#### The Geometry of Community Detection

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#### Information Theory and Inference

Symmetric SBM

Degree-Balanced SBM

Key steps in proof

Conclusion

Spectrum of research on network inference



Spectrum of research on network inference

flexible models limited theory		toy models extensive theory
	corrected SBM mixed-membership SBM	k-community 2-community symm. SBM symm. SBM
applied network analysis scientific modeling	statistical modeling	computer science information theory statistical physics

# Our Goals

- Broad class of network models (beyond symmetric models)
- Multivariate measures of performance
- Exact expressions for asymptotic performance
- Explore computational gaps

Paper on arxiv https://arxiv.org/abs/1907.02496

# The 'Bayes optimal' setting

Assume joint distribution on  $(\boldsymbol{X},\boldsymbol{G})$  where

- $\blacktriangleright$  G is adjacency matrix of simple graph with n vertices
- $\boldsymbol{X} = (X_1, \dots, X_n)$  contains vertex labels

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How much do we learn?

$$\begin{split} P(\boldsymbol{X} \mid \boldsymbol{G}) & \text{versus} \quad P(\boldsymbol{X}) \\ I(\boldsymbol{X}; \boldsymbol{G}) = \mathbb{E} \bigg[ \log \frac{P(\boldsymbol{X}, \boldsymbol{G})}{P(\boldsymbol{X}) P(\boldsymbol{G})} \bigg] \end{split}$$

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How well can we recover labels?

$$\hat{X}$$
 verus  $X$ 

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# A network with three similar communities



### A network with three similar communities



Recent literature on detection / recovery thresholds

Incomplete list:

- A. Decelle, F. Krzakala, C. Moore, and L. Zdeborová, 2011
- E. Mossel, J. Neeman, and A. Sly, 2014
- Deshpande, E. Abbe, and A. Montanari, 2015
- ▶ J. Barbier, M. Dia, N. Macris, F. Krzakala, T. Lesieur, and L. Zdeborová, 2016
- F. Krzakala, J. Xu, L. Zdeborová, 2016
- J. Banks, C. Moore, J. Neeman, and P. Netrapalli, 2017
- E. Abbe and C. Sandon, 2017
- F. Caltagirone, M. Lelarge and L. Miolane, 2017
- F. Ricci-Tersenghi, G. Semerjian, and L. Zdeborová, 2018

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Normalize such that  $\mathbb{E}[X_i] = 0$  and  $Cov(X_i) = I$ , and hence

$$X_i^{\top} X_j = \begin{cases} k - 1, & X_i = X_j \\ -1, & X_i \neq X_j \end{cases}$$

Entries of adjacency matrix are conditionally independent:

$$G_{ij} \sim \mathsf{Bernoulli}\left(rac{d}{n} + rac{r\sqrt{d(1 - d/n)}}{n} X_i^{\top} X_j
ight), \quad i < j$$

- $\blacktriangleright$  d is the expected degree of each node
- r characterizes "community structure"
  - $r = 0 \implies$  no dependence
  - $r > 0 \implies$  assortative
  - $r < 0 \implies$  disassortative

Two-community SBM as  $n, d \rightarrow \infty$  [Deshpande et al. 2015]



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Where do these formulas come from?

### The signal-plus-noise model

$$Y_i \sim \mathcal{N}(X_i, s^{-1}I), \quad i = 1, \dots, n$$

where s > 0 is the signal-to-noise ratio.





high SNR

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Mutual information and MMSE functions (can approximate numerically)

$$I_X(s) = I(X_1; Y_1)$$
  

$$m_X(s) = \mathbb{E} \Big[ \|X_1 - \mathbb{E}[X_1 \mid Y_1]\|^2 \Big]$$

Theorem (Deshpande et al. 2015)

