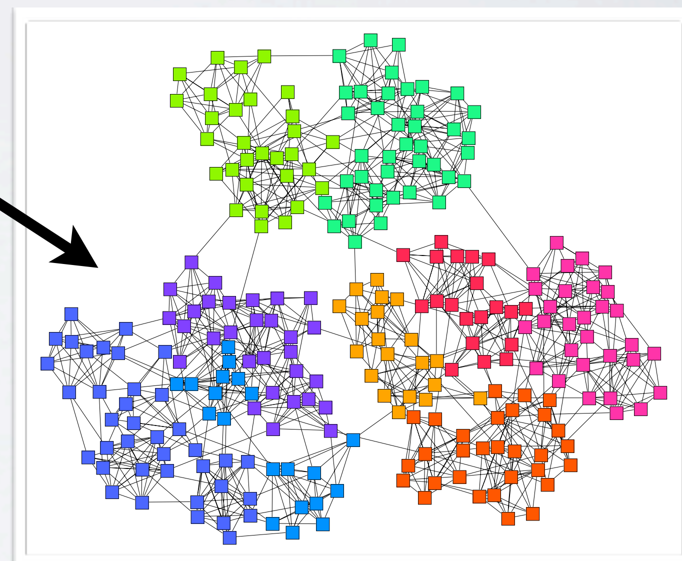
model



hierarchical random graph

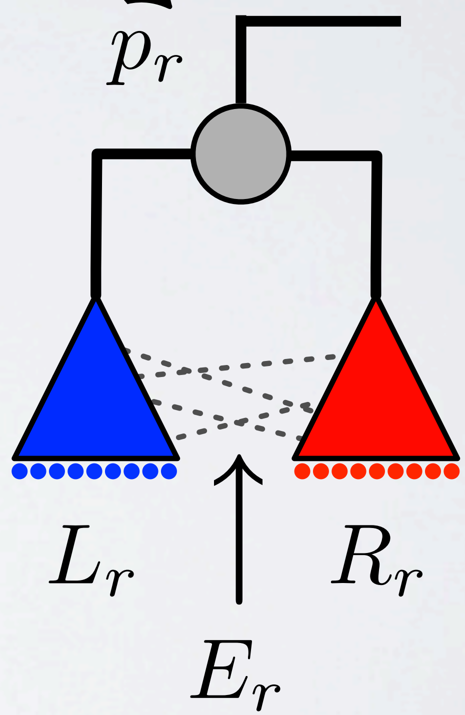


instance



$$\Pr(i, j \text{ connected}) = p_r$$
$$= p_{(\text{lowest common ancestor of } i,j)}$$

$$\mathcal{L}(\mathcal{D},\, \{p_r\}) = \prod_r \underline{p_r^{E_r}\,(1-p_r)^{L_r R_r - E_r}}$$



L_r = number nodes in left subtree

R_r = number nodes in right subtree

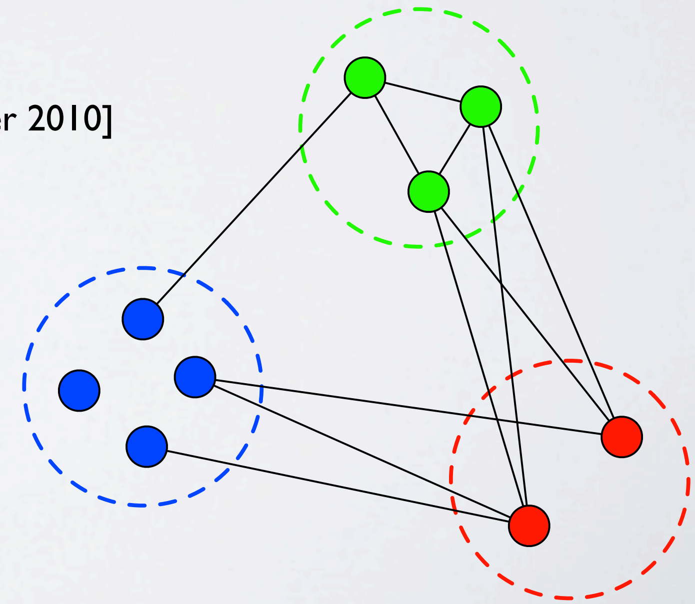
E_r = number edges with r as lowest common ancestor

classes of generative models

- stochastic block models

k types of vertices, $P(A_{ij} \,|\, z_i, z_j)$ depends only on types of *i, j*
originally invented by sociologists [Holland, Laskey, Leinhardt 1983]

many, many flavors, including
mixed-membership SBM [Airoldi, Blei, Feinberg, Xing 2008]
hierarchical SBM [Clauset, Moore, Newman 2006,2008]
restricted hierarchical SBM [Leskovec, Chakrabarti, Kleinberg, Faloutsos 2005]
infinite relational model [Kemp, Tenenbaum, Griffiths, Yamada, Ueda 2006]
restricted SBM [Hofman, Wiggins 2008]
degree-corrected SBM [Karrer, Newman 2011]
SBM + topic models [Ball, Karrer, Newman 2011]
SBM + vertex covariates [Mariadassou, Robin, Vacher 2010]
SBM + edge weights [Aicher, Jacobs, Clauset 2013]
+ many others



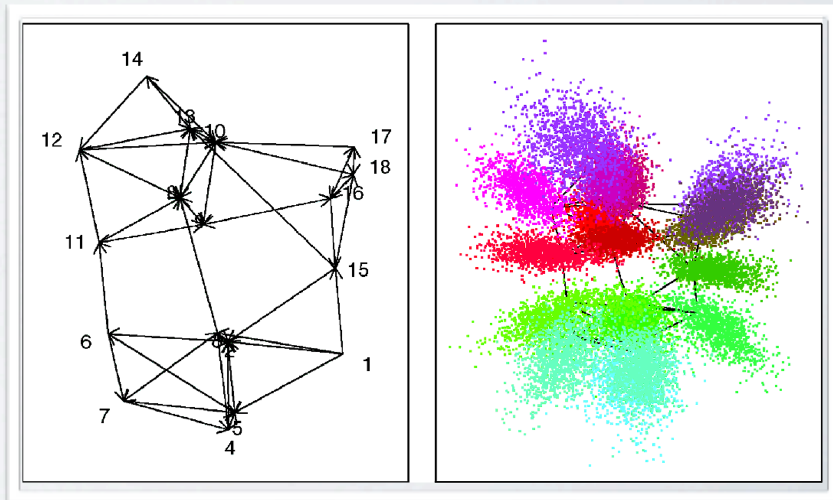
classes of generative models

- latent space models

  nodes live in a latent space, $P(A_{ij} \mid f(x_i, x_j))$ depends only on vertex-vertex proximity

  many, many flavors, including

  logistic function on vertex features [Hoff, Raftery, Handcock 2002]
  social status / ranking [Ball, Newman 2013]
  nonparametric metadata relations [Kim, Hughes, Sudderth 2012]
  multiple attribute graphs [Kim, Leskovec 2010]
  nonparametric latent feature model [Miller, Griffiths, Jordan 2009]
  infinite multiple memberships [Morup, Schmidt, Hansen 2011]
  ecological niche model [Williams, Anandanadesan, Purves 2010]
  hyperbolic latent spaces [Boguna, Papadopoulos, Krioukov 2010]



opportunities and challenges

- richly annotated data

  edge weights, node attributes, time, etc.

  = new classes of generative models

- generalize from $n = 1$ to ensemble

  useful for modeling checking, simulating other processes, etc.

