Optimization and learning techniques for clustering problems

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Statistical Physics and Machine Learning back together
Cargèse, August 2018

Clustering

"Next AI revolution is unsupervised" Yann LeCun

Main task in unsupervised machine learning:

- Finding structure in unlabeled data.

k-means clustering

- Simple objective
- Useful for "generic data"

Clustering stochastic block model

- Specialized objective
- Algorithms get more precise but less robust to model changes

Data-driven clustering methods.

Clustering

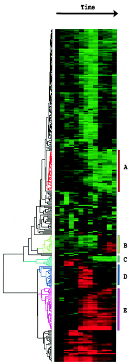
"Next AI revolution is unsupervised" Yann LeCun

Main task in unsupervised machine learning:

- Finding structure in unlabeled data.

Example:
Cluster analysis and display of genome-wide expression patterns.

- Gene expression as a function of time for different conditions.
- Clustering gene expression data groups together genes of known similar functionality.



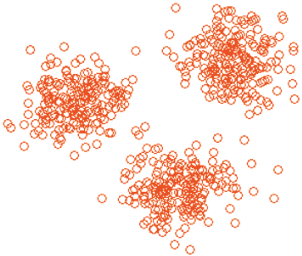
Eisen, Spellman, Brown, Botstein, PNAS, 1998

Summary

- k-means clustering
  - Landscape of manifold optimization
  - Lower bounds certificates from SDPs (data-driven)
- Clustering stochastic block model
  - AMP $\longrightarrow$ Spectral methods $\longrightarrow$ Graph neural networks
- Quadratic assignment

The k-means problem

Given a point cloud $\{x_i\}$, partition the points in clusters $C_1, \ldots, C_k$



k-means objective:

$$\min_{C_1,\ldots C_k} \sum_{t=1}^{k} \sum_{i \in C_t} \left\| x_i - \frac{1}{|C_t|} \sum_{j \in C_t} x_j \right\|^2$$

- NP-hard to minimize in general (even in the plane).

Lloyd's algorithm

1. Choose k centers at random.
2. Assign points to closest center.
3. Compute new centers are clusters centroids.

k-means++ is Lloyd's with smarter initialization.

Pros:

- Fast.
- Very easy to implement.
- Widely used and it works for most applications.

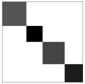
Cons:

- No guarantee of convergence (local minima).
- In extreme cases it may take exponentially many steps.
- Solutions depend heavily on initialization.
- Its output doesn't say how good of a solution it may be.

Optimization formulation

Taking $D_{ij} := \|x_i - x_j\|^2$, then

$$\sum_{t=1}^{k} \sum_{i \in C_t} \left\| x_i - \frac{1}{|C_t|} \sum_{j \in C_t} x_j \right\|^2 = \frac{1}{2} \operatorname{Tr}\left(D \underbrace{\sum_{t=1}^{k} \frac{1}{|C_t|} 1_{C_t} 1_{C_t}^\top} \right)$$



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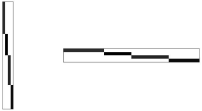


$$\begin{array}{ll} \text{minimize} & \operatorname{Tr}(D Y Y^\top) \\ \text{subject to} & Y \in \mathbb{R}^{n \times k} \\ & Y^\top Y = I_k \\ & Y Y^\top 1 = 1 \\ & Y \geq 0 \end{array}$$

Set of Y's is discrete.

Manifold optimization implementation

$$\begin{array}{ll} \text{minimize} & \mathrm{Tr}(DYY^\top) + \lambda \|Y_-\|^2 \\ \text{subject to} & Y \in M = \{Y \in \mathbb{R}^{n\times k} : Y^\top Y \ = I_k, \quad YY^\top 1 = 1\} \end{array}$$

To implement the manifold optimization one needs:

$$\mathrm{grad}_f : M \to TM,$$
$$\mathrm{retr}_Y : T_Y M \to M,$$

where

$$\mathrm{retr}_Y(0) = 0, \quad \left.\frac{d}{dt}\right|_{t=0} \mathrm{retr}_Y(tV) = V.$$

Gradient descent:

$$Y_{n+1} = \mathrm{retr}_{Y_n}(-\alpha_n \, \mathrm{grad}_f(Y_n)).$$

Sepulchre, Absil, Mahony, 2008

Carson, Mixon, V., Ward, SampTA, 2017

Manifold optimization, retraction implementation

Homogeneous structure of M.
Let $O(1_n)$ be the $n \times n$ orthogonal matrices that fix 1.

$$\begin{aligned} M \times O(1_n) \times O(k) &\to M \\ (Y, Q, R) &\mapsto QYR \quad \text{(transitive action)} \end{aligned}$$

Multiplication of Y on the right by R is equivalent to multiplication on the left by $R' = YRY^\top \in O(1_n)$.

