

Network Inference

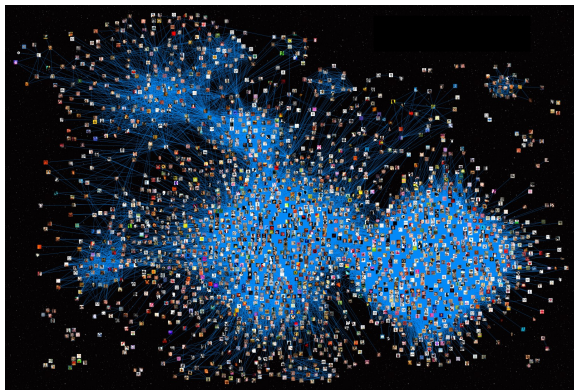
Part 2

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Tehran, August 2018

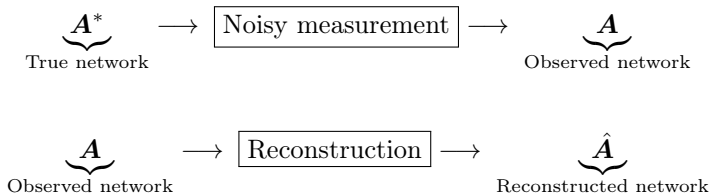
NETWORK MEASUREMENTS ARE NOISY



(A social network)

- ▶ As with any empirical measurement, network data are unreliable.
- ▶ However, very few datasets contain any kind of error estimate!
- ▶ We know there must be errors, but we do not know how many, or where they are located.

NETWORK RECONSTRUCTION TASK



So that $\hat{\mathbf{A}}$ is as close as possible to \mathbf{A}^* .

Caveats:

- ▶ With a single copy of \mathbf{A} .
- ▶ Without knowing how strong the noise is (i.e. the number of missing or spurious edges).

HOW IS RECONSTRUCTION POSSIBLE?



(a)



(b)

HOW IS RECONSTRUCTION POSSIBLE?



(a)



(b)

We need:

- ▶ A model for structure.
- ▶ A model for noise.

HOW IS RECONSTRUCTION POSSIBLE?



(a)



(b)

We need:

- ▶ A model for structure.
- ▶ A model for noise.

(but for networks)

NONPARAMETRIC BAYESIAN INFERENCE

- ▶ A model for structure, $P(\mathbf{A}|\theta)$
- ▶ A model for noise, $P(\mathcal{D}|\mathbf{A}, \phi)$

$\mathbf{A} \rightarrow$ Network, $\mathcal{D} \rightarrow$ Measured data, $(\theta, \phi) \rightarrow$ Parameters

Posterior distribution:

$$P(\mathbf{A}|\mathcal{D}) = \frac{P(\mathcal{D}|\mathbf{A})P(\mathbf{A})}{P(\mathcal{D})}$$

Marginal probabilities:

$$P(\mathcal{D}|\mathbf{A}) = \int P(\mathcal{D}|\mathbf{A}, \phi)P(\phi)d\phi$$

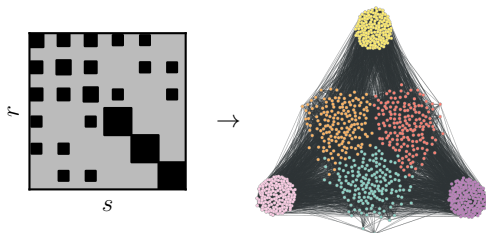
$$P(\mathbf{A}) = \int P(\mathbf{A}|\theta)P(\theta)d\theta$$

STRUCTURE: THE STOCHASTIC BLOCK MODEL (SBM)

Planted partition: N nodes divided into B groups.

Parameters: $b_i \rightarrow$ group membership of node i

$\lambda_{rs} \rightarrow$ edge probability from group r to s .



Degree-corrected: Arbitrary degree sequence: $\{\kappa_i\}$

-
- ▶ Not restricted to assortative structures (“communities”).
 - ▶ Easily generalizable (edge direction, overlapping groups, etc.)

BAYESIAN SBM

$$P(\mathbf{A}|\boldsymbol{\lambda}, \boldsymbol{\kappa}, \mathbf{b}) = \prod_{i < j} \frac{(\kappa_i \kappa_j \lambda_{b_i b_j})^{A_{ij}} e^{-\kappa_i \kappa_j \lambda_{b_i b_j}}}{A_{ij}!} \times \prod_i \frac{(\kappa_i^2 \lambda_{b_i b_i} / 2)^{A_{ii}/2} e^{-\kappa_i^2 \lambda_{b_i b_i} / 2}}{(A_{ii}/2)!}$$

Noninformative priors:

$$P(\boldsymbol{\lambda}|\mathbf{b}) = \prod_{r \leq s} e^{-\lambda_{rs} / (1 + \delta_{rs}) \bar{\lambda}} / (1 + \delta_{rs}) \bar{\lambda}$$

$$P(\boldsymbol{\kappa}|\mathbf{b}) = \prod_r (n_r - 1)! \delta(\sum_i \kappa_i \delta_{b_i, r} - 1)$$

