Cut Improvement and Clustering using Compressive Sensing

Math. of Data Science Virtual Lecture Series
Tufts University

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Clusters in Graphs

- All graphs G = (V, E) are finite and $V := [n] = \{1, \dots, n\}$.
- A denotes (possibly weighted) adjacency matrix of G.
- For any data set $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\} \subset \mathbb{R}^D$ can make graph:

$$A_{ij} = \exp\left(-\|\boldsymbol{x}_i - \boldsymbol{x}_j\|^2/\sigma^2\right)$$

• A cluster $C \subset V$ has "many" internal edges and "few" external edges.

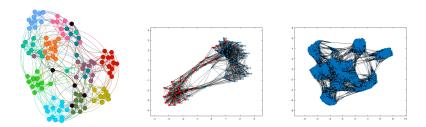


Figure: From left to right: College Football (2000 season) Girvan and Newman [2002], Senate Co-voting data for 97th congress Lewis et al. [2020], OptDigits made into a graph.

Quantifying Good Clusters

A cluster $C \subset V$ has "many" internal edges and "few" external edges.

- **Volume:** $vol(C) := \sum_{i \in C} d_i$ where $d_i = \text{degree of } i = \sum_j A_{ij}$
- Cut: Cut(C) = $\sum_{i \in C, j \in \bar{C}} A_{ij}$
- Normalized Cut: $NCut(C) = \frac{Cut(C)}{vol(C)vol(\overline{C})}$
- Conductance: $Cond(C) = \frac{Cut(C)}{\min(vol(C), vol(\bar{C}))}$
- Finding $C^{\#} = \min_{C \subset V} Cut(C)$ possible but non-informative.
- Finding $C^\# = \min_{C \subset V} \mathsf{NCut}(C)$ or $\min_{C \subset V} \mathsf{Cond}(C)$ informative but NP-Hard

Finding Good Clusters—Local and Global

- Global clustering (e.g. Spectral Clustering ¹).
 - Operates on full adj. matrix, run time $\sim O(n^2)$.
 - Typically unsupervised.
- Strongly local clustering (e.g. Nibble, CRD, LocalImprove²).
 - Semi-supervised: Given $\Gamma \subset V$ returns $C^{\#}$ containing Γ .
 - Only operates on neighbourhood of $C^{\#}$, run time $\sim O(\operatorname{vol}(C^{\#}))$.
- Weakly local clustering (e.g. PPR, HK-flow, <u>CP+RWT</u>³).
 - Semi-supervised: Given $\Gamma \subset V$ returns $C^{\#}$ containing Γ .
 - Operate on whole graph, run time $\sim \tilde{O}(n)$.
- Cut improvement (e.g. FlowImprove, LocalFlow, ClusterPursuit) 4
 - Given $\Omega \approx C$ returns $C^{\#}$ better approx to C.
 - Can be local, run time $= O(Vol(\Omega)^{\alpha})$, or global, run time $= \tilde{O}(n)$.

¹Shi and Malik [2000], Ng et al. [2002]

²Spielman and Teng [2004, 2013], Wang et al. [2017], Veldt et al. [2016]

³Andersen et al. [2007],Kloster and Gleich [2014],Lai and Mckenzie [2019]

⁴Andersen and Lang [2008], Orecchia and Allen-Zhu [2014], Lai and Mckenzie [2019]

Overview of this talk

- We rephrase cut improvement as a compressive sensing problem.
- We introduce a new algorithm for cut improvement: ClusterPursuit.
- This algorithm enjoys theoretical guarantees on accuracy and run time.
- Numerical results are good.
- We use ClusterPursuit to design local & global clustering algorithms.
- Code available at: http://danielmckenzie.github.io/.