Assume k = 2 communities. Let  $s^* \ge 0$  be global minimizer of

$$I_X(s) + \frac{1}{4}\left(r - \frac{s}{r}\right)^2$$

Then, MMSE of pairwise interactions satisfies

$$\frac{1}{n^2} \mathbb{E}\left[\left\|\boldsymbol{X}\boldsymbol{X}^{\top} - \mathbb{E}\left[\boldsymbol{X}\boldsymbol{X}^{\top} \mid \boldsymbol{G}\right]\right\|_F^2\right] = 1 - \frac{(s^*)^2}{r^4} + o_{n,d}(1),$$

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Furthermore

$$\inf_{\hat{\boldsymbol{X}}(\cdot)} \mathbb{E}\left[\min_{\pi \in \{+1,-1\}} \frac{1}{n} \left\| \boldsymbol{X} - \pi \hat{\boldsymbol{X}}(\boldsymbol{G}) \right\|^2 \right] \le m(s^*) + o_{n,d}(1),$$

where the minimum over  $\pi$  resolves label invariance problem.

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#### Parameterization of degree-balanced SBM

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Represent labels using k points in (k-1) dimensions normalized to zero mean and identity covariance:



### Parameterization of degree-balanced SBM

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ight), \quad i < j$$

- d is the expected degree of each vertex
- ▶ *R* is a symmetric matrix that characterizes "community structure"
  - $R = 0 \implies$  no dependence
  - $R \succ 0 \implies$  assortative
  - $R \prec 0 \implies$  disassortative

# Multivariate performance metric

$$\mathsf{MMSE}(\boldsymbol{X} \mid \boldsymbol{G}) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \Big[ (X_i - \mathbb{E}[X_i \mid \boldsymbol{G}]) (X_i - \mathbb{E}[X_i \mid \boldsymbol{G}])^\top \Big]$$

Data processing inequality + normalization of vertex labels:

$$0 \preceq \mathsf{MMSE}(\boldsymbol{X} \mid \boldsymbol{G}) \preceq I_{k-1}$$

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Trace corresponds to usual (scalar) MMSE

$$\operatorname{tr}(\mathsf{MMSE}(\boldsymbol{X} \mid \boldsymbol{G})) = \frac{1}{n} \mathbb{E} \big[ \|\boldsymbol{X} - \mathbb{E}[\boldsymbol{X} \mid \boldsymbol{G}]\|^2 \big]$$

### The signal-plus-noise model with matrix SNR

$$Y_i \sim \mathcal{N}(X_i, \mathbf{S}^{-1}I), \quad i = 1, \dots, n$$

where S is positive semidefinite signal-to-noise ratio matrix.



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$$I_X(S) = I(X_1; Y_1)$$
  

$$M_X(S) = \mathbb{E}\Big[(X_1 - \mathbb{E}[X_1 \mid Y_1])(X_1 - \mathbb{E}[X_1 \mid Y_1])^\top\Big]$$

Theorem (R., Mayya, Volfovsky, 2019)

Assume that R is definite and let  $S^*$  be the global minimizer of

$$I_X(S) + \frac{1}{4} \operatorname{tr} ((R - R^{-1}S)^2).$$

Then, the MMSE matrix satisfies<sup>1</sup>

$$\mathsf{MMSE}(\boldsymbol{X} \mid \boldsymbol{G}) \preceq M_X(\boldsymbol{S}^*) + o_{n,d}(1),$$

where  $o_{n,d}(1)$  denotes a symmetric matrix that converges to zero as  $n, d \rightarrow \infty$ .

<sup>&</sup>lt;sup>1</sup>after resolving label invariances

# Comparison of theoretical and empirical results



$$p = (1/3, 1/3, 1/3)$$
  $p = (0.6, 0.3, 0.1)$ 

Bound on tr(MMSE( $X \mid G$ )) (contour lines) and empirical MSE of belief propagation (heat map) with  $n = 10^5$ , average degree d = 30.