BAYESIAN SBM

$$P(\mathbf{A}|\boldsymbol{\lambda}, \boldsymbol{\kappa}, \mathbf{b}) = \prod_{i < j} \frac{(\kappa_i \kappa_j \lambda_{b_i b_j})^{A_{ij}} e^{-\kappa_i \kappa_j \lambda_{b_i b_j}}}{A_{ij}!} \times \prod_i \frac{(\kappa_i^2 \lambda_{b_i b_i} / 2)^{A_{ii} / 2} e^{-\kappa_i^2 \lambda_{b_i b_i} / 2}}{(A_{ii} / 2)!}$$

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$$P(\boldsymbol{\kappa}|\mathbf{b}) = \prod_r (n_r - 1)! \delta(\sum_i \kappa_i \delta_{b_i, r} - 1)$$

Marginal likelihood:

$$\begin{aligned} P(\mathbf{A}|\mathbf{b}) &= \int P(\mathbf{A}|\boldsymbol{\lambda}, \boldsymbol{\kappa}, \mathbf{b}) P(\boldsymbol{\lambda}|\mathbf{b}) P(\boldsymbol{\kappa}|\mathbf{b}) \, d\boldsymbol{\lambda} d\boldsymbol{\kappa} \\ &= \frac{\bar{\lambda}^E}{(\bar{\lambda} + 1)^{E + B(B+1)/2}} \times \frac{\prod_{r < s} e_{rs}! \prod_r e_{rr}!!}{\prod_{i < j} A_{ij}! \prod_i A_{ii}!!} \times \prod_r \frac{(n_r - 1)!}{(e_r + n_r - 1)!} \times \prod_i k_i! \\ &= P(\mathbf{A}|\mathbf{k}, \mathbf{e}, \mathbf{b}) P(\mathbf{k}|\mathbf{e}, \mathbf{b}) P(\mathbf{e}) \end{aligned}$$

BAYESIAN SBM

$$P(\mathbf{A}|\boldsymbol{\lambda}, \boldsymbol{\kappa}, \mathbf{b}) = \prod_{i < j} \frac{(\kappa_i \kappa_j \lambda_{b_i b_j})^{A_{ij}} e^{-\kappa_i \kappa_j \lambda_{b_i b_j}}}{A_{ij}!} \times \prod_i \frac{(\kappa_i^2 \lambda_{b_i b_i} / 2)^{A_{ii} / 2} e^{-\kappa_i^2 \lambda_{b_i b_i} / 2}}{(A_{ii} / 2)!}$$

Noninformative priors:

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Marginal likelihood:

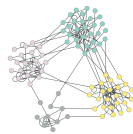
$$\begin{aligned} P(\mathbf{A}|\mathbf{b}) &= \int P(\mathbf{A}|\boldsymbol{\lambda}, \boldsymbol{\kappa}, \mathbf{b}) P(\boldsymbol{\lambda}|\mathbf{b}) P(\boldsymbol{\kappa}|\mathbf{b}) d\boldsymbol{\lambda} d\boldsymbol{\kappa} \\ &= \frac{\bar{\lambda}^E}{(\bar{\lambda} + 1)^{E+B(B+1)/2}} \times \frac{\prod_{r < s} e_{rs}! \prod_r e_{rr}!!}{\prod_{i < j} A_{ij}! \prod_i A_{ii}!!} \times \prod_r \frac{(n_r - 1)!}{(e_r + n_r - 1)!} \times \prod_i k_i! \\ &= P(\mathbf{A}|\mathbf{k}, \mathbf{e}, \mathbf{b}) P(\mathbf{k}|\mathbf{e}, \mathbf{b}) P(\mathbf{e}) \end{aligned}$$



Edge counts \mathbf{e} .

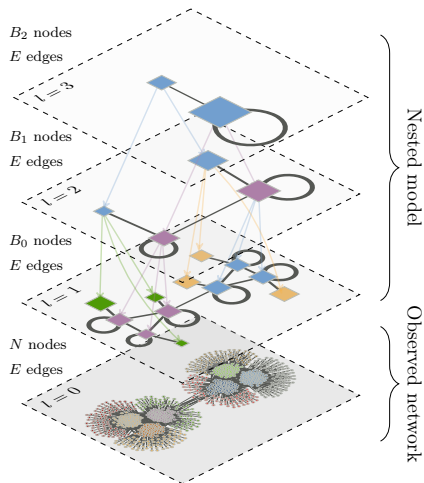


Degrees, \mathbf{k} .



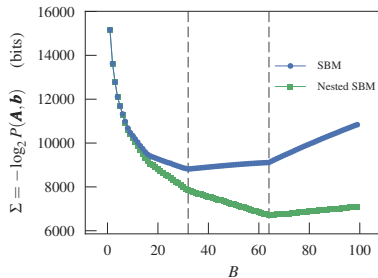
Network, \mathbf{A} .

NESTED SBM: GROUP HIERARCHIES



Deeper Bayesian hierarchy:

- ▶ Prevents underfitting.
- ▶ Multiple scales of description.