In cluster and between cluster graphs

- Graph Laplacian: $L = I D^{-1}A$.
- Suppose G has clusters C_1, \ldots, C_k .
- **Key Idea:** Split $G = G^{in} \coprod G^{out}$.
- Here $E^{\text{in}} = \{\{i, j\} : i, j \in C_a \text{ for } a = 1, ..., k\} \text{ and } G^{\text{in}} := (V, E^{\text{in}}).$
- $E^{\text{out}} = E \setminus E^{\text{in}}$ and $G^{\text{out}} = (V, E^{\text{out}})$.
- Let A^{in} (resp. L^{in}) denote adj. matrix (resp. Laplacian) of G^{in} .
- Then $A = A^{in} + A^{out}$ and $L = L^{in} + M$.
- **Theorem**⁵ $L^{\text{in}} \mathbf{1}_{C_a} = 0$ for a = 1, ..., k.
- Observation: $\|\mathbf{1}_{C_a}\|_0 := |\{i: (\mathbf{1}_{C_a})_i \neq 0\}| = |C_a| := n_a$

⁵See, for example, Von Luxburg [2007]

(Totally Perturbed) Compressive Sensing

Compressive Sensing gives theory and algorithms for solving problem:

$$\mathbf{x}^{\#} = \arg\min\{\|\Phi \mathbf{x} - \mathbf{y}\|_2 : \|\mathbf{x}\|_0 \le s\}$$
 (1)

• Restricted Isometry Constant, $\delta_s(\Phi)$: smallest $\delta \in (0,1)$ s.t.

$$(1-\delta)\|\mathbf{x}\|_{2}^{2} \leq \|\Phi\mathbf{x}\|_{2}^{2} \leq (1+\delta)\|\mathbf{x}\|_{2}^{2} \text{ for all } \mathbf{x} \in \mathbb{R}^{n} \text{ with } \|\mathbf{x}\|_{0} \leq s$$

- Fast, greedy algorithms for (1): OMP, CoSaMP, SubspacePursuit 6.
- Robust to (additive and multiplicative) noise 7:

If
$$\mathbf{x}^* = \arg\min\left\{\|\hat{\Phi}\mathbf{x} - \hat{\mathbf{y}}\|_2 : \|\mathbf{x}\|_0 \le s\right\}$$
 and $\mathbf{x}^\# = \arg\min\left\{\|\Phi\mathbf{x} - \mathbf{y}\|_2 : \|\mathbf{x}\|_0 \le s\right\}$ with $\mathbf{y} = \hat{\mathbf{y}} + \mathbf{e}$ and $\Phi = \hat{\Phi} + M$ then $\frac{\|\mathbf{x}^* - \mathbf{x}^\#\|_2}{\|\mathbf{x}^*\|_2} \le C(\delta_s(\Phi), \epsilon_\Phi^s, \epsilon_\mathbf{y})$ where $\epsilon_\Phi^s \approx \frac{\|M\|_2}{\|\Phi\|_2}$ and $\epsilon_\mathbf{y} = \frac{\|\mathbf{e}\|_2}{\|\mathbf{y}\|_2}$

⁶Tropp [2004], Needell and Tropp [2009], Dai and Milenkovic [2009]

⁷Herman and Strohmer [2010], Li [2016]

Recall:

- $L = L^{in} + M$. (Think $\hat{\Phi} = L^{in}$ and $\Phi = L$)
- $L^{in} \mathbf{1}_{C_a} = 0$.

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 - $L^{in} \mathbf{1}_{C_a} = 0.$
- Assume $\Omega \approx C_a$ given. Let $U = C_a \setminus \Omega$ and $W = \Omega \setminus C_a$. Then:

$$\mathbf{1}_{\Omega} = \mathbf{1}_{C_a} + \mathbf{1}_W - \mathbf{1}_U \implies L^{\text{in}} \, \mathbf{1}_{\Omega} = L^{\text{in}} \, \mathbf{1}_{C_a} + L^{\text{in}} \, (\mathbf{1}_W - \mathbf{1}_U)$$

$$\implies L^{\text{in}} \, \mathbf{1}_{\Omega} = 0 + L^{\text{in}} \, (\mathbf{1}_W - \mathbf{1}_U)$$

$$\implies \mathbf{y}^{\text{in}} = L^{\text{in}} \, (\mathbf{1}_W - \mathbf{1}_U) \quad (\text{if } \mathbf{y}^{\text{in}} := L^{\text{in}} \, \mathbf{1}_{\Omega})$$

$$\implies \mathbf{y} \approx L \, (\mathbf{1}_W - \mathbf{1}_U) \quad (\text{if } \mathbf{y} := L \, \mathbf{1}_{\Omega})$$