- many familiar techniques

  frequentist and Bayesian frameworks

  makes probabilistic statements about observations, models

  predicting missing links $\approx$ leave-*k*-out cross validation

  approximate inference techniques (EM, VB, BP, etc.)

  sampling techniques (MCMC, Gibbs, etc.)

- learn from partial or noisy data

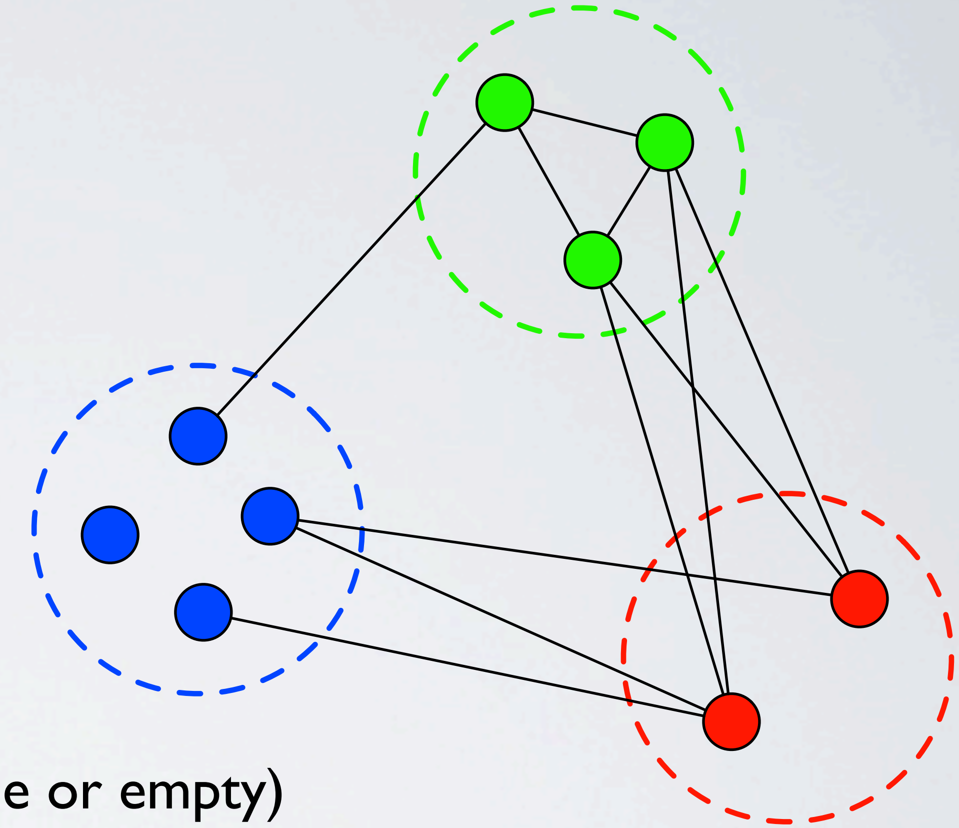
  extrapolation, interpolation, hidden data, missing data

opportunities and challenges

- only two classes of models
  - stochastic block models
  - latent space models
- bootstrap / resampling for network data
  - critical missing piece
  - depends on what is independent in the data
- model comparison
  - naive AIC, BIC, marginalization, LRT can be wrong for networks
  - what is goal of modeling: realistic representation or accurate prediction?
- model assessment / checking?
  - how do we know a model has done well? what do we check?
- what is *v*-fold cross-validation for networks?
  - Omit n^2/v edges? Omit n/v nodes? What?

- what is structure?
- generative models for complex networks
    - ➤ general form
    - ➤ types models
    - ➤ opportunities and challenges
- **weighted stochastic block models**
    - ➤ a parable about thresholding
    - ➤ learning from data (approximately)
    - ➤ checking our models

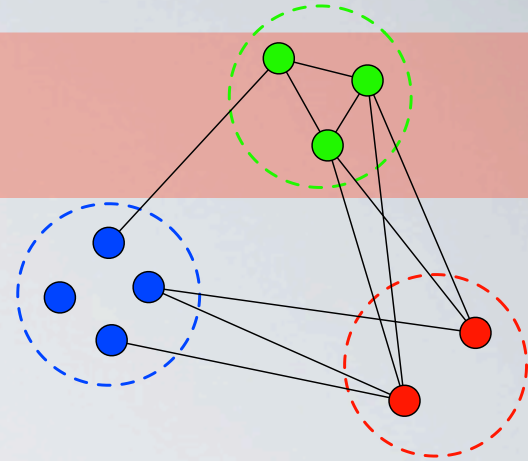
stochastic block models



functional groups, not just clumps

- social "communities" (large, small, dense or empty)
- social: leaders and followers
- word adjacencies: adjectives and nouns
- economics: suppliers and customers

classic stochastic block model



nodes have discrete attributes

each vertex i has type $t_i \in \{1, \ldots, k\}$

$k \times k$ matrix p of connection probabilities

if $t_i = r$ and $t_j = s$, edge $(i \to j)$ exists with probability p_{rs}

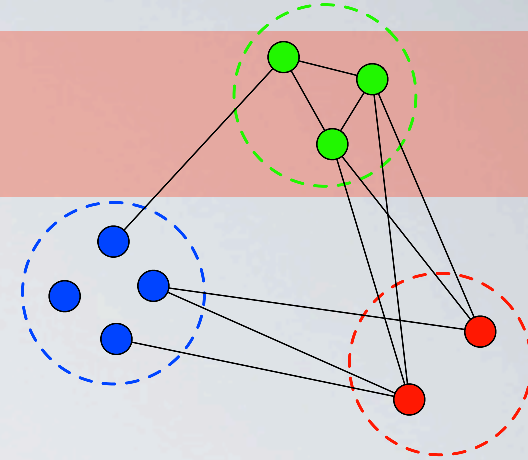
p not necessarily symmetric, and we do not assume $p_{rr} > p_{rs}$

given some G, we want to simultaneously

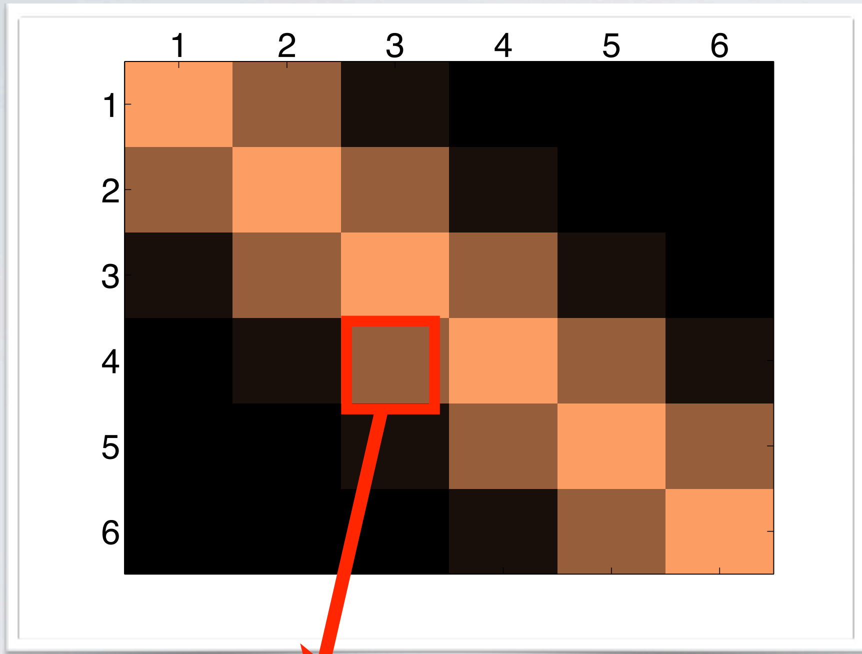
label nodes (infer type assignment $t : V \to \{1, \ldots, k\}$)