MEASUREMENT MODEL

Edge-o-meter

$p \rightarrow$ probability of a missing edge ($1 \rightarrow 0$)

$q \rightarrow$ probability of a spurious edge ($0 \rightarrow 1$)

$n_{ij} \rightarrow$ number of measurements of pair (i, j)

$x_{ij} \rightarrow$ number of edges recorded

$$P(x_{ij}|n_{ij}, A_{ij}, p, q) = \binom{n_{ij}}{x_{ij}} [(1-p)^{x_{ij}} p^{n_{ij}-x_{ij}}]^{A_{ij}} [q^{x_{ij}} (1-q)^{n_{ij}-x_{ij}}]^{1-A_{ij}}$$

$$P(\mathbf{x}|\mathbf{n}, \mathbf{A}, \alpha, \beta, \mu, \nu) = \int P(\mathbf{x}|\mathbf{n}, \mathbf{A}, p, q) P(p|\alpha, \beta) P(q|\mu, \nu) dp dq$$

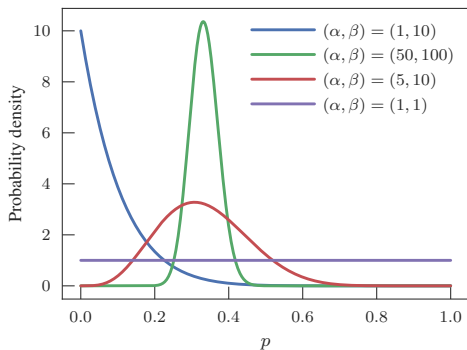
$P(p|\alpha, \beta), P(q|\mu, \nu) \rightarrow$ Beta priors



THE EDGE-O-METER

$$P(p|\alpha, \beta) = \frac{p^{\alpha-1}(1-p)^{\alpha-1}}{\mathcal{B}(\alpha, \beta)}$$

$$P(q|\mu, \nu) = \frac{q^{\mu-1}(1-q)^{\mu-1}}{\mathcal{B}(\mu, \nu)}$$



- ▶ $(\alpha, \beta) = (1, 10) \rightarrow$ accurate measurement (low noise)
- ▶ $(\alpha, \beta) = (50, 100) \rightarrow$ high noise, good calibration
- ▶ $(\alpha, \beta) = (5, 10) \rightarrow$ high noise, bad calibration
- ▶ $(\alpha, \beta) = (1, 1) \rightarrow$ noninformative (i.e. uniform distribution)

THE FULL RECONSTRUCTION METHOD

Posterior distribution:

$$P(\mathbf{A}, \mathbf{b} | \mathbf{n}, \mathbf{x}, \alpha, \beta, \mu, \nu) = \frac{P(\mathbf{x} | \mathbf{n}, \mathbf{A}, \alpha, \beta, \mu, \nu) P(\mathbf{A} | \mathbf{b}) P(\mathbf{b})}{P(\mathbf{x} | \alpha, \beta, \mu, \nu)}.$$

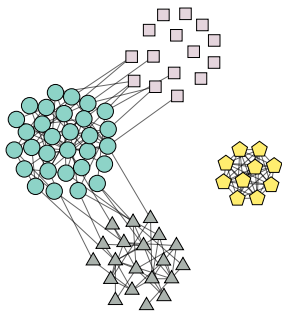
We infer both the network \mathbf{A} as well as the SBM latent variables \mathbf{b} via MCMC:

Move proposals $P(\mathbf{b}' | \mathbf{A}, \mathbf{b})$ and $P(\mathbf{A}' | \mathbf{A}, \mathbf{b})$, accept with probability

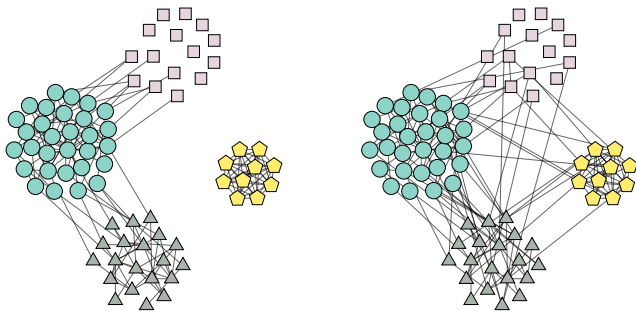
$$\min \left(1, \frac{P(\mathbf{A}', \mathbf{b}' | \mathcal{D}) P(\mathbf{A} | \mathbf{A}', \mathbf{b}') P(\mathbf{b} | \mathbf{A}', \mathbf{b}')}{P(\mathbf{A}, \mathbf{b} | \mathcal{D}) P(\mathbf{A}' | \mathbf{A}, \mathbf{b}) P(\mathbf{b}' | \mathbf{A}, \mathbf{b})} \right).$$

(Efficient, scales to very large networks.)

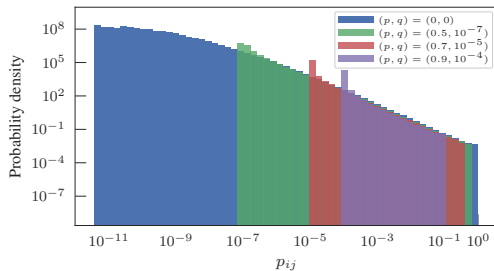
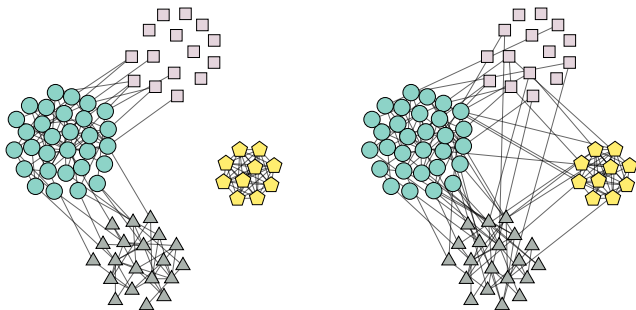
HOW DOES IT WORK?