$V \in T_Y M$ can be written as $V = BY + YA$ where $A \in \mathfrak{so}(k)$, $B \in \mathfrak{so}(1_n)$ where BY and YA are orthogonal. We compute A, B explicitly.

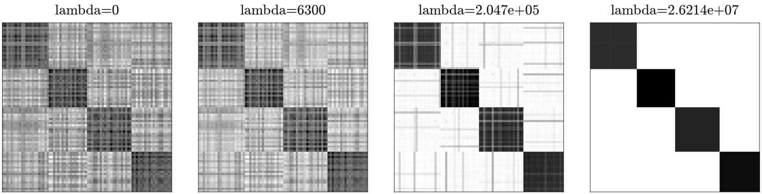
$$\begin{aligned} A &= Y^\top V \\ B &= VY^\top - YV^\top - 2YAY^\top \end{aligned}$$

$\mathrm{retr}_Y(V) = \exp(B)\exp(A')Y \in M$

Manifold optimization algorithm

$\lambda_0 \leftarrow 0$
repeat
  $Y_{n+1} \leftarrow \text{GradientDescent}(f_\lambda)$ {Initialized at Y_n}
  $\lambda_{n+1} \leftarrow 2\lambda_n + 1$
until $\|Y_-\|_F < \epsilon$

$$\begin{aligned} &\text{minimize}_Y \quad f_\lambda(Y) = \text{Tr}(DYY^\top) + \lambda \|Y_-\|^2 \\ &\text{subject to} \quad Y \in M = \{Y \in \mathbb{R}^{n\times k} : Y^\top Y = I_k, \quad YY^\top 1 = 1\} \end{aligned}$$



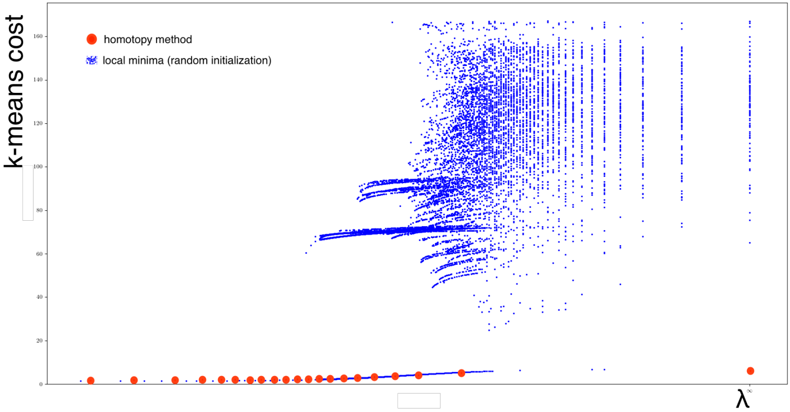
Problem structure allows to do each iteration in linear-time.

Carson, Mixon, V., Ward, SampTA, 2017

Claim: clustering is (maybe) not (that) hard

Optimization landscape

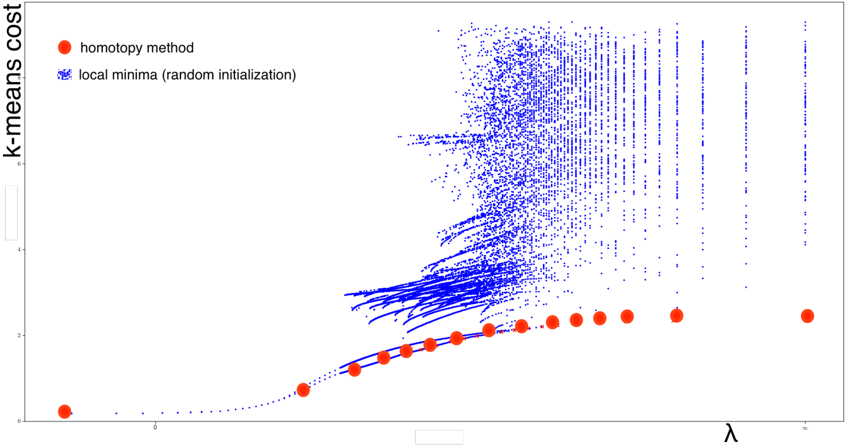
Points from three well-separated unit balls in small dimension.