learn the latent matrix p

classic stochastic block model



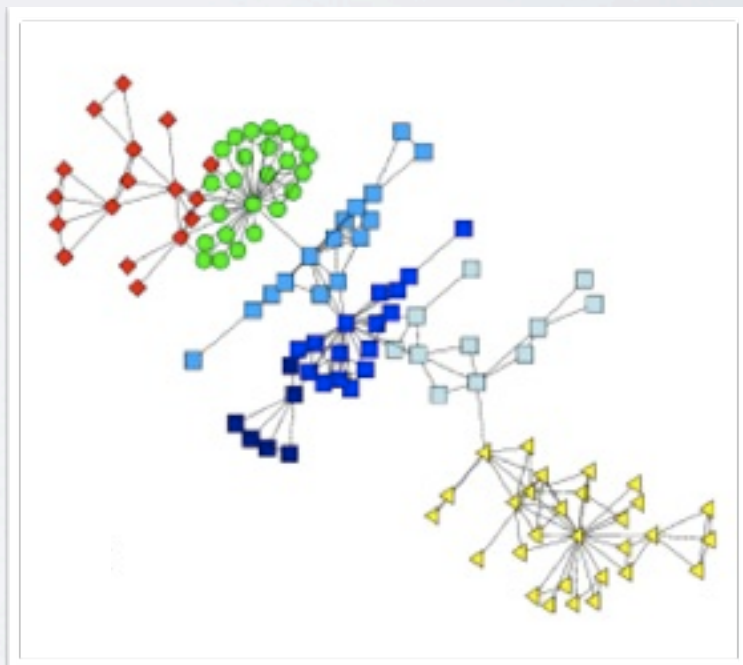
model



assortative modules

$$\Pr(\text{node in } i \text{ connected to node in } j) = p_{i,j}$$

instance



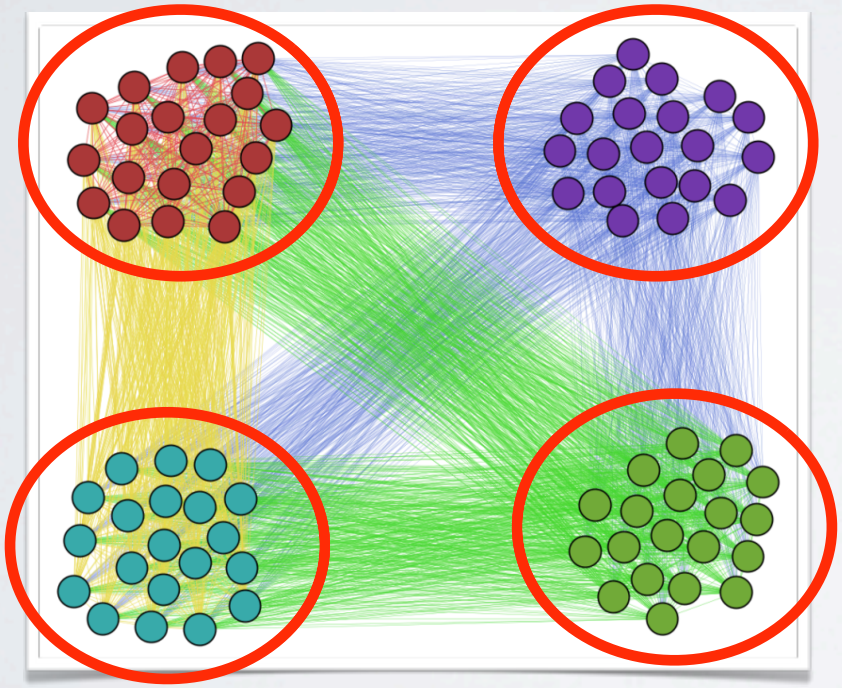
likelihood

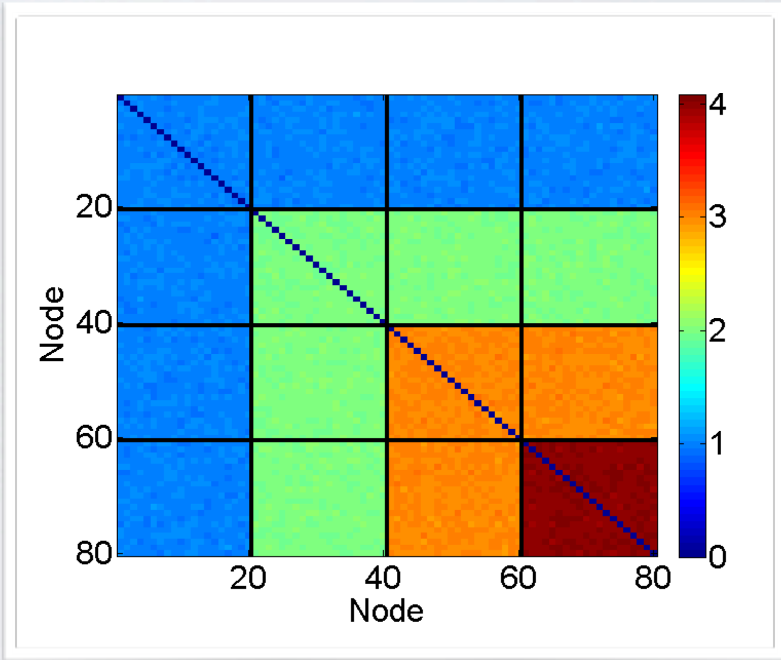
$$P(G \,|\, t, \theta) = \prod_{(i,j) \in E} p_{t_i,t_j} \prod_{(i,j) \notin E} (1 - p_{t_i,t_j})$$

thresholding edge weights

- 4 groups
- edge weights $\sim N(\mu_i, \sigma^2)$ with $\mu_1 < \mu_2 < \mu_3 < \mu_4$

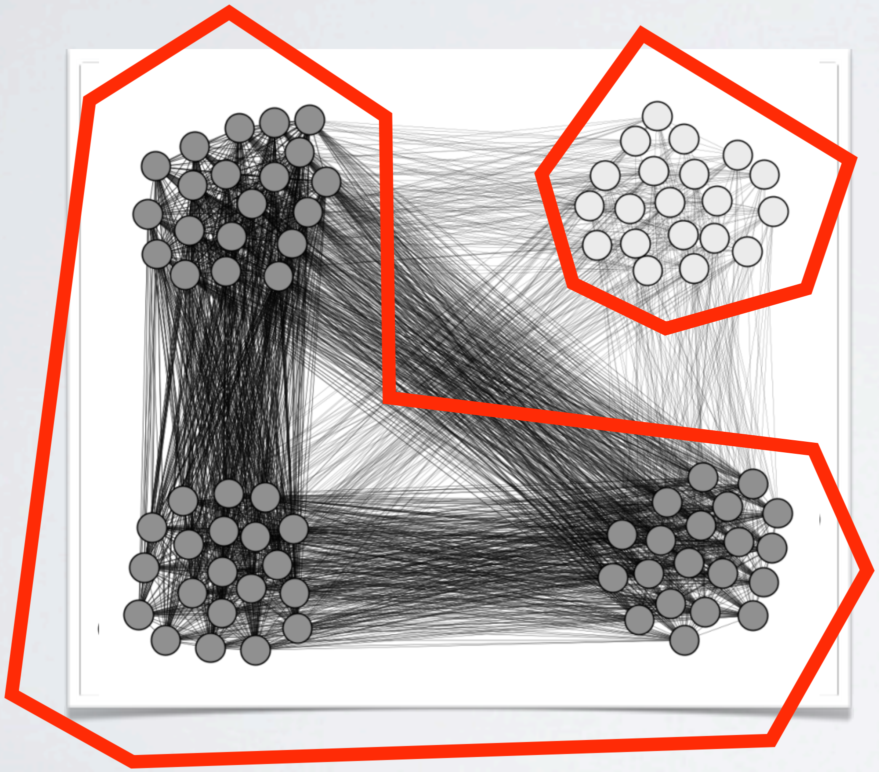
➤ what threshold t should we choose? $t = 1, 2, 3, 4$