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# Express MMSE as gradient of mutual information

Signal-plus-noise problem (in matrix notation)

$$\underbrace{\boldsymbol{Y}}_{n \times \ell} = \underbrace{\boldsymbol{X}}_{n \times \ell} \underbrace{S^{1/2}}_{\ell \times \ell} + \underbrace{\text{Gaussian noise}}_{n \times \ell}$$

### Express MMSE as gradient of mutual information

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By Matrix I-MMSE relation [R. Pfister, Dytso 2018],

$$\mathsf{MMSE}(\boldsymbol{X} \mid \boldsymbol{G}) = \frac{2}{n} \nabla_{\boldsymbol{S}} I(\boldsymbol{X}; \boldsymbol{G}, \boldsymbol{Y}) \Big|_{\boldsymbol{S}=\boldsymbol{0}}$$

Holds for any joint distribution on (X, G)!

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Holds for any joint distribution on (X, G)!

$$\mathsf{Goal:} \quad \lim_{n \to \infty} \frac{1}{n} I(\boldsymbol{X}; \boldsymbol{G}, \boldsymbol{Y}), \qquad S \succeq 0$$

### Channel universality

Comparison between SBM and noisy matrix estimation

$$oldsymbol{G} \sim \mathsf{Bernoulli}\left(rac{d}{n} + rac{\sqrt{d(1-d/n)}}{n}oldsymbol{X}Roldsymbol{X}^{ op}
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Theorem (R., Mayya, Volfovsky, 2019) If t = 1, then

$$\lim_{n,d\to\infty}\frac{1}{n}|I(\boldsymbol{X};\boldsymbol{G},\boldsymbol{Y})-I(\boldsymbol{X};\boldsymbol{Y},\boldsymbol{Z})|=0$$

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Generalizes prior work [Deshpande et al. 2015], [Krzakala et al. 2016]

#### Interpolation via mutual information

$$m{Y} = m{X}S^{1/2} + {\sf Gaussian}$$
 noise  
 $m{Z} = \sqrt{rac{t}{n}}m{X}Rm{X}^T + {\sf Gaussian}$  noise

Define interpolating function  $\mathcal{I}:\mathbb{S}^d_+\times[0,\infty)\to[0,\infty)$ 

$$\mathcal{I}(S,t) = \frac{1}{n}I(\boldsymbol{X};\boldsymbol{Y},\boldsymbol{Z})$$

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• t = 0 is signal-plus-noise model:

$$\mathcal{I}(S,0) = \frac{1}{n}I(\boldsymbol{X};\boldsymbol{Y})$$

• t = 1 is desired goal (by channel universality):

$$\mathcal{I}(S,1) = \frac{1}{n}I(\boldsymbol{X};\boldsymbol{G},\boldsymbol{Y}) + o_{n,d}(1)$$

# Estimation inequality for gradients

By I-MMSE relation,

$$\nabla_{S} \mathcal{I}(S, t) = \frac{1}{2} \operatorname{MMSE}(\boldsymbol{X} \mid \boldsymbol{Y}, \boldsymbol{Z})$$
$$\nabla_{t} \mathcal{I}(S, t) = \frac{1}{4} \frac{1}{n^{2}} \mathbb{E} \left[ \left\| \boldsymbol{X} R \boldsymbol{X}^{\top} - \mathbb{E} \left[ \boldsymbol{X} R \boldsymbol{X}^{\top} \mid \boldsymbol{G} \right] \right\|^{2} \right]$$

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Rearranging terms + Jensen's inequality yields

$$\nabla_t \mathcal{I}(S,t) \le \frac{1}{4}g(2\nabla_S \mathcal{I}(S,t)),$$

where  $g:\mathbb{S}^d_+\to [0,\infty)$  is given by

$$g(U) = \frac{1}{n^2} \operatorname{tr} \left( \mathbb{E} \left[ \left( R \boldsymbol{X}^T \boldsymbol{X} \right)^2 \right] \right) - \operatorname{tr} \left( \left( R \left( \frac{1}{n} \mathbb{E} \left[ \boldsymbol{X} \boldsymbol{X}^T \right] - U \right) \right)^2 \right).$$