Claim: clustering is (maybe) not (that) hard

No clustering structure

Points drawn from unit ball into three clusters in small dimension.

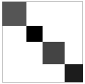


And it's optimal! How do I know that?

k-means optimization formulation

Recall $D_{ij} := \|x_i - x_j\|^2$, then

$$\sum_{t=1}^{k} \sum_{i \in C_t} \left\| x_i - \frac{1}{|C_t|} \sum_{j \in C_t} x_j \right\|^2 = \frac{1}{2} \operatorname{Tr}\left(D \underbrace{\sum_{t=1}^{k} \frac{1}{|C_t|} 1_{C_t} 1_{C_t}^\top} \right)$$



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$$\begin{aligned} \text{minimize} \quad & \operatorname{Tr}(D Y Y^\top) \\ \text{subject to} \quad & Y \in \mathbb{R}^{n \times k} \\ & Y^\top Y = I_k \\ & Y Y^\top 1 = 1 \\ & Y \geq 0 \end{aligned}$$

Set of Y's is discrete.

A semidefinite programming relaxation

Recall $D_{ij} := \|x_i - x_j\|^2$, then

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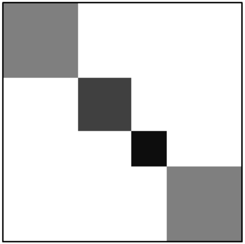
Relax to SDP:

$$\begin{array}{ll} \text{minimize} & \operatorname{Tr}(DX) \\ \text{subject to} & \operatorname{Tr}(X) = k \\ & X1 = 1 \\ & X \geq 0 \\ & X \succeq 0 \end{array}$$

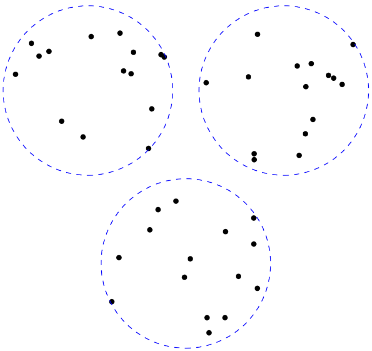


Peng, Wei, SIAM J. Optim., 2007

Stochastic ball model

$(\mathcal{D}, \gamma, n)$-**stochastic ball model**

- $\mathcal{D}$ = rotation-invariant distribution over unit ball in $\mathbb{R}^m$
- $\gamma_1, \ldots, \gamma_k$ = ball centers in $\mathbb{R}^m$
- Draw $r_{t,1}, \ldots, r_{t,n}$ i.i.d. from $\mathcal{D}$ for each $i \in \{1, \ldots, k\}$
- $x_{t,i} = \gamma_t + r_{t,i}$ = ith point from cluster t



Nellore, Ward, Information and Computation, 2015

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Nellore, Ward, Information and Computation, 2015

k-means SDP. *Stochastic ball model*

Exact recovery

SDP is tight for k unit balls in $\mathbb{R}^m$ with centers $\gamma_i \dots \gamma_k$

$$\min_{i \neq j} \|\gamma_i - \gamma_j\| \geq \min \left\{ 2\sqrt{2}(1 + \tfrac{1}{\sqrt{m}}),\ 2 + \tfrac{k^2}{m},\ 2 + \sqrt{\tfrac{2k}{m+2}} \right\}$$

Conjecture (Li, Li, Ling, Strohmer)

Phase transition for exact recovery (under stochastic ball model) at

$$\min_{i \neq j} \|\gamma_i - \gamma_j\| \geq 2 + \frac{c}{m}$$

Awasthi, Bandeira, Charikar, Krishnaswamy, V., Ward, Proc. ITCS, 2015

Iguchi, Mixon, Peterson, V., Mathematical Programming, 2016

Li, Li, Ling, Strohmer, `arXiv:1710.06008` 2017

k-means SDP. *Subgaussian mixtures*

Relax and "round" (weak recovery).

