# Maximum Likelihood Estimation and Graph Matching in Errorfully Observed Networks

Jesús Arroyo

September 20th, 2020





#### Joint work with:



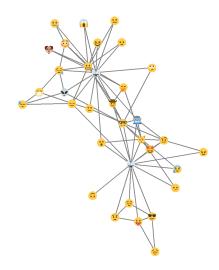
Daniel L. Sussman (Boston University)

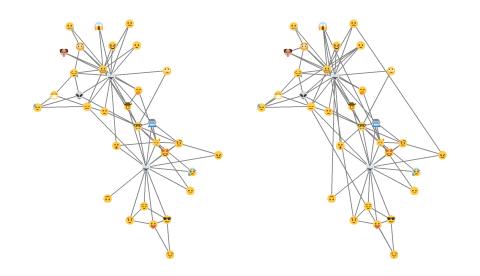


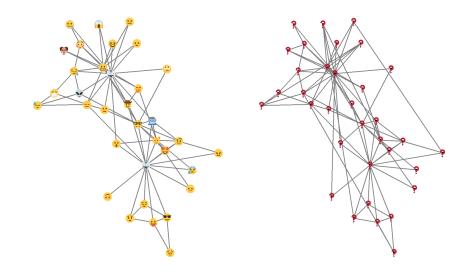
Carey E. Priebe (Johns Hopkins University)

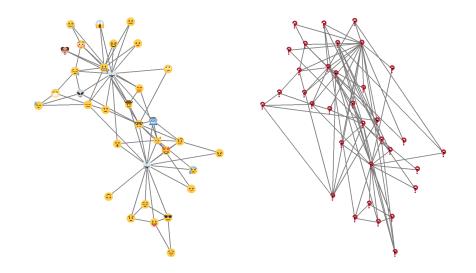


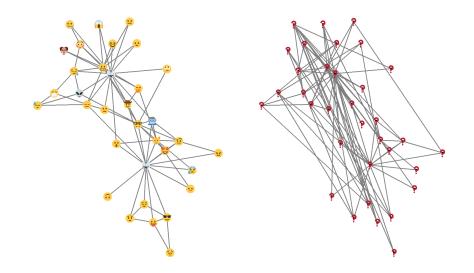
Vince Lyzinski (University of Maryland)

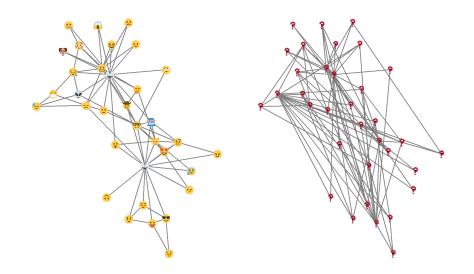


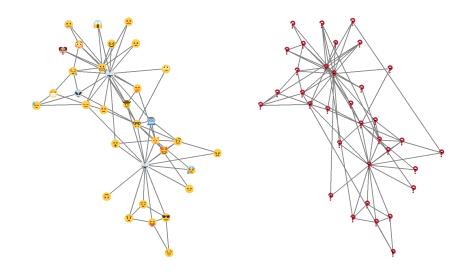


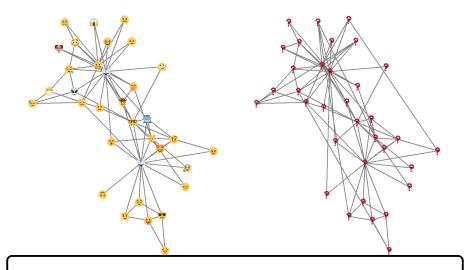












- How can we formulate a statistical model for graph matching?
- When is statistically feasible to solve the problem?

# Graph matching problem

Goal: find a meaningful correspondence between the vertices of the graphs

 Typically defined as the permutation that minimizes the number of edge disagreements:

$$\begin{split} \widehat{Q}_{\mathsf{GM}} &= \underset{Q \in \Pi_n}{\operatorname{argmin}} \, \|A - QBQ^T\|_F^2 \\ &= \underset{Q \in \Pi_n}{\operatorname{argmin}} \sum_{i \neq j} (A_{ij} - B_{\sigma(i),\sigma(j)})^2 \end{split}$$

- $A, B \in \{0, 1\}^{n \times n}$  adjacency matrices
- $\blacktriangleright \ Q$  is a permutation matrix,  $\sigma$  is the associated permutation function