#### Information inequality via duality Conjugate function

$$\mathcal{J}(U,t) = \sup_{S \succeq 0} \left\{ \mathcal{I}(S,t) - \frac{1}{2} \langle S, U \rangle \right\}$$

Dual variable  $\boldsymbol{U}$  corresponds to MMSE matrix

$$U = \nabla_S \mathcal{I}(S^*, t) \quad \iff \quad \mathcal{J}(U, t) = \mathcal{I}(S^*, t) - \frac{1}{2} \langle S^*, U \rangle$$

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By envelope theorem + inequality for gradients

$$\nabla_t \mathcal{J}(U,t) = \nabla_t \mathcal{I}(S^*,t) \le \frac{1}{4}g(\nabla_S \mathcal{I}(S^*,t)) = \frac{1}{4}g(U)$$

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Dual variable U corresponds to MMSE matrix

$$U = \nabla_S \mathcal{I}(S^*, t) \quad \iff \quad \mathcal{J}(U, t) = \mathcal{I}(S^*, t) - \frac{1}{2} \langle S^*, U \rangle$$

By envelope theorem + inequality for gradients

$$\nabla_t \mathcal{J}(U,t) = \nabla_t \mathcal{I}(S^*,t) \le \frac{1}{4}g(\nabla_S \mathcal{I}(S^*,t)) = \frac{1}{4}g(U)$$

Integrating gives simple upper bound:

$$\mathcal{J}(U,1) \le \mathcal{J}(U,0) + \frac{1}{4}g(U)$$

For any joint distribution on  $(\boldsymbol{X}, \boldsymbol{G})$ ,

$$\mathcal{I}(S,1) = \inf_{U \succeq 0} \left\{ \mathcal{J}(U,1) + \frac{1}{2} \langle S, U \rangle \right\}$$

•

$$I(\cdot,1)$$
 is concave

For any joint distribution on  $(\boldsymbol{X}, \boldsymbol{G})$ ,

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If rows of  $\boldsymbol{X}$  are IID with  $\mathbb{E} \big[ X_1 X_1^\top \big] = I$ , then

$$\mathcal{I}(S,0) = I_X(S), \qquad h(\Delta) = \operatorname{tr}\left((R - R^{-1}\Delta)^2\right) + o_n(1)$$

### Final steps in proof

We showed that for all  $S \succeq \mathbf{0}\text{,}$ 

$$\limsup_{n,d\to\infty}\frac{1}{n}I(\boldsymbol{X};\boldsymbol{G},\boldsymbol{Y}) \leq \inf_{\Delta\succeq 0} \left\{ I_X(S+\Delta,0) + \frac{1}{4}\operatorname{tr}\left((R-R^{-1}\Delta)^2\right) \right\}$$

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Matching lower bound is much more difficult! We use matrix estimation result of Lelarge, Miolane 2018 to show inequality is tight for S = 0.

$$\lim_{n,d\to\infty}\frac{1}{n}I(\boldsymbol{X};\boldsymbol{G}) = \inf_{\Delta\succeq 0} \left\{ I_X(\Delta,0) + \frac{1}{4}\operatorname{tr}\left((R - R^{-1}\Delta)^2\right) \right\}$$

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Comparing these expressions gives asymptotic upper bound on the gradient of the mutual information, which is the MMSE matrix.

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Contributions

- Study broad class of network models beyond the symmetric SBM.
- Characterize asymptotic performance via MMSE matrix.
- Novel interpolation method.
- Explore computation gap in asymmetric networks.

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Future directions

- Bridge gaps in theory / statistics / applied network inference
- Use geometric insight to inform methodology
- Covariate information and other types of community structure.

Paper on arxiv https://arxiv.org/abs/1907.02496