# Phase transitions in inference: Tree reconstruction and community detection

Laurent Massoulié

Inria, MSR-Inria Joint Centre

January 9, 2019

Laurent Massoulié

# Context: inference of structure hidden in random noise



Analysis of random instances

- $\rightarrow$  reveals phase transitions on feasibility and hardness of task
- $\rightarrow$  suggests new algorithms

## Phase diagram for community detection



## Tree reconstruction

- Census reconstruction and Kesten-Stigum threshold
- Belief Propagation and Information-Theoretic threshold
- Community detection
  - Relation to tree reconstruction
  - The hard phase
  - Above the Kesten-Stigum threshold
  - Links to random matrix theory

# The tree reconstruction problem [Evans et al.'00]



Genealogy tree  $\mathcal{T}$  with root r, "Spins"  $\sigma_i \in [q]$  transmitted independently:  $\mathbb{P}(\sigma_i = t | \sigma_{p(i)} = s) = P_{st}$  for stochastic irreducible matrix P

Root spin  $\sigma_r \sim \nu$  where  $\nu$ : stationary distribution of *P* 

 $\rightarrow$  Can one infer  $\sigma_r$  non-trivially from  $\mathcal{G}_d := (\mathcal{T}_d, \sigma_{\mathcal{L}_d})$  as  $d \rightarrow \infty$ ?

#### Definition

Reconstructibility:  $\lim_{d\to\infty} I(\sigma_r; \mathcal{G}_d) > 0$ where *I*: mutual information

**Census** at generation *d*:

$$X_d := \{X_{s,d}\}_{s \in [q]}$$
 where  $X_{s,d} = \sum_{i \in \mathcal{L}_d} \mathbb{I}_{\sigma_i = s}$ 

#### Definition

Census reconstructibility:  $\lim_{d\to\infty} I(\sigma_r; X_d) > 0$ 

In the sequel:  $\mathcal{T}$  a Galton-Watson branching tree with mean number of children  $\alpha$  (e.g.  $\mathcal{S}(i) \sim \text{Poi}(\alpha)$ )

伺 ト イヨト イヨト

# Kesten-Stigum threshold for census reconstructibility [Mossel-Peres'03]

## Spectrum of *P*: $\lambda_i(P)$ , with $\lambda_1 = 1 \ge |\lambda_2| \cdots \ge |\lambda_q|$

#### Theorem

Census reconstructibility holds if  $\alpha |\lambda_2|^2 > 1$ , fails if  $\alpha |\lambda_2|^2 < 1$ .

[Proof elements for Poisson Galton-Watson tree]

## Reconstruction and belief propagation [Pearl'82]

 $\nu_{s,d}^i = \mathbb{P}(\sigma_i = s | \sigma_{\mathcal{L}_{i,d}}, \mathcal{T}_d)$  satisfy "belief propagation" recursion

$$\nu_{s,d}^{i} := \begin{cases} \frac{1}{Z^{i}} \nu_{s} \prod_{j \in \mathcal{S}(i)} \sum_{s_{j} \in [q]} \frac{\nu_{s_{j}}^{i}}{\nu_{s_{j}}} P_{ss_{j}}, & i \in V_{d} \setminus \mathcal{L}_{d}, \\ \mathbb{I}_{s=\sigma_{i}}, & i \in \mathcal{L}_{d}. \end{cases}$$

Both an algorithm and an analysis tool: let  $\pi_{t,d} = \operatorname{Law}\left(\left(\nu_{s,d}^{r}\right)_{s\in[q]} \middle| \sigma_{r} = t\right)$ 

#### Theorem

 $\pi_d$  satisfies density evolution equation  $\pi_{d+1} = F(\pi_d)$ :

$$\begin{aligned} \pi_{\tau,d+1} &= Law\left(\left\{U_s/(\sum_{s'\in[q]}U_{s'})\right\}_{s\in[q]}\right) \text{ where:} \\ U_s &= \nu_s \prod_{j=1}^D \sum_{s_j\in[q]} \frac{X_{s_j}^{i_j}}{\nu_{s_j}} P_{ss_j}, \ D \sim \text{Poi}(\alpha), \ \sigma_1 \dots, \sigma_D \text{ i.i.d. } \sim P_{\tau}, \\ X^1, \dots, X^D: \text{ independent, and } X^j \sim \pi_{\sigma_j,d}, \ j \in [D]. \end{aligned}$$

Non-reconstructibility  $\Leftrightarrow \forall t \in [q], \ \lim_{d \to \infty} \pi_{t,d} = \delta_{\nu}$ 

Hence: Uniqueness of fixed point of density evolution,  $\pi = F(\pi)$  implies non-reconstructibility

Converse [Mézard-Montanari'06]: For  $\nu$  uniform on [q], non-uniqueness (for unconditional version of fixed point equation) implies reconstructibility

[Sly'09]: For symmetric Potts model with q, reconstruction differs from census reconstruction (3 distinct phases).