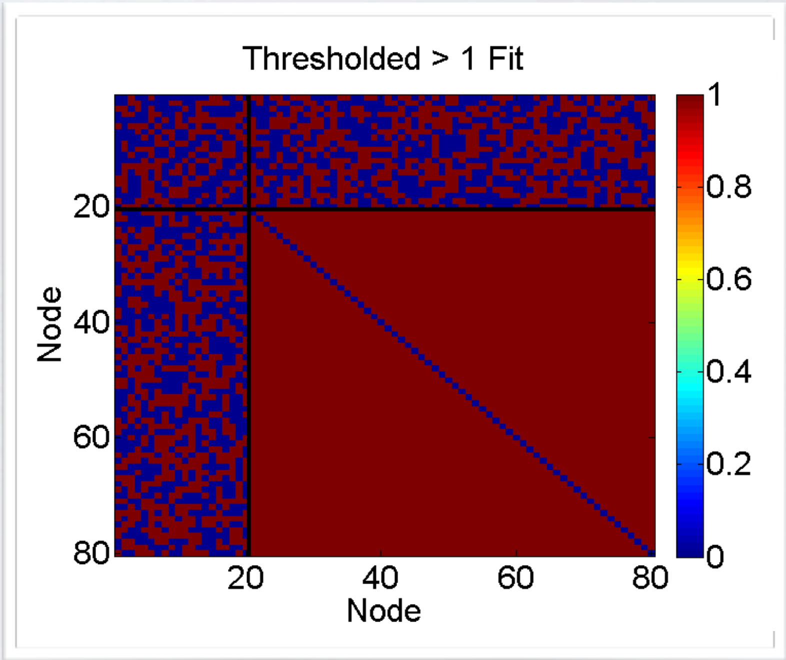




- 4 groups
- edge weights $\sim N(\mu_i, \sigma^2)$ with $\mu_1 < \mu_2 < \mu_3 < \mu_4$

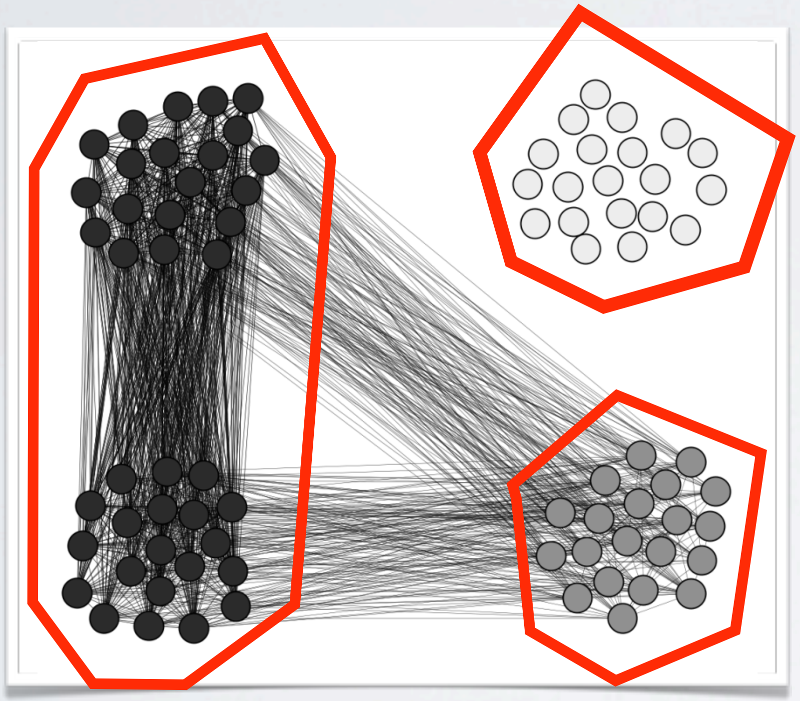
➤ set threshold $t \leq 1$, fit SBM

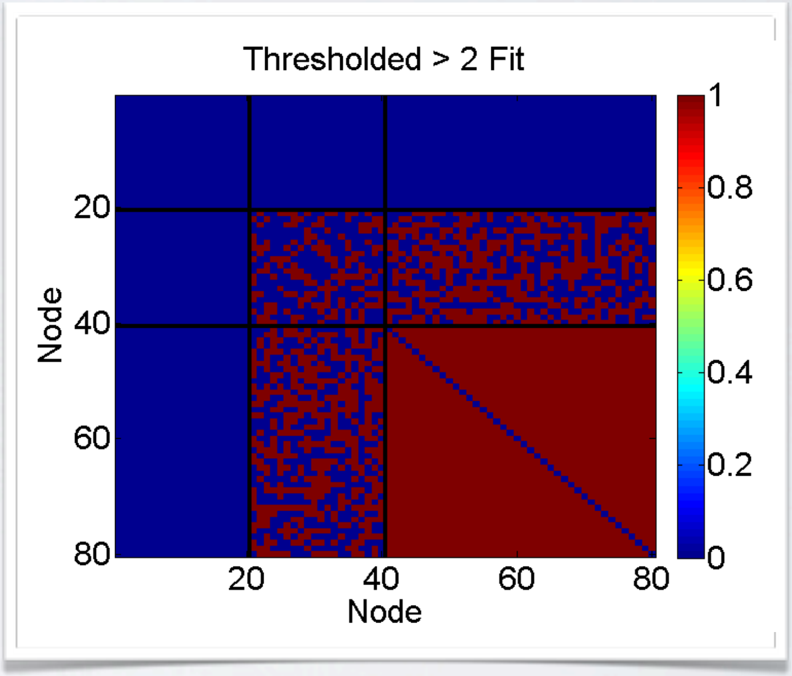




- 4 groups
- edge weights $\sim N(\mu_i, \sigma^2)$ with $\mu_1 < \mu_2 < \mu_3 < \mu_4$