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- Define $\mathbf{x}^* = \arg\min \left\{ \| L^{\text{in}} \mathbf{x} \mathbf{y}^{\text{in}} \|_2 : \| \mathbf{x} \|_0 \le |W| + |U| \right\}.$
- Will show that $\mathbf{x}^* = \mathbf{1}_W \mathbf{1}_U$.
- Define $\mathbf{x}^{\#} = \arg\min \{ \|L\mathbf{x} \mathbf{y}\|_2 : \|\mathbf{x}\|_0 \le |W| + |U| \}.$
- Will show that $x^{\#} \approx x^{*}$.

Algorithm 1: ClusterPursuit

Input: Adj. matrix A, initial cut Ω , estimate $s \approx |C_a \triangle \Omega|$ and $R \in [0,1)$.

Output: Subset $C_a^{\#}$ that approximates C_a

- 1 $L \leftarrow I D^{-1}A$ and $\mathbf{y} \leftarrow L \mathbf{1}_{\Omega}$.
- 2 $\mathbf{x}^{\#} \leftarrow \arg\min \{ \|L\mathbf{x} \mathbf{y}\|_2 : \|\mathbf{x}\|_0 \}$ using $m = O(\log(n))$ iterations of SubspacePursuit.
- 3 $U^{\#} \leftarrow \{i: x_i^{\#} < -R\} \text{ and } W^{\#} \leftarrow \{i: x_i^{\#} > R\}.$
- 4 $C_a^\# \leftarrow (\Omega \setminus W^\#) \cup U^\#$.
 - $|C_a \triangle \Omega| = |C_a \setminus \Omega| + |\Omega \setminus C_a| = |W| + |U|$.
 - Robust w.r.t parameters.
 - Run time = $O(d_{\text{max}} n \log n)$.

Recall:

- $\Omega \approx C_a$.
- $\mathbf{y}^{in} = \mathbf{L}^{in} \, \mathbf{1}_{\Omega}$

Theorem (Lai & M.)

 $\mathbf{1}_W - \mathbf{1}_U$ is the unique solution to:

$$\arg\min\left\{\|\boldsymbol{L}^{in}\boldsymbol{x}-\boldsymbol{y}^{in}\|_2:\ \|\boldsymbol{x}\|_0\leq s\right\}$$

for any G with clusters C_1, \ldots, C_k , as long as $|C_a \triangle \Omega| \le s < n_1/2$.

- Not a practical result! Don't know $L^{\rm in}$.
- Getting from Lⁱⁿ to L requires a data model.

The Data Model

- Let $\{\mathcal{G}_n\}_{n=1}^{\infty}$ where \mathcal{G}_n is prob. dist. on graphs on n vertices.
- Suppose exists $\epsilon_i = o_n(1)$ for i = 1, 2, 3 such that for $G \sim \mathcal{G}_n$:
- (A1) $V = C_1 \cup \ldots \cup C_k$ where C_a are disjoint clusters and $k = O_n(1)$.
- (A2) For all $a \in [k]$ $\lambda_2(L_{G_{C_a}}) \ge 1 \epsilon_1$ and $\lambda_{n_a}(L_{G_{C_a}}) \le 1 + \epsilon_1$ almost surely.
- (A3) letting $r_i := d_i^{\text{out}}/d_i^{\text{in}}$, $r_i \le \epsilon_2$ for all $i \in [n]$ almost surely.
- (A4) If $d_{\mathsf{av}}^\mathsf{in} := \mathbb{E}[d_i^\mathsf{in}]$ then $d_{\mathsf{max}}^\mathsf{in} \leq (1+\epsilon_3) d_{\mathsf{av}}^\mathsf{in}$ and $d_{\mathsf{min}}^\mathsf{in} \geq (1-\epsilon_3) d_{\mathsf{av}}^\mathsf{in}$ a.s.

From L^{in} to L

Recall:

- $M := L L^{\text{in}}$ and $e := y y^{\text{in}}$.
- $\epsilon_y = \frac{\|e\|_2}{\|\mathbf{y}^{\text{in}}\|_2}$ and $\epsilon_L^s = \frac{\|M\|_2^{(s)}}{\|L^{\text{in}}\|_2^{(s)}}$
- Key parameters for perturbed compressive sensing are ϵ_y, ϵ_L^s and $\delta_s(L)$

Theorem (Lai & M.)