HOW DOES IT WORK?

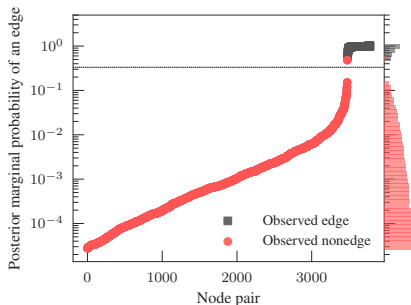
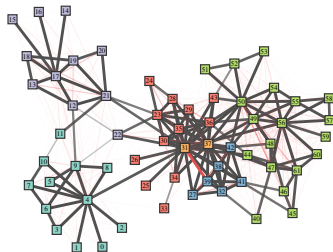
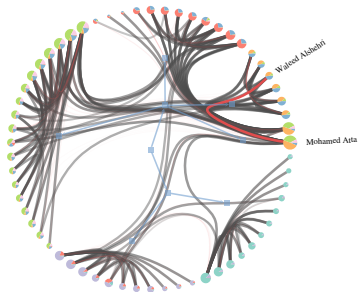


HOW DOES IT WORK?



$$p'_{ij} = (1 - p - q)p_{ij} + q$$

EXAMPLE: TERRORIST ASSOCIATIONS



WAIT! IS THIS JUST EDGE PREDICTION?

It *is* edge prediction, but it yields a full posterior distribution $P(\mathbf{A}|\mathbf{n}, \mathbf{x})$ that is **nonparametric**.

We can:

- ▶ Perform maximum marginal posterior estimation,

$$\hat{A}_{ij} = \begin{cases} 1 & \text{if } \pi_{ij} > 1/2 \\ 0 & \text{if } \pi_{ij} < 1/2, \end{cases}$$

where $\pi_{ij} = \sum_{\mathbf{A}} A_{ij} P(\mathbf{A}|\mathbf{n}, \mathbf{x})$ is the marginal posterior edge probability.

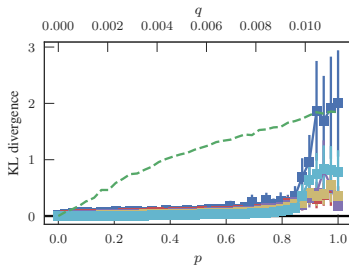
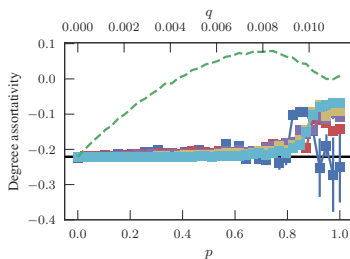
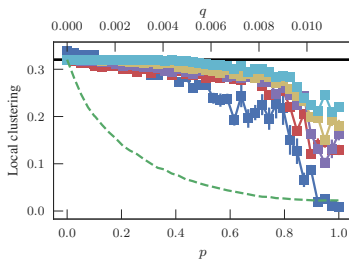
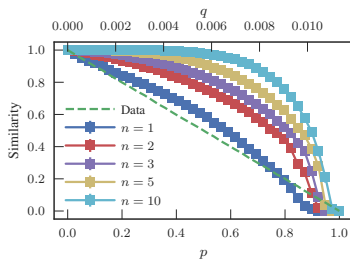
- ▶ Estimate network properties $y(\mathbf{A})$ and their error estimates:

$$\hat{y} = \sum_{\mathbf{A}} y(\mathbf{A}) P(\mathbf{A}|\mathbf{n}, \mathbf{x})$$
$$\sigma_y^2 = \sum_{\mathbf{A}} (\hat{y} - y(\mathbf{A}))^2 P(\mathbf{A}|\mathbf{n}, \mathbf{x}).$$

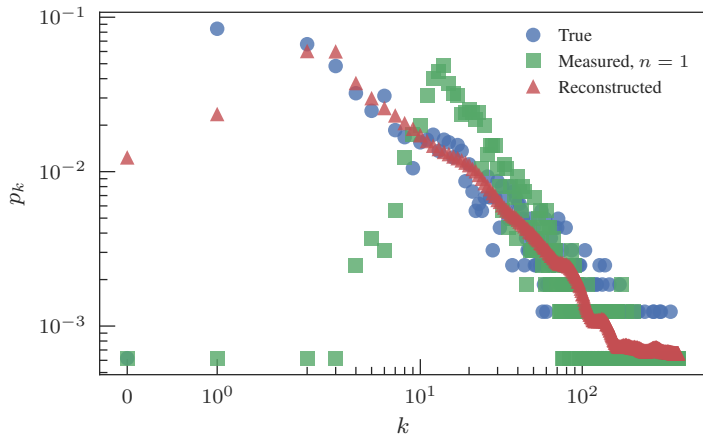
RECONSTRUCTION PERFORMANCE

Real network (political blogs) + simulated noise:

$$p \in [0, 1], q = pE / \left[\binom{N}{2} - E \right]$$

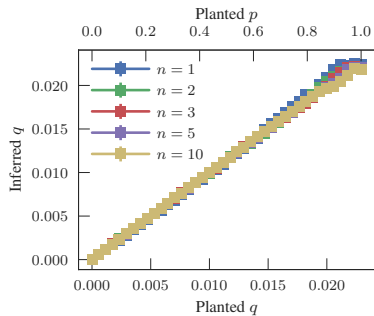
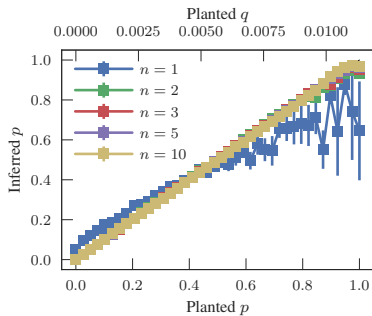