# Graph matching problem

Goal: find a meaningful correspondence between the vertices of the graphs

 Typically defined as the permutation that minimizes the number of edge disagreements:

$$\begin{split} \widehat{Q}_{\mathsf{GM}} &= \underset{Q \in \Pi_n}{\operatorname{argmin}} \, \|A - QBQ^T\|_F^2 \\ &= \underset{Q \in \Pi_n}{\operatorname{argmin}} \sum_{i \neq j} (A_{ij} - B_{\sigma(i),\sigma(j)})^2 \end{split}$$

- $A, B \in \{0, 1\}^{n \times n}$  adjacency matrices
- $\,\blacktriangleright\, Q$  is a permutation matrix,  $\sigma$  is the associated permutation function

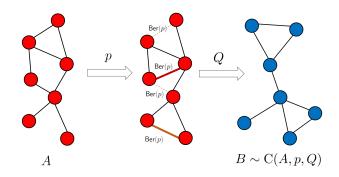
#### Some applications:

- Aligning biological networks
- De-anonymization in social networks
- Unsupervised word translation

# Corrupting channel model

**Model:** B is an edge and vertex-label corrupted version of A

- lacktriangle Edges and non-edges of A are independently flipped with probability p.
- $oldsymbol{Q}$  Vertices are shuffled with a permutation Q.



### Maximum likelihood estimation

Consider the maximum likelihood estimator for the parameters

$$(\widehat{p}_{\mathsf{MLE}}, \widehat{Q}_{\mathsf{MLE}}) := \operatorname*{argmax}_{p,Q} \sum_{u > v} \log \mathbb{P}_p \left( A_{uv} = (QBQ^T)_{uv} \right).$$

ullet  $\widehat{Q}_{\mathsf{MLE}}$  is the matching estimator via MLE.

### Maximum likelihood estimation

Consider the maximum likelihood estimator for the parameters

$$(\widehat{p}_{\mathsf{MLE}}, \widehat{Q}_{\mathsf{MLE}}) := \operatorname*{argmax}_{p,Q} \sum_{u > v} \log \mathbb{P}_p \left( A_{uv} = (QBQ^T)_{uv} \right).$$

- ullet  $\widehat{Q}_{\mathsf{MLE}}$  is the matching estimator via MLE.
- The MLE is equivalent to the typical graph matching formulation!

$$\widehat{Q}_{\mathsf{MLE}} = \mathop{\mathrm{argmin}}_{Q \in \Pi_n} \|A - QBQ^T\|_F^2.$$

### Maximum likelihood estimation

Consider the maximum likelihood estimator for the parameters

$$(\widehat{p}_{\mathsf{MLE}}, \widehat{Q}_{\mathsf{MLE}}) := \operatorname*{argmax}_{p,Q} \sum_{u > v} \log \mathbb{P}_p \left( A_{uv} = (QBQ^T)_{uv} \right).$$

- ullet  $\widehat{Q}_{\mathsf{MLE}}$  is the matching estimator via MLE.
- The MLE is equivalent to the typical graph matching formulation!

$$\widehat{Q}_{\mathsf{MLE}} = \operatorname*{argmin}_{Q \in \Pi_n} \|A - QBQ^T\|_F^2.$$

- Extensions of the model to non-uniform corrupting probabilities
  - ► This result also holds with non-uniform corrupting probabilities.

### When is the MLE correct?

ullet The difficulty of the problem depends on how different is A from  $QAQ^T$  for any  $Q \neq I$ , measured by

$$||A - QAQ^T||_F^2 = \sum_{i \neq j} (A_{ij} - A_{\sigma(i),\sigma(j)})^2.$$

### When is the MLE correct?

ullet The difficulty of the problem depends on how different is A from  $QAQ^T$  for any Q 
eq I, measured by

$$||A - QAQ^T||_F^2 = \sum_{i \neq j} (A_{ij} - A_{\sigma(i),\sigma(j)})^2.$$

 $\bullet$   $\Pi_{n,k}$  is the set of permutations that permute exactly k nodes.

#### Examples:

- k = 2
- $||A QAQ^T||_F^2 = 4$ .





### When is the MLE correct?

ullet The difficulty of the problem depends on how different is A from  $QAQ^T$  for any  $Q \neq I$ , measured by

$$||A - QAQ^T||_F^2 = \sum_{i \neq j} (A_{ij} - A_{\sigma(i),\sigma(j)})^2.$$

•  $\Pi_{n,k}$  is the set of permutations that permute exactly k nodes.