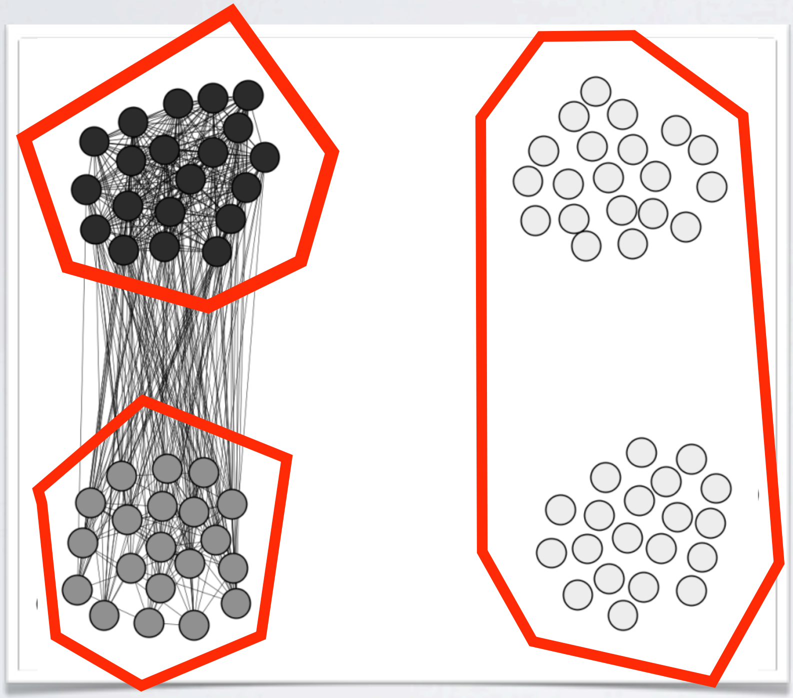
➤ set threshold $t = 2$, fit SBM

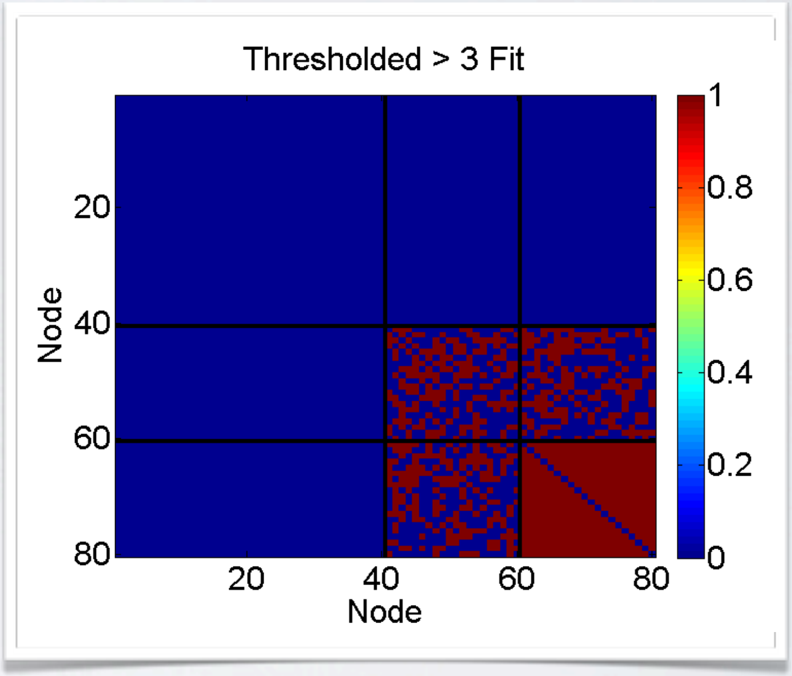




- 4 groups
- edge weights $\sim N(\mu_i, \sigma^2)$ with $\mu_1 < \mu_2 < \mu_3 < \mu_4$

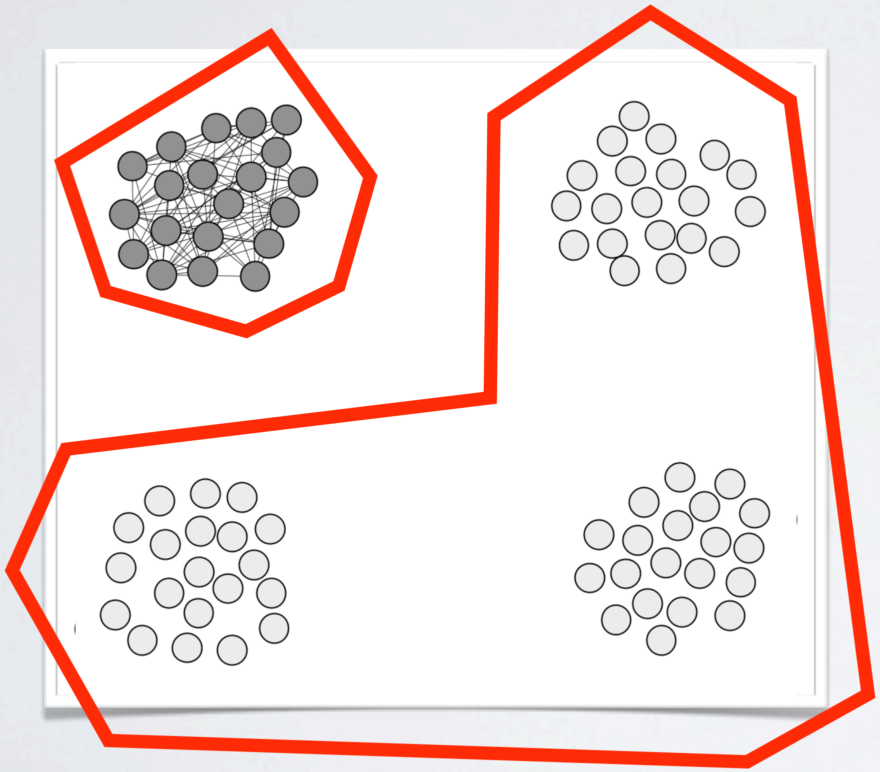
➤ set threshold $t = 3$, fit SBM

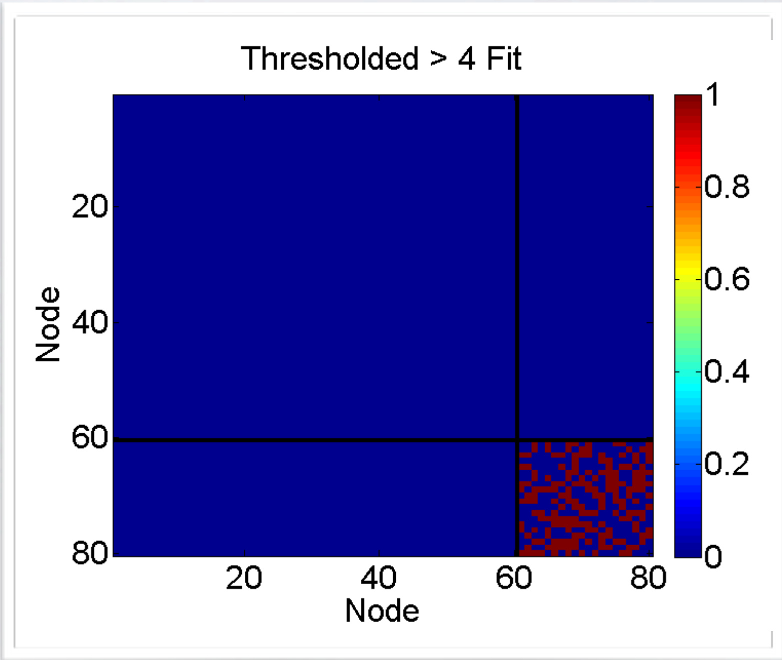




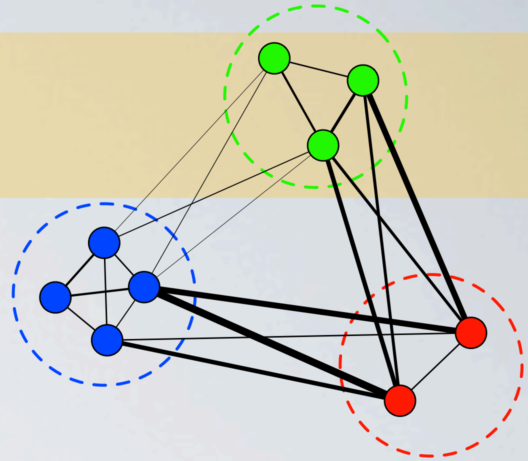
- 4 groups
- edge weights $\sim N(\mu_i, \sigma^2)$ with $\mu_1 < \mu_2 < \mu_3 < \mu_4$

➤ set threshold $t \geq 4$, fit SBM





weighted stochastic block model



adding auxiliary information:

each edge has weight $w(i,j)$

let $w(i,j) \sim f(x|\theta)$

$$= h(x) \exp(T(x) \cdot \eta(\theta))$$

➤ covers all exponential-family type distributions:

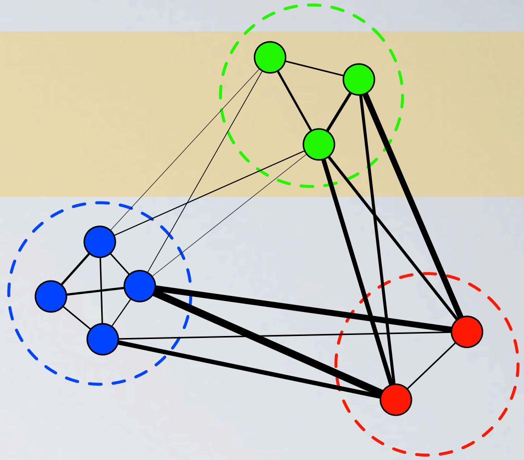
bernoulli, binomial (classic SBM), multinomial

poisson, beta

exponential, power law, gamma

normal, log-normal, multivariate normal

weighted stochastic block model



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let $w(i,j) \sim f(x|\theta)$

$$= h(x)\exp(T(x)\cdot\eta(\theta))$$

- examples of weighted graphs:

  frequency of social interactions (calls, txt, proximity, etc.)

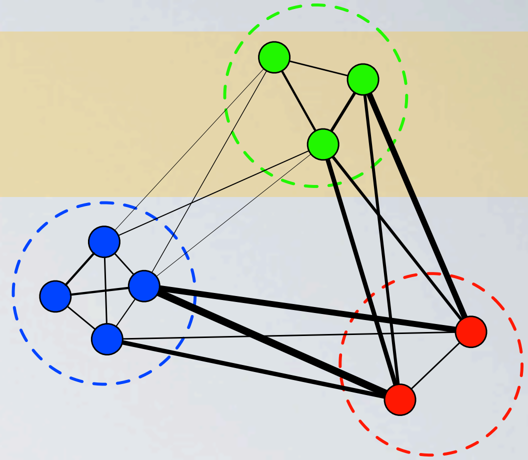
  cell-tower traffic volume

  other similarity measures

  time-varying attributes

  missing edges, active learning, etc.

weighted stochastic block model



block structure $\mathcal{R} : k \times k \to \{1, \ldots, R\}$

weight distribution f

block assignment z

weighted graph G

likelihood function: $P(G \mid z, \theta, f) = \prod_{i<j} f\left(G_{i,j} \mid \theta_{\mathcal{R}(z_i, z_j)}\right)$

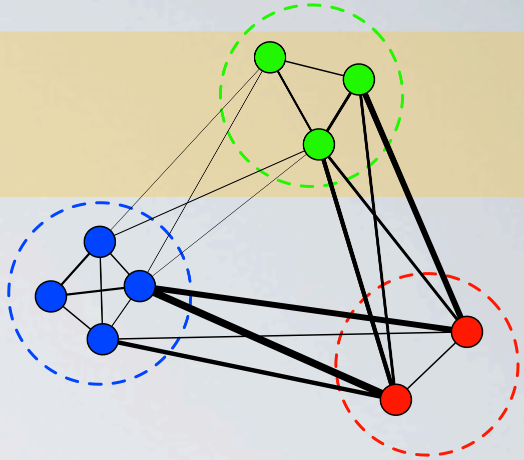
➤ given G and choice of f, learn z and θ

technical difficulties:

degeneracies in likelihood function

(variance can go to zero. oops)

approximate learning

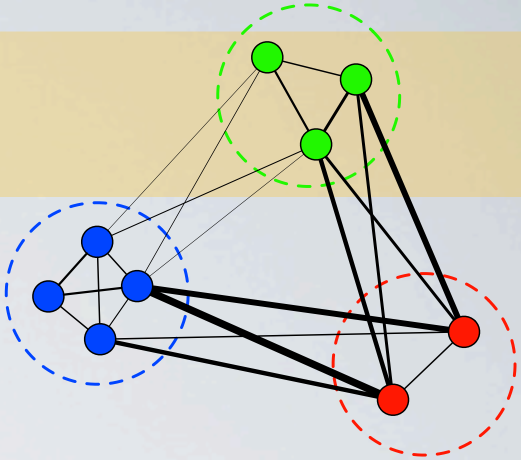


- **edge generative model** $P(G \,|\, z, \theta, f)$
- **estimate model** via variational Bayes

  conjugate priors solve degeneracy problem

  algorithms for dense and sparse graphs

dense weighted SBM



approximate posterior distribution

$$\pi^*(z,\theta\,|\,G) \approx q(z,\theta) = \prod_i q_i(z_i) \prod_r q(\theta_r)$$

- estimate q by minimizing

$$D_{\mathrm{KL}}(q||\pi^*) = \ln P(G\,|\,z,\theta,f) - \mathcal{G}(q)$$

where $\mathcal{G}(q) = \mathbb{E}_q(\mathcal{L}) + \mathbb{E}_q\left(\log \frac{\pi(z,\theta)}{q(z,\theta)}\right)$

for (conjugate) prior π for exponential family distribution f

- taking derivative yields update equations for z,θ
- iterating equations yields local optima

checking the model

synthetic network with known structure

- given synthetic graph with known structure
- run VB algorithm to convergence
- compare against choose threshold + SBM (and others)

compute Variation of Information (partition distance)

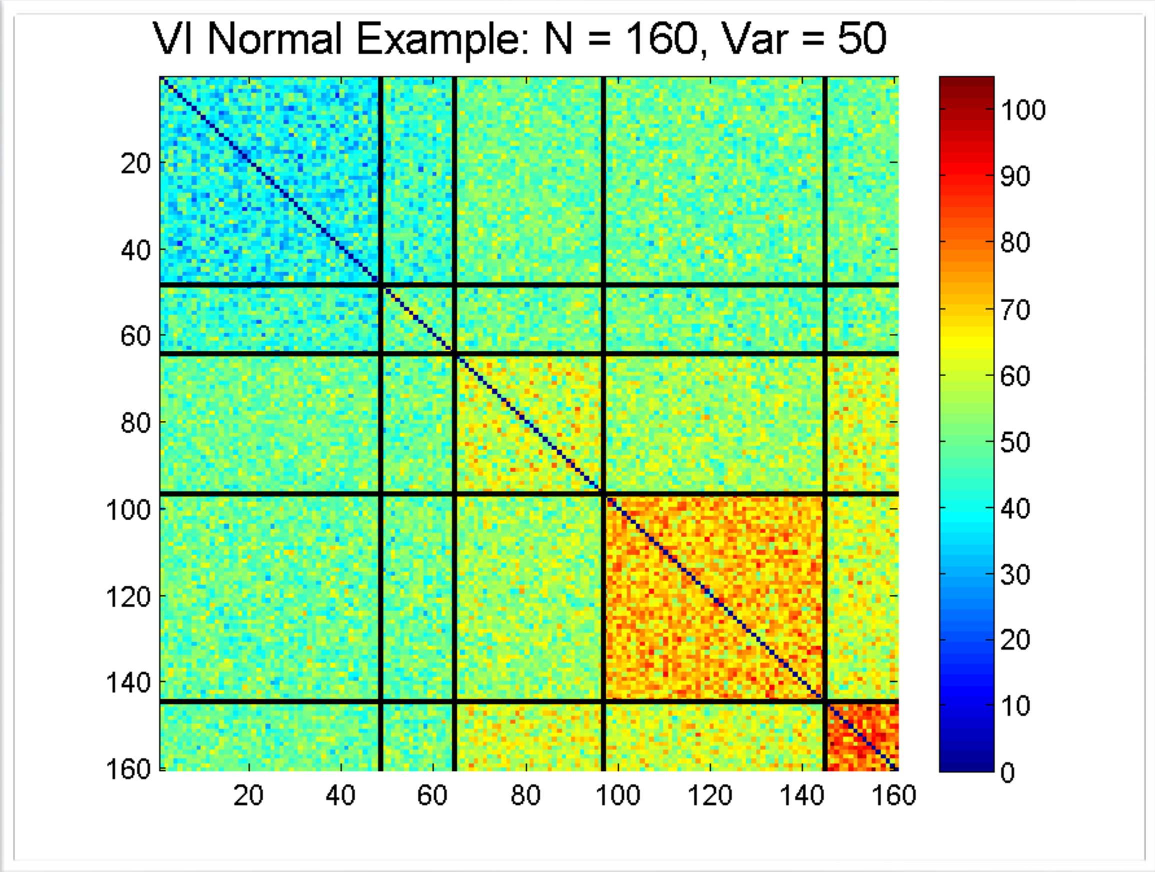
$$\mathrm{VI}(P_1, P_2) \in [0, \ln N]$$