RECONSTRUCTION PERFORMANCE: DEGREES



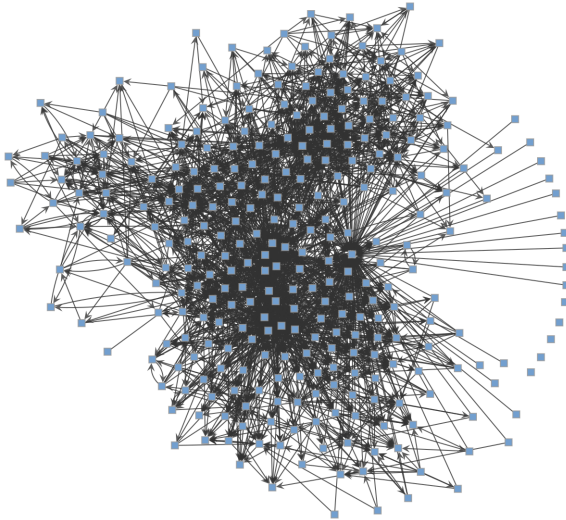
$$(p, q) = (0.41, 0.0094)$$

INFERRING THE NOISE



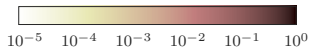
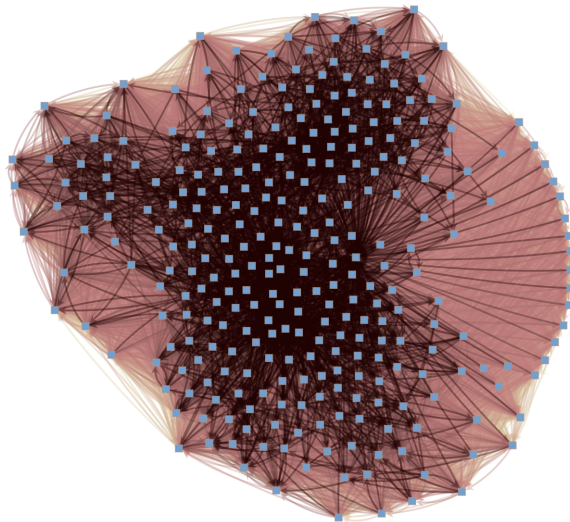
EMPIRICAL RECONSTRUCTION REDUX

C. elegans NEURAL NETWORK



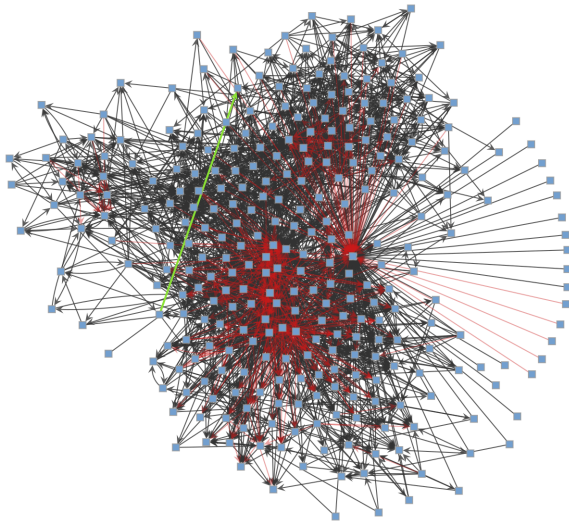
EMPIRICAL RECONSTRUCTION REDUX

C. elegans NEURAL NETWORK

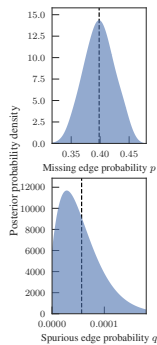
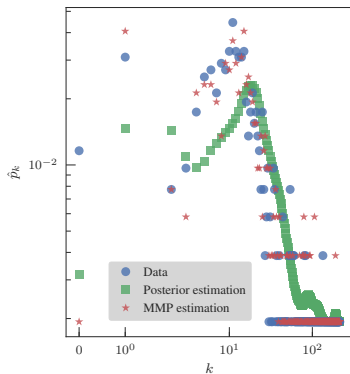
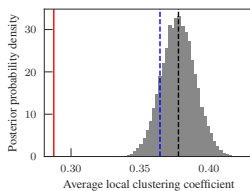
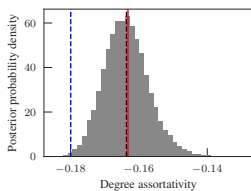