#### Examples:

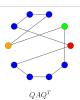
- k = 2
- $||A QAQ^T||_F^2 = 4.$





- k = 3
- $||A QAQ^T||_F^2 = 10.$





### Consistency of the MLE

Consider a sequence of networks  $\{A_n\}$  with n vertices, and parameters  $\{p_n,Q_n\}$ 

#### **Definition**

$$\{\widehat{Q}_n\}$$
 is consistent if  $\|\widehat{Q}_n - Q_n\|_F \stackrel{a.s.}{\longrightarrow} 0$  as  $n \to \infty$ .

Consistency: all vertices are correctly matched in the limit.

# Consistency of the MLE

Consider a sequence of networks  $\{A_n\}$  with n vertices, and parameters  $\{p_n,Q_n\}$ 

### Definition

$$\{\widehat{Q}_n\}$$
 is consistent if  $\|\widehat{Q}_n - Q_n\|_F \stackrel{a.s.}{\longrightarrow} 0$  as  $n \to \infty$ .

Consistency: all vertices are correctly matched in the limit.

#### Theorem

ullet  $\widehat{Q}_{\mathit{MLE}}$  is consistent if

$$\min_{Q \in \Pi_{n,k}} \|A_n - QA_nQ^T\|_F^2 \ge \frac{6k \log n}{(1/2 - p_n)^2}, \qquad \forall k \ge 2.$$

# Consistency of the MLE

Consider a sequence of networks  $\{A_n\}$  with n vertices, and parameters  $\{p_n,Q_n\}$ 

#### Definition

$$\{\widehat{Q}_n\}$$
 is consistent if  $\|\widehat{Q}_n - Q_n\|_F \stackrel{a.s.}{\longrightarrow} 0$  as  $n \to \infty$ .

Consistency: all vertices are correctly matched in the limit.

#### Theorem

ullet  $\widehat{Q}_{\mathit{MLE}}$  is consistent if

$$\min_{Q \in \Pi_{n,k}} \|A_n - QA_nQ^T\|_F^2 \ge \frac{6k \log n}{(1/2 - p_n)^2}, \qquad \forall k \ge 2.$$

ullet  $\widehat{Q}_{\mathit{MLE}}$  is not consistent if there exists  $m=\Omega(n)$  disjoint permutations  $Q_1,\ldots,Q_m$ 

$$\max_{i \in [m]} \|A_n - Q_i A_n Q_i^T\|_F^2 = o\left(\frac{\log n}{(1/2 - p_n)^2}\right).$$

# Relaxed consistency of the MLE

Matching all vertices correctly can be hard or impossible, for example:

- low-degree vertices
- automorphisms in the graph

# Definition (Relaxed consistency)

$$\{\widehat{Q}_n\}_{n=n_0}^{\infty} \text{ is } \{\underline{k}_n\}\text{-consistent if } \tfrac{\|\widehat{Q}_n-Q_n\|_F}{k_n} \xrightarrow{a.s.} 0. \text{ as } n\to\infty$$

**Relaxed consistency**: at most  $o(k_n)$  misaligned vertices.

# Relaxed consistency of the MLE

Matching all vertices correctly can be hard or impossible, for example:

- low-degree vertices
- automorphisms in the graph

### Definition (Relaxed consistency)

$$\{\widehat{Q}_n\}_{n=n_0}^{\infty} \text{ is } \{\underline{k}_n\}\text{-consistent if } \xrightarrow{\|\widehat{Q}_n-Q_n\|_F} \xrightarrow{a.s.} 0. \text{ as } n \to \infty$$

**Relaxed consistency**: at most  $o(k_n)$  misaligned vertices.

#### Theorem

$$\widehat{Q}_{MLE}$$
 is  $k_n$ -consistent if

$$\min_{Q \in \Pi_{n,k}} \|A_n - QA_nQ^T\|_F^2 \ge \frac{6k \log n}{(1/2 - p_n)^2}, \qquad \forall k \ge k_n.$$