in this case $\mathrm{VI}(P_1, P_2) \in [0, \ln k^* + 1.5] = [0, 3.1]$

checking the model

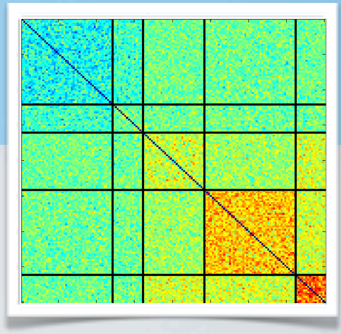
synthetic network with known structure

- variation of Newman's four-groups test
- $k^* = 5$ latent groups
  $n_r = [48, 16, 32, 48, 16]$
- Normal edge weights:
  $f = \mathcal{N}(\mu_r, \sigma_r^2)$



in this case $\mathrm{VI}(P_1, P_2) \in [0, \ln k^* + 1.5] = [0, 3.1]$

learn better with more data

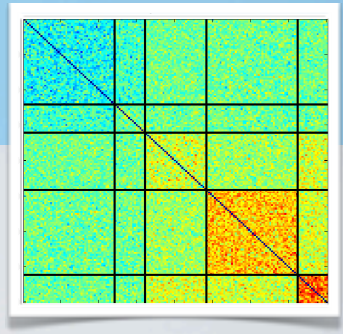


increase network size N

- fix $k = k^*$, $f = \mathcal{N}$
- bigger network, more data

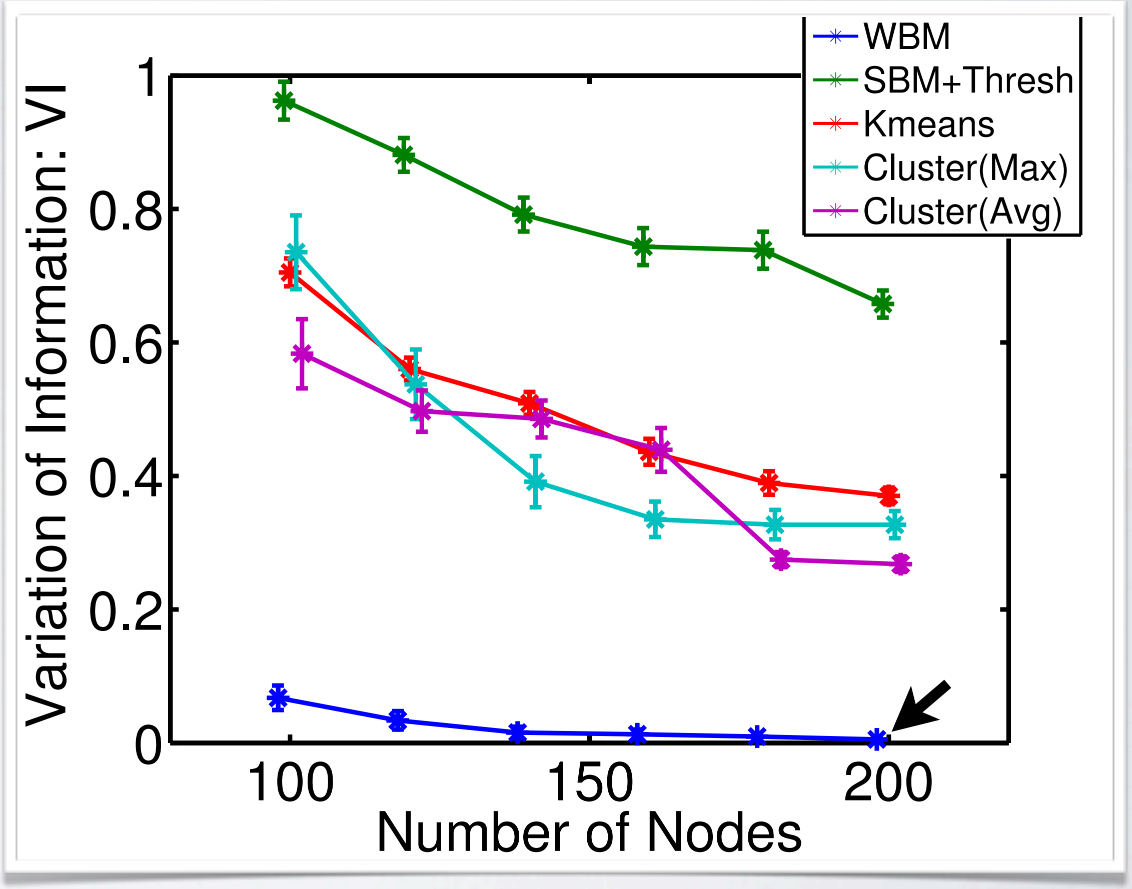
we keep the n_r/N *constant*

learn better with more data



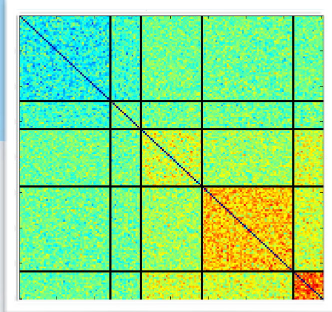
increase network size N

- fix $k = k^*$, $f = \mathcal{N}$
- bigger network, more data
- WSBM converges on correct solution more quickly
- thresholding + SBM particularly bad