EMPIRICAL RECONSTRUCTION REDUX

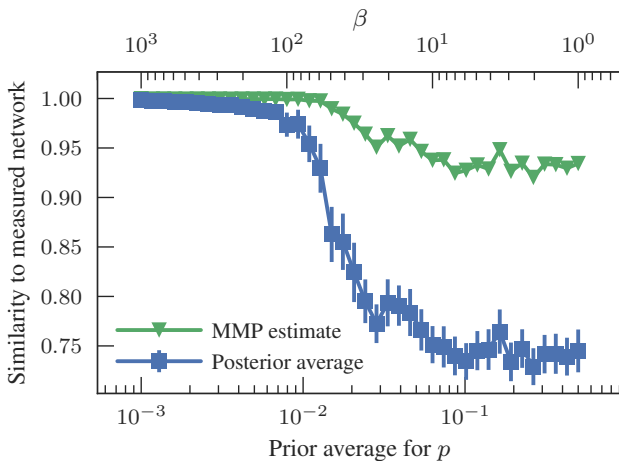
C. elegans NEURAL NETWORK



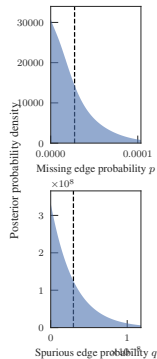
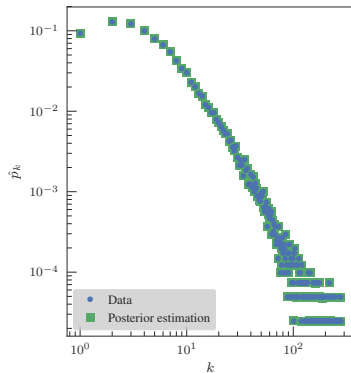
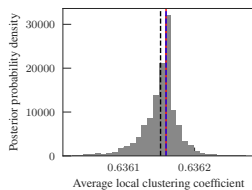
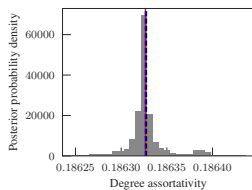
C. elegans NEURAL NETWORK



C. elegans NEURAL NETWORK



ARXIV.ORG CO-AUTHORSHIP NETWORK



UNCERTAINTY ASSESSMENT OF EMPIRICAL DATA

Dataset	Similarity	Nodes	Edges		Degree assortativity		Local clustering		B_e	\hat{p}	\hat{q}
			Direct	Estimated	Direct	Estimated	Direct	Estimated			
karate	0.94(4)	34	78	77(7)	-0.475 61	-0.49(5)	0.570 64	0.58(5)	2.7(6)	0.06(5)	0.012(10)
terrorists	0.96(2)	62	152	154(8)	-0.080 48	-0.096(20)	0.486 37	0.50(2)	5.4(5)	0.05(4)	0.003(2)
football	0.857(16)	115	613	500(18)	0.162 44	0.18(7)	0.403 22	0.68(4)	12.7(3)	0.05(3)	0.0226(19)
netscience	0.9981(17)	379	914	915(3)	-0.081 68	-0.0823(18)	0.741 23	0.741(3)	29.6(14)	0.004(3)	$3.1(19) \times 10^{-5}$
celegans	0.754(20)	302	2345	3850(150)	-0.163 20	-0.165(7)	0.287 52	0.374(12)	17.25(19)	0.39(3)	$6(3) \times 10^{-5}$
malaria	0.9981(15)	1103	2965	2973(9)	-0.300 13	-0.2997(20)	0	0(0)	30.8(3)	0.004(3)	$4(3) \times 10^{-6}$
power	0.80(7)	4941	6594	9900(1300)	0.003 46	0.043(17)	0.080 10	0.058(7)	15.6(7)	0.33(10)	$2.5(19) \times 10^{-7}$
polblogs	0.965(5)	1222	16 714	17 860(190)	-0.221 33	-0.2226(16)	0.320 25	0.343(5)	16.6(3)	0.066(10)	$4.4(17) \times 10^{-5}$
dlib	0.64(1)	12 590	49 744	106 000(2000)	-0.045 72	-0.0559(19)	0.117 18	0.164(7)	86.4(20)	0.529(11)	$9(5) \times 10^{-9}$
openflights	0.9916(9)	3286	39 430	40 100(70)	-0.005 31	-0.0071(11)	0.496 47	0.507(2)	117.1(5)	0.0167(18)	$1.0(3) \times 10^{-7}$
reactome	0.999 977(10)	6327	146 160	146 164(3)	0.244 87	0.244 87(4)	0.588 38	0.5887(3)	318.7(10)	$4.1(18) \times 10^{-5}$	$1.3(8) \times 10^{-7}$
cond-mat	0.999 986(13)	40 421	175 693	175 695(4)	0.186 33	0.186 33(2)	0.636 16	0.636 15(3)	1014(6)	$3(2) \times 10^{-5}$	$3(2) \times 10^{-9}$
Enron	0.999 86(5)	36 692	183 831	183 885(18)	-0.110 76	-0.110 75(2)	0.496 98	0.496 92(8)	188.9(11)	0.000 28(10)	$2.9(19) \times 10^{-9}$
linux	0.9973(3)	30 837	213 424	214 600(120)	-0.174 68	-0.174 67(7)	0.128 49	0.1322(10)	351.2(7)	0.0055(5)	$1.7(10) \times 10^{-9}$
brightkite	0.9985(3)	58 228	214 078	214 740(80)	0.010 82	0.011 00(11)	0.172 33	0.172 34(10)	151(3)	0.0029(5)	$1.7(12) \times 10^{-8}$
pgp	0.997 99(9)	39 796	301 498	301 660(60)	0.000 76	0.000 49(8)	0.461 09	0.461 7(2)	929(2)	0.002 27(16)	$3.35(18) \times 10^{-7}$
caida	0.999 67(13)	53 387	496 731	497 070(130)	-0.186 97	-0.186 959(17)	0.680 97	0.681 26(14)	218.0(16)	0.0007(3)	$1.0(8) \times 10^{-9}$
web-Stanford	0.999 998 7(8)	281 903	2 312 497	2 312 494(4)	-0.112 44	-0.112 444 7(2)	0.597 63	0.597 634(3)	4168(2)	$1.0(2) \times 10^{-6}$	$7(5) \times 10^{-11}$
flickr	0.999 976(13)	105 938	2 316 948	2 316 830(60)	0.246 85	0.246 823(16)	0.089 13	0.089 138(7)	617(2)	$6(3) \times 10^{-7}$	$2.0(11) \times 10^{-8}$