## Stochastic block model and community detection

Matrix *P* assumed reversible  $(\nu_s P_{st} = \nu_t P_{ts})$ 

#### Definition

Stochastic block model  $\mathcal{G} = \mathcal{G}(n, P, \alpha)$ : random graph  $\mathcal{G}$  on [n], s.t.  $\sigma_{[n]}$  i.i.d.  $\sim \nu$ , and Conditionally on  $\sigma_{[n]}$ , edges present independently,  $\mathbb{P}(i \sim j | \sigma_{[n]}) = \frac{R_{\sigma_i \sigma_j}}{n}$ , where  $R_{st} = \alpha P_{st} / \nu_t$ .



## Block reconstruction

#### Definition

Block reconstruction feasible if can compute estimates  $\hat{\sigma}_i, i \in [n]$ from observed graph  $\mathcal{G}$  such that with high probability

$$\liminf_{n\to\infty} I_n(\sigma;\hat{\sigma}) > 0, \text{ where } I_n(\sigma;\hat{\sigma}) := \sum_{s,t\in[q]} p_n(s,t) \ln\left(\frac{p_n(s,t)}{q_n(s)\nu_t}\right).$$

Alternative notion:

#### Definition

 $\begin{aligned} & \operatorname{overlap}(\hat{\sigma}_{[n]}): \text{ max over permutations } \pi \text{ of } [q] \text{ of } \\ & \frac{1}{n} \sum_{i \in [n]} \mathbb{I}_{\pi(\sigma_i) = \hat{\sigma}_i} - \sup_{s \in [q]} \nu_s. \\ & \text{Strong reconstruction holds if with high probability for some } \hat{\sigma}_{[n]}, \\ & \lim \inf_{n \to \infty} \operatorname{overlap}(\hat{\sigma}_{[n]}) > 0 \end{aligned}$ 

Strong reconstruction implies reconstruction; the two coincide for uniformly distributed  $\nu$ .

#### Theorem (Mossel-Neeman-Sly'15)

Block reconstruction in  $\mathcal{G}(n, P, \alpha)$  implies tree reconstruction in Poisson Galton-Watson tree with parameters  $P, \alpha$ .

Proof ideas:

-local structure of  $\mathcal{G}(n, P, \alpha)$ 

-approximate Markov random field property of  $\sigma_{[n]}$  on  $\mathcal{G}$ 

## Existence of hard phase

Mean progeny matrix:  $M = \alpha P$ Kesten-Stigum threshold:  $|\lambda_2(M)|^2 > \lambda_1(M) = \alpha$ .

Consider symmetric SBM:  $R_{st} = \begin{cases} c_{in} & \text{if } s = t, \\ c_{out} & \text{if } s \neq t. \end{cases}, \ \alpha = \frac{c_{in} + (q-1)c_{out}}{q}.$ 

### Theorem (Banks et al.'16)

For the symmetric SBM with  $q \ge 4$ , strong reconstruction holds strictly below the Kesten-Stigum threshold for some  $\hat{\sigma}_{[n]}$  that can be computed in exponential time.

Proof idea: **good partition** of [n]= balanced partition with interand intra-group edge counts close to target values; show with first moment method sufficient condition for all good partitions to achieve positive overlap.

## Above Kesten-Stigum threshold: belief propagation

Belief propagation iteration:  $\psi_s^{i \to j} \propto \nu_s \prod_{k \sim i, k \neq j} \sum_{s_k \in [q]} \psi_{s_k}^{k \to i} R_{ss_k}$ .

When converged, predicted distribution:  $\mathbb{P}(\sigma_i = s | \mathcal{G}) \approx \psi_s^i \propto \nu_s \prod_{j \sim i} \sum_{s_i \in [q]} \psi_{s_j}^{j \to i} R_{ss_j}$ 

## Conjecture (Decelle et al.'11)

Above Kesten-Stigum threshold, belief propagation on  $\mathcal{G}(n, P, \alpha)$ with random initialization converges, and fixed points  $\psi^i$  such that with high probability  $\liminf_{n\to\infty} I_n(\sigma; \psi) > 0$ .



Standard spectral method: Associate  $u \in [n]$  with  $x_i(u), i \in [r]$ where eigenvector  $x_i \leftrightarrow \lambda_i(A)$ 



 $\rightarrow$  fails to correlate with  $\sigma_i$ :

For  $\alpha = O(1)$ , largest eigenvalues  $\lambda_i(A) \sim \sqrt{\frac{\log n}{\log \log n}}$  induced by highest degree nodes,  $\sup_{j \in [n]} d_j \sim \frac{\log n}{\log \log n}$ 

Corresponding eigenvector uncorrelated with  $\sigma_{[n]}$ 

# Spectral redemption [Krzakala et al'13]

Linearization of BP around trivial fixed point:  $\psi_s^{i \to j} = \nu_s (1 + \epsilon_s^{i \to j})$ 

 $\rightarrow \epsilon = B \otimes P\epsilon$ , where B: non-backtracking matrix indexed by oriented edges  $i \rightarrow j \in \vec{E}$  of  $\mathcal{G}$ ,

 $B_{u\to v,x\to y} = \mathbb{I}_{v=x}\mathbb{I}_{y\neq u}$ 



Asymmetric, such that  $B_{ef}^k$  = number of non-backtracking walks on  $\mathcal{G}$  of k + 1 edges starting with e and ending with f

. . . . . . . . . .