Theorem

Centers: $\hat{\gamma}_1, \ldots, \hat{\gamma}_k$. Estimated centers $v_1, \ldots, v_k$

$$\frac{1}{k}\sum_{i=1}^{k} \|v_i - \hat{\gamma}_i\|^2 \lesssim k^2\sigma^2 \text{ whp provided } \min_{i \neq j} \|\gamma_i - \gamma_j\| \gtrsim k\sigma.$$

Example: `http://solevillar.github.io/2016/07/05/Clustering-MNIST-SDP.html`

Mixon, V., Ward, Information and Inference, 2017

Proof technique: Guédon, Vershynin, Probability Theory and Related Fields, 2016

SDPs are slow!

Fast lower bound certificates

Want: Lower bound on k-means value,

Given $\{x_i\}_{i\in T} \subseteq \mathbb{R}^m$, let $W=$ value of k-means++ initialization

$$\mathrm{val}_{\mathrm{kmeans}}(\mathrm{T}) := \min \frac{1}{|T|} \sum_{t=1}^{k} \sum_{i\in C_t} \left\| x_i - \frac{1}{|C_t|} \sum_{j\in C_t} x_j \right\|^2 \geq \frac{1}{8(\log k + 2)} \mathbb{E} W$$

Running k-means++ on MNIST training set with $k = 10$ gives:

- Upper bound (by running the algorithm): 39.22
- Lower bound (estimated from above): 2.15

Can we get a better lower bound?

Arthur, Vassilvitskii, 2007

Idea

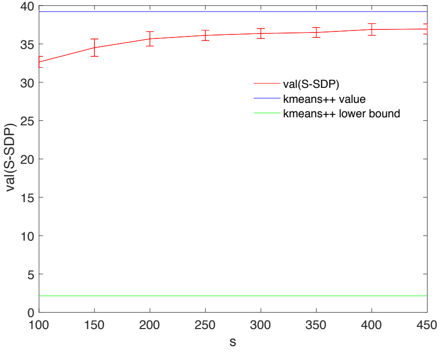
Given $\{x_i\}_{i \in T} \subseteq \mathbb{R}^m$, draw $S \sim \mathrm{Unif} \in \binom{T}{s}$.

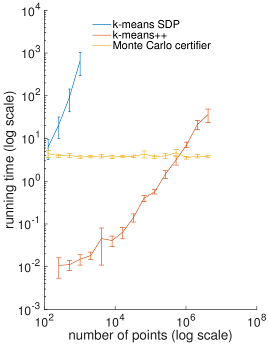
$$\begin{aligned}
\mathbb{E}\,\mathrm{val}_{\mathrm{SDP}}(\mathrm{S}) &\leq \mathbb{E}\,\mathrm{val}_{\mathrm{kmeans}}(\mathrm{S}) \\
&\leq \mathbb{E}\left[\frac{1}{s}\sum_{t=1}^{k}\sum_{i \in C_t^* \cap S}\left\|x_i - \frac{1}{|C_t^* \cap S|}\sum_{j \in C_t^* \cap S} x_j\right\|^2\right] \\
&\leq \mathbb{E}\left[\frac{1}{s}\sum_{t=1}^{k}\sum_{i \in C_t^* \cap S}\left\|x_i - \frac{1}{|C_t^*|}\sum_{j \in C_t^*} x_j\right\|^2\right] = \mathrm{val}_{\mathrm{kmeans}}(\mathrm{T})
\end{aligned}$$

Goal: Establish $\mathbb{E}\,\mathrm{val}_{\mathrm{SDP}}(\mathrm{S}) > B$ with small p-value.

Mixon, V., arXiv:1710.00956

Better performance, and fast!