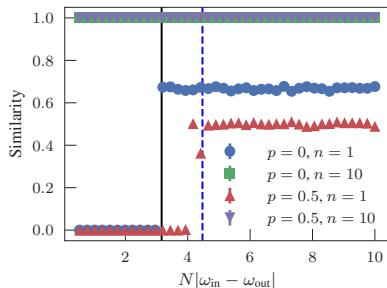
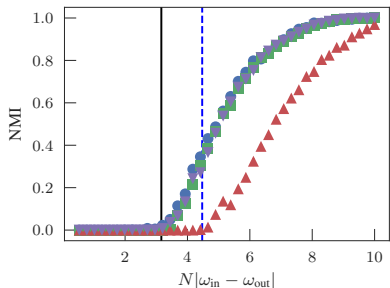
NOISE AND DETECTABILITY OF COMMUNITIES

Planted partition model:

$$\omega_{rs} = \omega_{\text{in}}\delta_{rs} + \omega_{\text{out}}(1 - \delta_{rs})$$

Single observation, $n = 1$, effectively:

$$\omega'_{rs} = (1 - p - q)\omega_{rs} + q$$



$$N|\omega_{\text{in}} - \omega_{\text{out}}| < B\sqrt{\langle k \rangle},$$

$$N|\omega_{\text{in}} - \omega_{\text{out}}| < \frac{B\sqrt{(1-p-q)\langle k \rangle + qN}}{(1-p-q)}.$$

MULTIPLE MEASUREMENTS AND HETEROGENEOUS ERRORS

Observational error does not need to be uniform for every pair (i, j) .

Non-uniform model, w/ pair-specific error rates: p_{ij} and q_{ij}

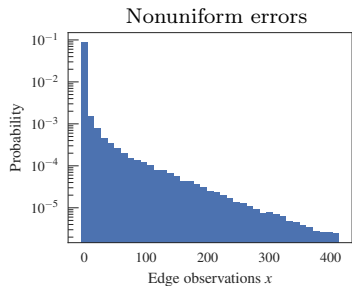
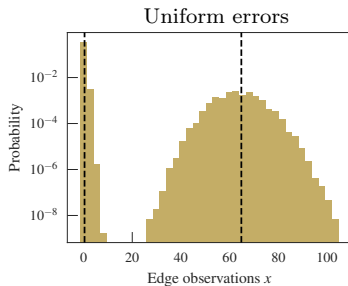
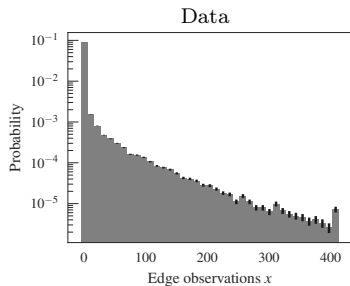
$$P(x_{ij}|n_{ij}, A_{ij}, p_{ij}, q_{ij}) = \binom{n_{ij}}{x_{ij}} \left[(1 - p_{ij})^{x_{ij}} p_{ij}^{n_{ij} - x_{ij}} \right]^{A_{ij}} \left[q_{ij}^{x_{ij}} (1 - q_{ij})^{n_{ij} - x_{ij}} \right]^{1 - A_{ij}}$$

Marginal probability,

$$\begin{aligned} P(x_{ij}|n_{ij}, A_{ij}, \alpha, \beta, \mu, \nu) &= \int P(x_{ij}|n_{ij}, A_{ij}, p_{ij}, q_{ij}) P(p_{ij}|\alpha, \beta) P(q_{ij}|\mu, \nu) dp_{ij} dq_{ij} \\ &= \binom{n_{ij}}{x_{ij}} \left[\frac{\mathcal{B}(n_{ij} - x_{ij} + \alpha, x_{ij} + \beta)}{\mathcal{B}(\alpha, \beta)} \right]^{A_{ij}} \times \\ &\quad \left[\frac{\mathcal{B}(x_{ij} + \mu, n_{ij} - x_{ij} + \nu)}{\mathcal{B}(\mu, \nu)} \right]^{1 - A_{ij}}. \end{aligned}$$

HUMAN CONNECTOME

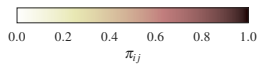
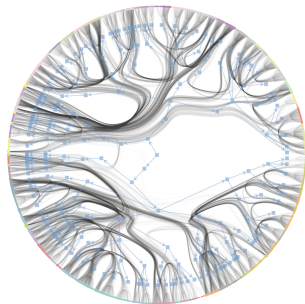
418 INDIVIDUALS