Suppose that \mathcal{G}_n satisfies (A1)–(A4) and that $|C_1 \triangle \Omega| \leq 0.13n_1$. Then for any $\gamma \in (0,1)$ the following hold almost surely:

- 1. $\epsilon_y = o(1)$ and $\epsilon_L^{\gamma n_1} = o(1)$.
- 2. $\delta_{\gamma n_1}(L) \leq \gamma + o(1)$.

(Think
$$s = \gamma n_1$$
.)

Recovery Guarantee for ClusterPursuit

Theorem (Lai & M.)

Suppose the following:

- \mathcal{G}_n satisfies (A1)–(A4) and $G \sim \mathcal{G}_n$.
- $|C_1 \triangle \Omega| = \epsilon n_1$ with $\epsilon \leq 0.13$.
- $s \le 0.13n_1$ and R = 0.5.

$$\textit{If } C_1^\# = \texttt{ClusterPursuit}(A, \Omega, s, R) \textit{ then } \frac{\left|C_1 \bigtriangleup C_1^\#\right|}{|C_1|} = \textit{o(1) a.s.}$$

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Proof.

- Know $\mathbf{x}^* = \arg\min\left\{\|\mathbf{L}^{\text{in}}\mathbf{x} \mathbf{y}^{\text{in}}\|_2: \|\mathbf{x}\|_0 \leq s\right\} = \mathbf{1}_W \mathbf{1}_U.$
- Data Model $\Rightarrow \epsilon_y, \epsilon_L^s$ and $\delta_s(L)$ are small.
- If $\mathbf{x}^{\#} = \arg\min \{ \|L\mathbf{x} \mathbf{y}\|_2 : \|\mathbf{x}\|_0 \le s \}$ then $\|\mathbf{x}^{\#} \mathbf{x}^*\|_2$ small.
- $\{i: x_i^\# > 0\} \approx W \text{ and } \{i: x_i^\# < 0\} \approx U$

The stochastic block model

- Specify cluster sizes $n_1 \leq n_2 \leq \ldots \leq n_k$.
- Specify connection probability matrix $P \in \mathbb{R}^{k \times k}$.
- Construct partition $V = C_1 \cup ... \cup C_k$ with $|C_a| = n_a$.
- Generate $G \sim \mathsf{SBM}(\mathbf{n}, P)$ with $\mathbb{P}\left[A_{ij} = 1 | i \in C_a, j \in C_b\right] = P_{ab}$.



Figure: Examples of adjacency matrices for different SBM(n, P).

Spectral Properties for L for SBM

Theorem (Lai & M.)

- Let $G_n = SBM(\mathbf{n}, P)$ with $|\mathbf{n}| = \sum_{a=1}^k n_a = n$.
- Assume:
 - $n_1 \to \infty$.
 - $P_{aa} = \omega \log(n)/n_a$ for any ω with $\omega \to \infty$.
 - $P_{ab} = (\beta + o(1)) \log(n)/n$ for all $a \neq b$
- Then: G_n satisfies assumptions (A1)–(A4).

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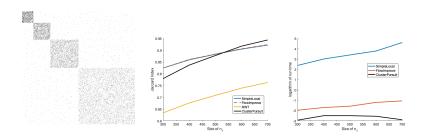
Proof.

- If $G \sim \mathsf{SBM}(n, P)$ then each $G_{C_a} \sim \mathsf{ER}(n_a, P_{aa})$.
- Concentration of measure for $d_i(G_{C_a})$.
- Concentration of measure for $\lambda_i(G_{C_a})$.

^aFrieze and Karoński [2016]

^bChung and Radcliffe [2011]

Experimental Results: Stochastic block model

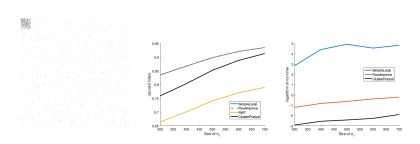


- $\operatorname{Jac}(C_1, C_1^\#) = |C_1 \cap C_1^\#| / |C_1 \cup C_1^\#|$. High is good.
- FlowImprove⁸ and SimpleLocal⁹ take essentially the same approach.
- SimpleLocal optimized for small clusters (i.e. $|C_a| = O_n(1)$).
- Yellow line is baseline (represents $Jac(\Omega, C_1)$).