we keep the n_r/N *constant*

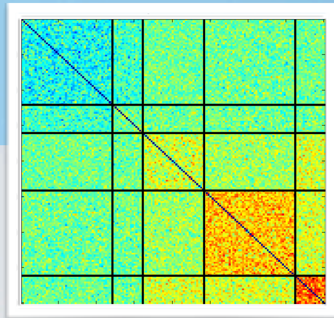
learning the number of groups



vary number of groups found k

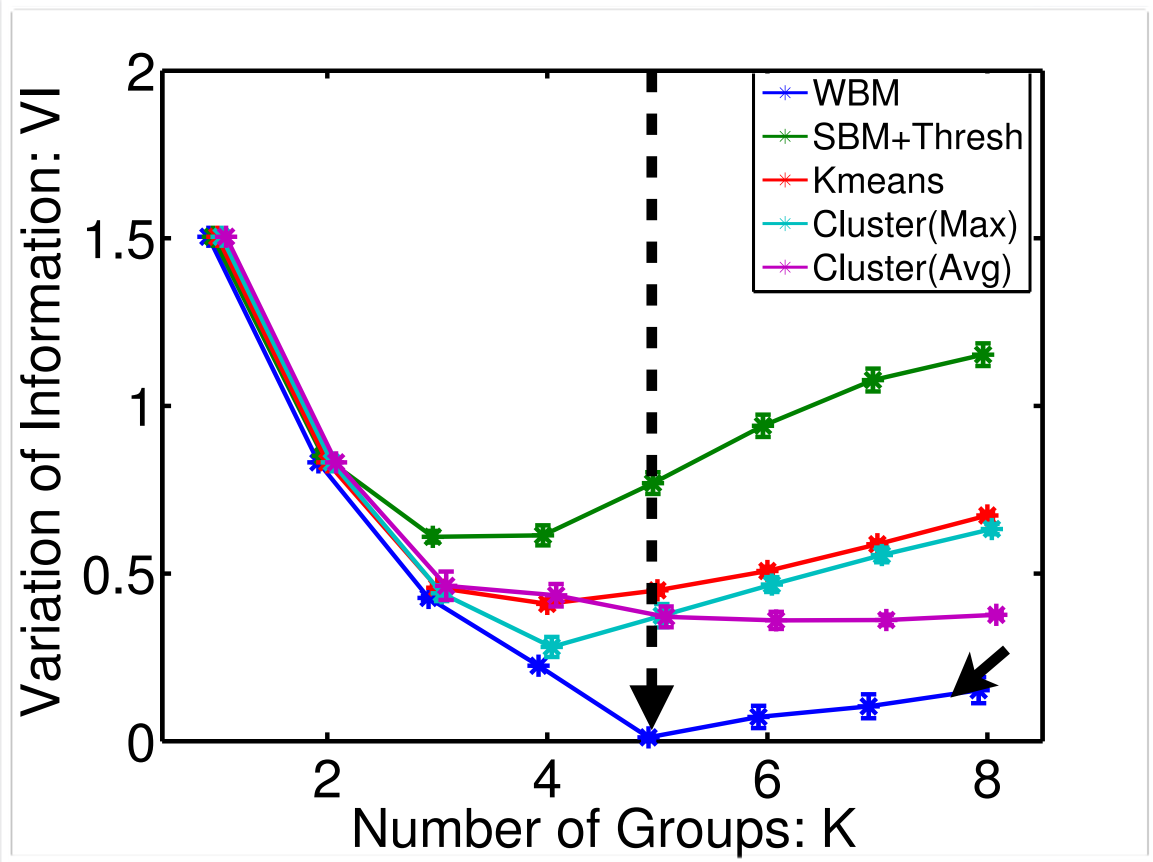
- fix $f = \mathcal{N}$
- too few / many blocks?

learning the number of groups



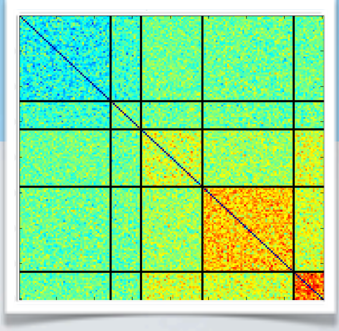
vary number of groups found k

- fix $f = \mathcal{N}$
- too few / many blocks?
- WSBM converges on correct solution
- WSBM fails gracefully when $k > k^*$
- others do poorly



In fact, Bayesian marginalization will correctly choose k=k* in this case.

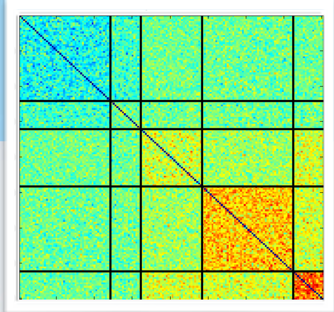
learning despite noise



increase variance in edge weights σ_r^2

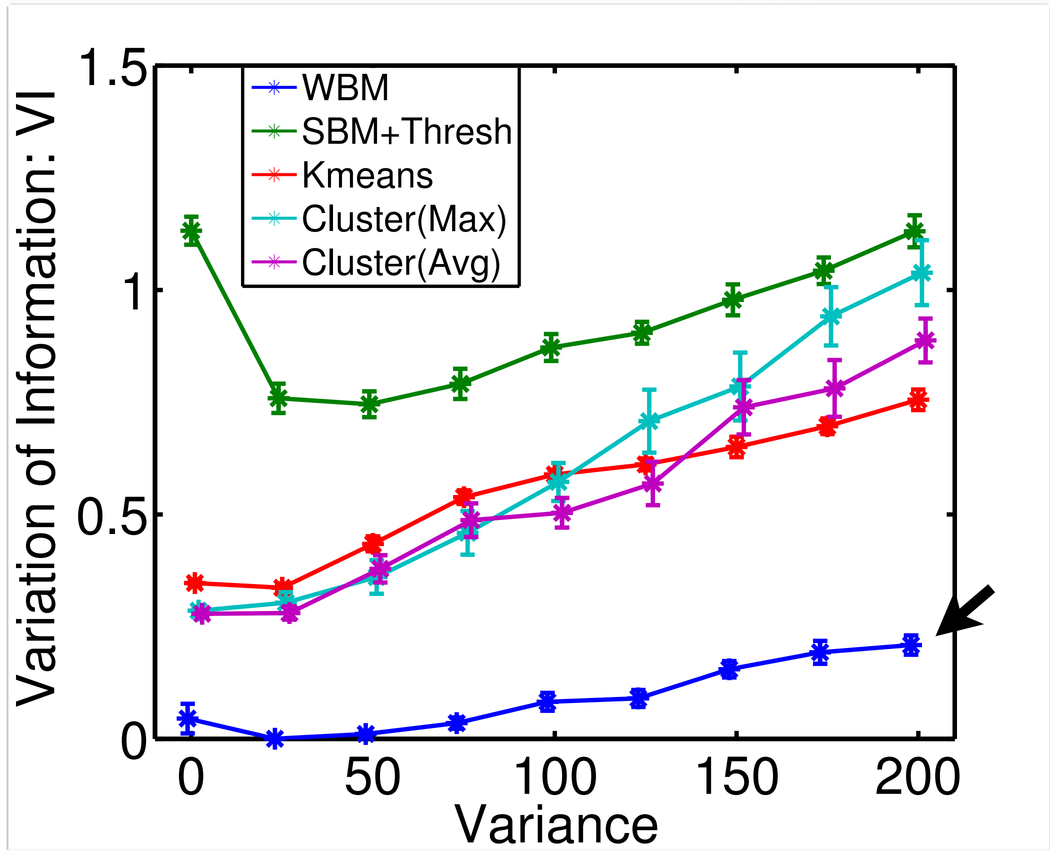
- fix $k = k^*$, $f = \mathcal{N}$
- bigger variance, less signal

learning despite noise



increase variance in edge weights σ_r^2

- fix $k = k^*$, $f = \mathcal{N}$
- bigger variance, less signal
- WSBM fails more gracefully than alternatives, even for very high variance
- thresholding + SBM particularly bad



comments

- single-scale structural inference

  mixtures of assortative, disassortative groups

- inference is cheap (VB)

  approximate inference works well

- thresholding edge weights is bad, bad, bad

  one threshold (SBM) vs. many (WSBM)

- generalizations also for sparse graphs, degree-corrections, etc.

generative models

- auxiliary information
  node & edge attributes, temporal dynamics (beyond static binary graphs)
- scalability
  fast algorithms for fitting models to big data (methods from physics, machine learning)
- model selection
  which model is better? is this model bad? how many communities?
- model checking
  have we learned correctly? check via generating synthetic networks
- partial or noisy data
  extrapolation, interpolation, hidden data, missing data
- anomaly detection
  low probability events under generative model

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some references

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