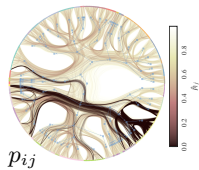
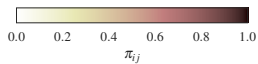
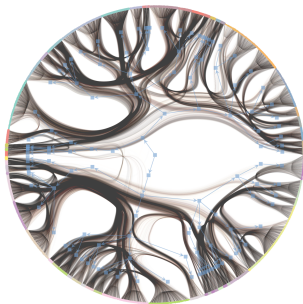
HUMAN CONNECTOME

418 INDIVIDUALS

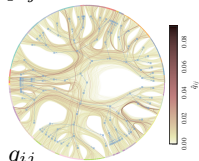
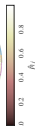
Uniform errors



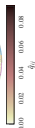
Nonuniform errors



p_{ij}



q_{ij}



EXTRINSIC ERROR ESTIMATES

$Q_{ij} \in [0, 1] \rightarrow$ experimentally determined uncertainties

$$P_{\mathbf{Q}}(\mathbf{A}|\mathbf{Q}) = \prod_{i < j} Q_{ij}^{A_{ij}} (1 - Q_{ij})^{1 - A_{ij}}.$$

Example:

STRING Protein-Protein interaction network database, Szklarczyk et al,
Nucleic Acids Research 45, D362–D368 (2017).

Errors are estimated via a combination of: (i) direct experiments, (ii) database curation, (iii) publication text-mining, (iv) co-expression data, (v) genome proximity, (vi) ortholog fusion, (vii) phylogenetic co-occurrence.

EXTRINSIC ERROR ESTIMATES

The distribution $P_Q(\mathbf{A}|\mathbf{Q})$ implies the following noisy measurement process,

$$P(\mathbf{Q}|\mathbf{A}) = \frac{P_Q(\mathbf{A}|\mathbf{Q})P_Q(\mathbf{Q})}{P_Q(\mathbf{A})},$$

with prior

$$P_Q(\mathbf{Q}) = \prod_{i<j} P(Q_{ij}),$$

and normalization constant

$$P_Q(\mathbf{A}) = \int P_Q(\mathbf{A}|\mathbf{Q})P_Q(\mathbf{Q}) \, d\mathbf{Q} = \prod_{i<j} \bar{Q}^{A_{ij}} (1 - \bar{Q})^{1-A_{ij}},$$

with $\bar{Q} = \int_0^1 Q P(Q) dQ$. Combining these together we have

$$P(\mathbf{Q}|\mathbf{A}) = P_Q(\mathbf{Q}) \prod_{i<j} \left(\frac{Q_{ij}}{\bar{Q}} \right)^{A_{ij}} \left(\frac{1 - Q_{ij}}{1 - \bar{Q}} \right)^{1-A_{ij}},$$

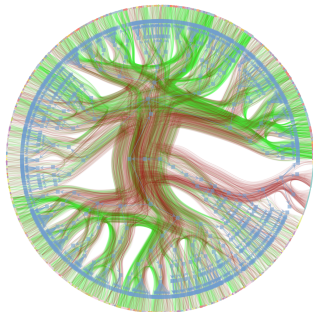
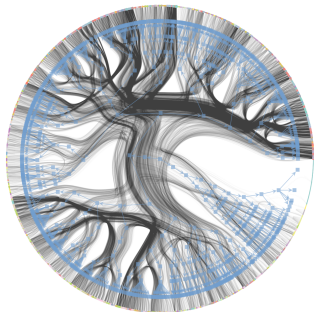
$$P(\mathbf{A}|\mathbf{Q}) = \frac{P(\mathbf{Q}|\mathbf{A})P(\mathbf{A})}{P(\mathbf{Q})}, \quad \bar{Q} = \frac{\sum_{i<j} Q_{ij}}{\binom{N}{2}}.$$

EXTRINSIC ERROR ESTIMATES

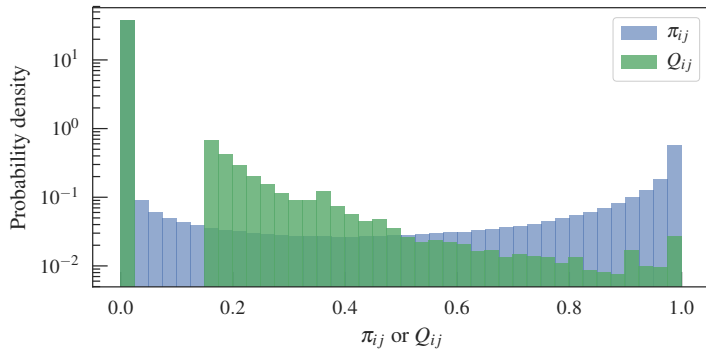
$$P(\mathbf{A}|\mathbf{Q}) = \frac{P(\mathbf{Q}|\mathbf{A})P(\mathbf{A})}{P(\mathbf{Q})}, \quad P(\mathbf{A}|\mathbf{Q}) \neq P_{\mathbf{Q}}(\mathbf{A}|\mathbf{Q})!$$

We are keeping the same noise generating process, but changing our prior assumption about the data.

E. coli proteins:



EXTRINSIC ERROR ESTIMATES



For code, see:

<https://graph-tool.skewed.de>

(See also HOWTO at: <https://graph-tool.skewed.de/static/doc/demos/inference/inference.html>)