⁸Andersen and Lang [2008]

⁹Veldt et al. [2016]

Experimental Results: Stochastic block model



- ClusterPursuit works well given $\Omega \approx \mathcal{C}_{a}$.
- How to find Ω ?

¹⁰Spielman and Teng [2004],Andersen et al. [2007], Kloster and Gleich [2014],Wang et al. [2017]

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- ClusterPursuit works well given $\Omega \approx C_a$.
- How to find Ω?
- Diffusion-based local clustering.
 - Given small set of seed vertices Γ.
 - Let $\mathbf{v}^{(0)} = |\Gamma|^{-1} \mathbf{1}_{\Gamma}$.
 - Run a diffusive process for t steps: $\mathbf{v}^{(t)} = P^t \mathbf{v}^{(0)}$.
 - $\Omega \leftarrow \{i : v_i^{(t)} \text{ "is large"}\}.$

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- Diffusive process? random walk, Pagerank, heat flow, CRD ¹⁰

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- Diffusive process? random walk, Pagerank, heat flow, CRD ¹⁰
- Two-step local clustering 11 : find $\Omega \approx C_a$ then refine to get $C_a^{\#}$.

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Random Walk Thresholding

Algorithm 2: RWThresh

Input: Adj. matrix A, thresh. param. $\epsilon \in (0,1)$, seeds $\Gamma \subset C_a, \hat{n}_a \approx n_a$ and t.

Output: $\Omega \approx C_a$

- 1 $P \leftarrow AD^{-1}$ and $\mathbf{v}^{(0)} \leftarrow D\mathbf{1}_{\Gamma}$.
- 2 $\mathbf{v}^{(t)} \leftarrow P^t \mathbf{v}^{(0)}$.
- з $\Omega \leftarrow \{i: v_i^{(t)} \text{ amongst } (1+\epsilon)\hat{n_1} \text{ entries}\}$
- 4 $\Omega \leftarrow \Omega \cup \Gamma$.

Random Walk Thresholding

Theorem (Lai & M.)

Suppose the following:

- \mathcal{G}_n satisfies Assumptions (A1)–(A4) and $G \sim \mathcal{G}_n$.
- t = O(1), $\hat{n}_1 = n_1$ and $\epsilon \in (0,1)$.
- $\Gamma \subset C_1$ with $|\Gamma| = g\epsilon_3^{2t-1}n_1$ for any $g \in (0,1)$ and ϵ_3 as in (A4)).

If $\Omega = \text{RWThresh}(A, \epsilon, \Gamma, \hat{n}_1, t)$ then $|\Omega \triangle C_1| \leq (\epsilon + o(1))n_1$ almost surely.

- For SBM $\epsilon_3 = 1/\log(n)$ so $|\Gamma| = n_1/\text{polylog}(n_1)$.
- In practice, take $|\Gamma| = 0.01 n_1$ or similar.
- Other diffusive algorithms¹² take $|\Gamma| = O(1)$, but return $|\Omega| = O(1)$.
- Run time = $O(n \log(n))$.

 $^{^{12}}$ Spielman and Teng [2004], Andersen et al. [2007], Kloster and Gleich [2014], Wang et al. [2017]

Cluster pursuit for local clustering

Algorithm 3: CP+RWT

Input: Adj. matrix A, seed vertices $\Gamma \subset C_1$, parameters $\epsilon, R, \hat{n}_1, t$

Output: $C_1^\# \approx C_1$

- 1 $\Omega \leftarrow \texttt{RWThresh}(A, \epsilon, \Gamma, \hat{n}_1, t)$
- 2 $C_1^\# \leftarrow \texttt{ClusterPursuit}(A, s = 2\epsilon \hat{n}_1, R)$

Theorem (Lai & M.)