- Taking $s = 100 \ll 60,000$ MNIST points already works
- Constant runtime in N, faster than k-means++ for $N \gtrsim 10^6$.
- Theorem for mixtures of Gaussians (additive bound)

Mixon, V., arXiv:1710.00956

Generic algorithms vs. model-dependent algorithms

Clustering the stochastic block model

- Sparse graph clustering (non-geometric)
- Similar generic algorithmic (SDP, manifold optimization)
- Model-tailored algorithms (AMP, spectral methods on Non-bactracking matrices and Bethe Hessian)
- Can we learn the algorithm from data?
  - Use graph neural networks

Decelle, Krzakala, Moore, Zdeborová, 2013

Krzakala, Moore, Mossel, Neeman, Sly, Zdeborová, Zhang, 2013

Saade, Krzakala, Zdeborová, 2014

Abbe, 2018

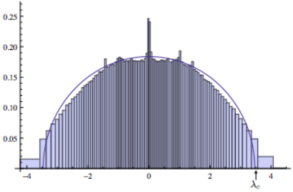
Spectral redemption

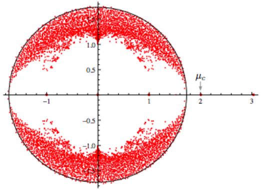
$A \sim SBM(a/n, b/n, n, 2)$ sparse.

Spectrum doesn't concentrate (high degree vertices dominate it)
Laplacian is not useful for clustering

Consider the non-backtracking operator (from linearized BP)

$$B_{(i \to j)(i' \to j')} = \begin{cases} 1 \text{ if } j = i' \text{ and } j' \neq i \\ 0 \text{ otherwise} \end{cases}$$





Second eigenvector of B reveals clustering structure

Krzakala, Moore, Mossel, Neeman, Sly, Zdeborová, Zhang, 2013

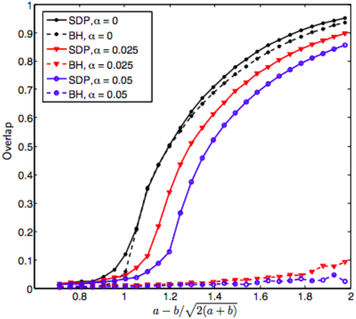
Bethe Hessian

$$BH(r) = (r^2 - 1)I - rA + D$$

Fixed points of BP $\longleftrightarrow$ Stationary points of Bethe free energy

Second eigenvector reveals clustering structure

Pitfall: highly dependent in the model



Goal: Combine graph operators $I, D, A, \ldots$ to generate robust "data-driven spectral methods" for problems in graphs

Saade, Krzakala, Zdeborová, 2014

Javanmard, Montanari, Ricci-Tersenghi, 2015

Graph neural networks

Power method: $v^{t+1} = Mv^t \qquad t = 1, \dots, T.$

Graph with adjacency matrix A. Set $\mathcal{M} = \{I_n, D, A, A^2, \dots A^{2^J}\}$,

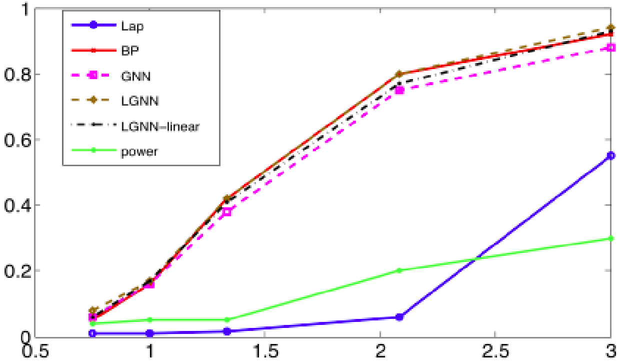
$$v_l^{t+1} = \rho\left(\sum_{M \in \mathcal{M}} M v^t {\theta_{M,l}}^t\right) \,, \, l = 1 \dots d_{t+1}$$

with $v^t \in \mathbb{R}^{n \times d_t}$,
$\Theta = \{\theta_1^t, \dots, \theta_{|\mathcal{M}|}^t\}_t$, $\theta_M^t \in \mathbb{R}^{d_t \times d_{t+1}}$ trainable parameters.

- Extension to line graph (GNN with non-backtracking).
- Covariant wrt permutations $G \mapsto \phi(G)$ then $G_\Pi \mapsto \Pi\phi(G)$.
- Preliminary theoretical analysis of energy landscape.
  - Strong assumptions $\Rightarrow$ local minima have low energy.