For  $\lambda_i(M)$  and associated eigenvector  $x_i$ , let  $y_i \in \mathbb{R}^{\vec{E}} : y_i(u \to v) = x_i(\sigma_u)$  $z_i = B^{\ell}B^{\top \ell}y_i, \ \ell = \Theta(\log n)$ Let  $r_0 = \sup\{i \in [q] : \lambda_i(M)^2 > \lambda_1(M)\}.$ 

#### Theorem (Bordenave, Lelarge, M.'15)

$$\begin{split} &i \in [r_0] \Rightarrow \lim_{n \to \infty} \lambda_i(B) = \lambda_i(M), \\ &i > r_0 \Rightarrow \lim_{n \to \infty} \sup_{n \to \infty} |\lambda_i(B)| \le \sqrt{\lambda_1(M)} \\ &For \ i \in [r_0] \ s.t. \ \lambda_i(M) \ simple: \\ &B \ admits \ eigenvector \ \xi_i \leftrightarrow \lambda_i(B) \ s.t. \\ &\lim_{n \to \infty} \frac{\langle \xi_i, z_i \rangle}{\|\xi_i\| \cdot \|z_i\|} = 1. \\ &If \ moreover \ i > 1, \ then \ \hat{\sigma}_u := \sqrt{n} \sum_{v \sim u} \xi_i(u \to v) \ s.t. \\ &\lim_{n \to \infty} \ln(\sigma; \hat{\sigma}) > 0. \end{split}$$

## Non-backtracking spectrum of SBM $\mathcal{G}(n, P, \alpha)$

Illustration for symmetric SBM, q = 2, above Kesten-Stigum threshold:



## Baik-Ben Arous-Péché phase transition

Low-rank deformation of random matrices:  $W_n \in \mathbb{R}^{n \times n}$  Wigner matrix, i.e. symmetric,  $\{W_{i,j}\}_{i < j}$  i.i.d.  $\mathcal{N}(0, \sigma^2/n)$ ,  $\{W_{ii}\}$  i.i.d.  $\mathcal{N}(0, 2\sigma^2/n)$ Spectral measure  $\rightarrow$  Wigner's semi-circle law  $\propto \sqrt{4\sigma^2 - x^2} \mathbb{I}_{|x| \le 2\sigma} dx$ 



Let  $P_n \in \mathbb{R}^{n \times n}$  symmetric, fixed rank q and spectrum. Let  $r_0 = \{\sup\{i \in [q] : \lambda_i(P)^2 > \sigma^2\}$ . Then:

Theorem (Benaych-Georges, Nadakuditi'11)

For  $i \in [r_0]$ ,  $\lim_{n\to\infty} \lambda_i (W_n + P_n) = \lambda_i (P_n) + \frac{\sigma^2}{\lambda_i (P_n)}$ . For  $i > r_0$ ,  $\limsup_{n\to\infty} |\lambda_i (W_n + P_n)| \le 2\sigma$ 

| 4 同 ト 4 ヨ ト 4 ヨ ト

## Parallel with SBM's non-backtracking spectrum

$$\sigma^2(BBP) \leftrightarrow \sum_{v \in [n]} \operatorname{var}(A_{uv} | \sigma_{[n]}) \to \alpha;$$

 $P_n \leftrightarrow \mathbb{E}(A|\sigma_{[n]}) \Rightarrow \operatorname{spectrum}(P_n) \rightarrow \operatorname{spectrum}(M)$ 

Hence:

KS condition  $\lambda_i(M)^2 > \alpha \leftrightarrow \text{ BBP condition } \lambda_i(P_n)^2 > \sigma^2$ 

伺 と く き と く き と … き

## Ihara-Bass formula

For any graph  $\mathcal{G}$  with *n* nodes and *m* edges, any  $z \in \mathbb{C}$ ,

$$(1-z^2)^{n-m}\det(I-zB) = \det(I-zA-z^2\mathsf{Diag}(\{d_i-1\}_{i\in[n]}))$$

#### Corollary

 $\lambda \notin \{-1, 0, 1\}$  is an eigenvalue of *B* if and only if  $det(\lambda^2 I - \lambda A - Diag(\{d_i - 1\}_{i \in [n]})) = 0.$ 

#### Corollary

If  $\alpha \gg 1$  s.t. node degrees  $d_i$  concentrate, i.e.  $\sup_{i \in [n]} |d_i - \alpha| = o(\alpha)$ , then for  $\lambda \in sp(B)$ ,  $|\lambda| \ll \alpha$ , one has  $\lambda + \frac{\alpha}{\lambda} + o(1) \in sp(A)$ .

Suggests that for non-sparse models  $\alpha \gg 1$ , spectral methods based on *A* succeed, and non-backtracking spectrum properties imply BBP transition

- for denser models, "Approximate Message Passing" [Montanari] an approach of choice
- Finer phase transitions occur [Ricci-Tersenghi et al'18]
- Hard phase needs better understanding (basins of attraction, alternative dynamics)
- Statistical physics brings rich perspective on computational complexity