Suppose the following:

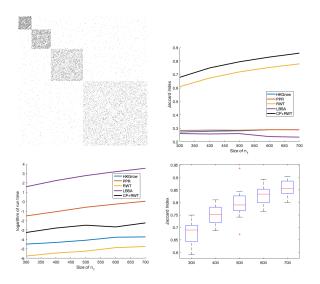
- \mathcal{G}_n satisfies Assumptions (A1)–(A4) and $G\sim\mathcal{G}_n$.
- $t = O_n(1)$, $\hat{n}_1 = n_1$, R = 0.5 and $\epsilon \in (0, 1)$.
- $\Gamma \subset C_1$ with $|\Gamma| = g\epsilon_3^{2t-1} n_1$ for any $g \in (0,1)$ and ϵ_3 as in (A4).

Then if $C_1^\# = \text{CP+RWT}(A, \Gamma, \epsilon, R, \hat{n}_1, t)$:

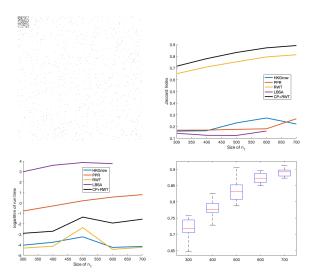
$$\frac{\left|C_1 \bigtriangleup C_1^{\#}\right|}{|C_1|} = o_n(1)$$

almost surely, for large enough n_1 .

Experimental Results: Stochastic block model



Experimental Results: Stochastic block model



Experimental Results: Social Networks

- Facebook100¹³ dataset: Facebook networks at American universities.
- Metadata used to define ground-truth clusters.
- Considered four clusters ¹⁴: two good, two moderately good.
- Always take $|\Gamma| = 0.02 n_1$.

School	Cluster	Size of graph	Size of Cluster	Conductance
Johns Hopkins	Class of 2009	5180	910	0.21
Rice	Dorm. 203	4087	406	0.47
Simmons	Class of 2009	1518	289	0.11
Colgate	Class of 2006	3482	557	0.49

Table: Basic properties of four clusters. Lower conductance is better.

¹³Traud et al. [2012]

¹⁴Wang et al. [2017]

Experimental Results: Social Networks

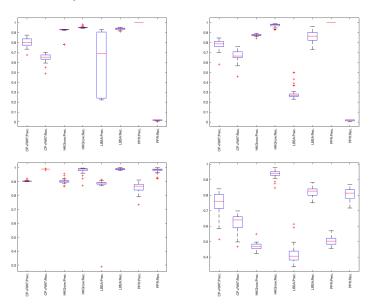


Figure: Clockwise from top left: Johns Hopkins, Rice, Colgate and Simmons.

Iterated CP+RWT for global clustering

Algorithm 4: ICP+RWT

Input: Adj. matrix A, labeled data $\Gamma_a \subset C_a$ for a = 1, ..., k. Parameters.

Output:
$$C_1^\# \approx C_1, \ldots, C_k^\# \approx C_k$$

$$_{1}\ \textit{G}^{(1)} \leftarrow \textit{G} \ \text{and} \ \textit{A}^{(1)} \leftarrow \textit{A}.$$

2 for
$$a=1,\ldots k$$
 do

$$C_a^{\#} \leftarrow \text{CP+RWT}(A^{(a)}, \Gamma_a, \epsilon, R, \hat{n}_a, t)$$

4
$$G^{(a+1)} \leftarrow G^{(a)} \setminus C_a^{\#}$$
 and $A^{(a+1)}$ is adj. matrix of $G^{(a+1)}$.

% Labeled Data	0.5	1	1.5	2	2.5
MNIST	96.41%	97.32%	97.44%	97.52%	97.50%
OptDigits	91.88%	95.47%	97.16%	98.06%	98.08%

Table: Classification accuracy, as a function of amount of labeled data, for ICP+RWT on two well-studied benchmark data sets. Results essentially state-of-the-art. 16

¹⁵Rasmus et al. [2015], Jacobs et al. [2018], Yin and Tai [2018]

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Conclusion

- ClusterPursuit is a provably robust, provably efficient cut improvement algorithm.
- Can use ClusterPursuit as an algorithmic primitive to design clustering algorithms.
- Theoretical guarantees follow from novel connection between cut improvement and compressed sensing.

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- Thanks!
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