Scarselli, Tsoi, Hagenbuchner, Monfardini, IEEE Transactions on Neural Networks, 2009
Chen, Li, Bruna, 2017

Numerical performance. SBM $k = 2$

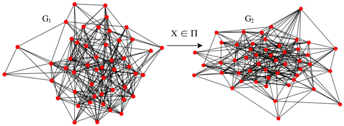


Overlap as function of SNR

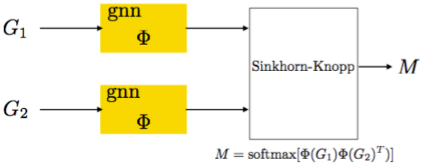
Chen, Li, Bruna, 2017

Extension to quadratic assignment

Graph matching: $\min_{X \in \Pi} \|G_1 X - X G_2\|_F^2 = \|G_1 X\|^2 + \|X G_2\|^2 - 2\langle G_1 X, X G_2 \rangle$



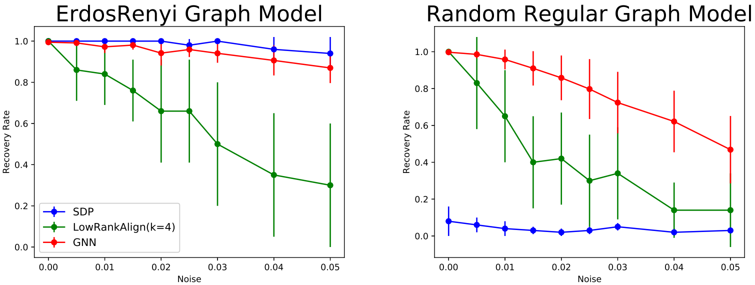
Siamese neural network:



$G_2 = \pi G_1 + N$ $\quad$ $N \sim$Erdos-Renyi
$G_1 \sim$ Erdos-Renyi
$G_1 \sim$ Random regular

Nowak, V., Bandeira, Bruna, 2017

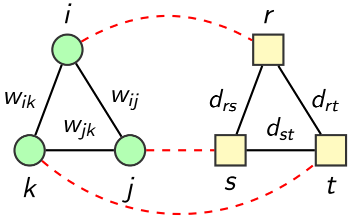
Numerical experiment



Our model runs in $O(n^2)$, LowRankAlign is $O(n^3)$, SDP in $O(n^4)$.

Nowak, V., Bandeira, Bruna, 2017

Quadratic Assignment Problem (QAP)



$$\min_{\pi} \quad \sum_{i\in A}\sum_{j\in A}\sum_{r\in B}\sum_{s\in B} \underbrace{w_{ij}\, d_{rs}}_{E_{ijrs}} \pi_{ir}\pi_{js}$$

$$\text{subject to} \quad \sum_{r} \pi_{ir} = 1 \quad \forall i \in A$$

$$\sum_{i} \pi_{ir} = 1 \quad \forall r \in B$$

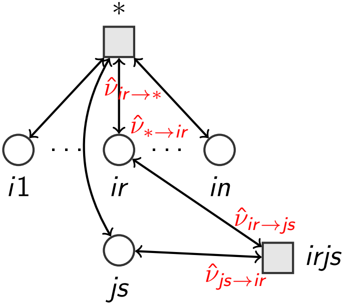
$$\pi_{ir} \in \{0, 1\}$$

Onaran, Villar, ongoing work

Max-Product Belief Propagation for QAP

- Posterior probability:

$$p(\pi) = \frac{1}{Z} \prod_i \mathbb{1}\{\sum_t \pi_{it} = 1\} \prod_r \mathbb{1}\{\sum_k \pi_{kr} = 1\} \prod_{j \neq i} \prod_{s \neq r} e^{-\beta \pi_{ir} \pi_{js} E_{ijrs}}$$



Max-Product Message Updates

- Variable to check nodes:

$$\nu_{ir\to *}(1) \cong \prod_{kt} e^{-\beta \hat{\nu}_{kt\to ir}(1) E_{irkt}}$$

$$\nu_{ir\to *}(0) \cong 1$$

- Check to variable nodes:

$$\nu_{*\to ir}(1) \cong \nu_{ir\to *}(1) \prod_{\ell \neq i} \nu_{\ell r\to *}(0) \prod_{t\neq r} \nu_{it\to *}(0)$$

$$\nu_{*\to ir}(0) \cong \nu_{ir\to *}(0) \max_{t\neq r, \ell\neq i} \nu_{it\to *}(1)\nu_{\ell r\to *}(1) \prod_{u\neq t,r} \nu_{iu\to *}(0) \prod_{m\neq \ell, i} \nu_{mr\to *}(0)$$