# Consistency in random graph models

#### Erdős-Rényi graph model: $A_n \sim G(n, \alpha_n)$







### Corollary

 $\widehat{Q}_{\mathrm{MLE}}$  is consistent if

$$\alpha_n \ge \frac{c_1 \log n}{n(1/2 - p_n)^2}.$$

### Newman-Watts small world graph model: $A_n \sim \mathrm{NW}(n, d_n, \beta_n)$ ,



 $\begin{aligned} d &= 4, \\ \beta &= 0 \end{aligned}$ 

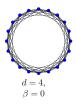


d = 4, $\beta = 0.05$ 

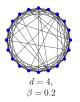


d = 4, $\beta = 0.2$ 

### Newman-Watts small world graph model: $A_n \sim NW(n, d_n, \beta_n)$ ,





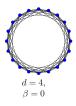


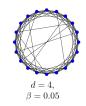
Corollary

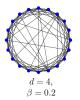
• For any  $\{d_n\}$ ,  $\widehat{Q}_{\mathsf{MLE}}$  is **not consistent** if  $(1/2-p_n)^2=o(\sqrt{\log n/n})$  and

$$\beta_n = o\left(\frac{\log n}{(1/2 - p_n)^2 n}\right).$$

### Newman-Watts small world graph model: $A_n \sim NW(n, d_n, \beta_n)$ ,







# Corollary

ullet For any  $\{d_n\},\ \widehat{Q}_{\mathsf{MLE}}$  is not consistent if  $(1/2-p_n)^2=o(\sqrt{\log n/n})$  and

$$\beta_n = o\left(\frac{\log n}{(1/2 - p_n)^2 n}\right).$$

•  $\widehat{Q}_{\mathrm{MLE}}$  is consistent if  $d_n = o(\beta_n^2 n)$  and

$$\beta_n \ge C\sqrt{\frac{\log n}{n\left(1/2 - p_n\right)^2}}.$$

# Relaxed consistency

#### Random regular graphs: $A \sim G_{n,d_n}$







d = 2

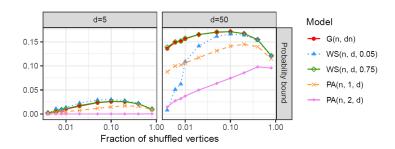
### Corollary

If  $d_n=c_1n^{2/3+\varepsilon}$  and  $(\frac12-p_n)^2\geq c_2\frac{\log n}{d_n},$  then  $\widehat Q_{\sf MLE}$  is  $\{n^{2/3+\varepsilon}\}$ -consistent.

A negligible fraction of the vertices  $(o(n^{-(1/3-\epsilon)}))$  might be incorrectly matched.

# Matchability on random graphs

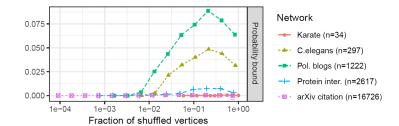
**Measure matching feasibility:** Upper bound for the noise probability tolerated by a graph based on the theory



#### Models considered

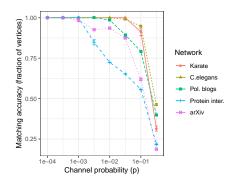
- ightharpoonup G(n,dn) Erdös-Rényi
- $WS(n,d,\beta)$ : Watts-Strogatz
- $ightharpoonup PA(n, \gamma, d)$ : preferential attachment

# Matchability on real networks



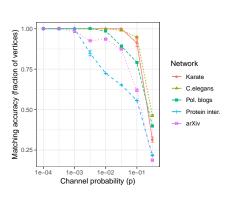
# Matchability on real networks

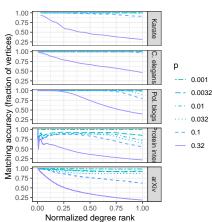
- $\bullet$  Sample B from corrupting channel, and approximately compute the MLE
- Evaluate percentage of correctly matched vertices (left) and large degree vertices that are correctly matched (right).



# Matchability on real networks

- $\bullet$  Sample B from corrupting channel, and approximately compute the MLE
- Evaluate percentage of correctly matched vertices (left) and large degree vertices that are correctly matched (right).





#### Conclusion

- Graph matching on errorfully observed networks is *statistically* feasible when:
  - ► The topology of the network is sufficiently irregular
  - ► The noise is small enough
- What are the computational limits?
- Matching on other relational data structures? multilayer networks, vertex or edge attributes, bipartite graphs, etc.
  - ► Graph matching between bipartite and unipartite networks: arXiv:2002.01648.

#### Conclusion

- Graph matching on errorfully observed networks is *statistically* feasible when:
  - ► The topology of the network is sufficiently irregular
  - ► The noise is small enough
- What are the computational limits?
- Matching on other relational data structures? multilayer networks, vertex or edge attributes, bipartite graphs, etc.
  - ► Graph matching between bipartite and unipartite networks: arXiv:2002.01648.

### Thank you!

Arroyo, J., Sussman, D. L., Priebe, C. E., Lyzinski, V. (2018). *Maximum Likelihood Estimation and Graph Matching in Errorfully Observed Networks*. arXiv:1812.10519.