- Variable back to variable nodes:

$$\hat{\nu}_{ir\to js}(1) \cong \nu_{*\to ir}(1) \prod_{ku\neq js} e^{-\beta \hat{\nu}_{ku\to ir}(1) E_{irku}}$$

$$\hat{\nu}_{ir\to js}(0) \cong \nu_{*\to ir}(0)$$

Simplifications (Min-Sum Algorithm)

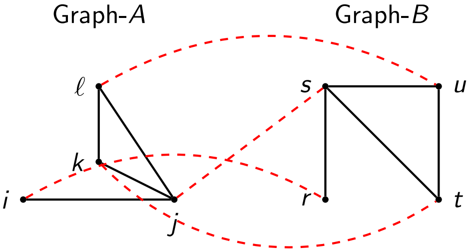
Introduce log-likelihood ratio:

$$\hat{\ell}_{ir\to js} = \frac{1}{\beta} \log \frac{\hat{\nu}_{ir\to js}(1)}{\hat{\nu}_{ir\to js}(0)}$$

Then the algorithm simplifies to one update step as follows,

$$\begin{aligned}\hat{\ell}_{ir\to js} \leftarrow \min_{t\neq r, l\neq i} & \sum_{ku} \frac{e^{\beta\hat{\ell}_{ku\to it}}}{1+e^{\beta\hat{\ell}_{ku\to it}}} E_{itku} + \frac{e^{\beta\hat{\ell}_{ku\to \ell r}}}{1+e^{\beta\hat{\ell}_{ku\to \ell r}}} E_{\ell rku} \\ & -2\sum_{ku\neq js} \frac{e^{\beta\hat{\ell}_{ku\to ir}}}{1+e^{\beta\hat{\ell}_{ku\to ir}}} E_{irku} + \frac{e^{\beta\hat{\ell}_{js\to ir}}}{1+e^{\beta\hat{\ell}_{js\to ir}}} E_{irjs}\end{aligned}$$

A special case: Graph Matching (Isomorphism)



When $A \sim \mathrm{ER}(n, 0.5)$ and

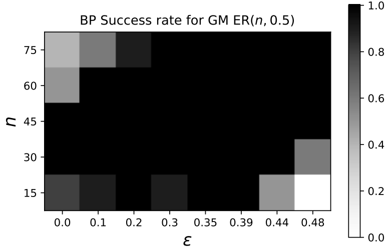
$$B = PAP^T \oplus Z$$

for some $P \in \Pi$ where $Z \sim \mathrm{Ber}(\epsilon)$. Find P given unlabeled graphs.

$$\min_{P} \quad \|A - PBP^T\|_F$$

$$\text{subject to} \quad P \in \Pi$$

equivalent to QAP with $E_{ijrs} = A_{ij} \oplus B_{rs}$.



Summary

- k-means clustering
  - Nice manifold optimization landscape
  - Lower bounds certificates from SDPs (data-driven)
- Clustering stochastic block model
  - AMP $\longrightarrow$ Spectral methods $\longrightarrow$ Graph neural networks
- Quadratic assignment

Thank you

Relax no need to round: Integrality of clustering formulations
P. Awasthi, A. S. Bandeira, M. Charikar, R. Krishnaswamy, S. Villar, R. Ward
arXiv:1408.4045, Innovations in Theoretical Computer Science (ITCS) 2015

Probably certifiably correct *k*-means clustering
T. Iguchi, D. G. Mixon, J. Peterson, S. Villar
arXiv:1509.07983, Mathematical Programming, 2016

Clustering subgaussian mixtures by semidefinite programming
D. G. Mixon, S. Villar, R. Ward
arXiv:1602.06612, Information and Inference: A Journal of the IMA, 2017

Monte Carlo approximation certificates for k-means clustering
D. G. Mixon, S. Villar
arXiv:1710.00956

Supervised Community Detection with Hierarchical Graph Neural Networks
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