A doubly non-negative relaxation for modularity density maximization

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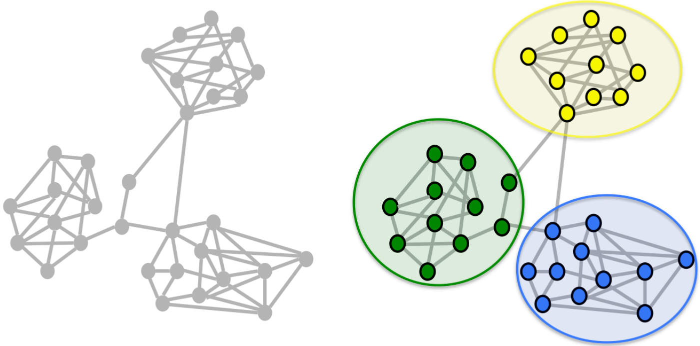
Introduction (Community detection)

Community detection is grouping nodes of a graph into several parts:



- each part (community) consists of tightly connected nodes
- communities are loosely connected each other

Introduction (Quality measure)

Ratio cut (Cheng and Wei '91)

Normalized cut (Shi and Malik '00)

Min-max cut (Ding et al. '01)

Modularity (Newman and Girvan '04)

- degeneracy
- resolution limit (Fortunato and Barthelemy '07)
- NP-hard (Brandes et al. '08)

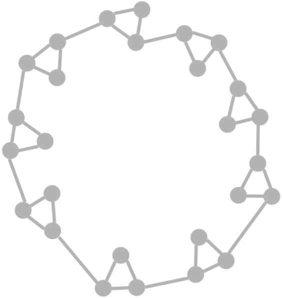
Modularity density (Li et al. '08)

- avoids the resolution limit
- NP-hard ?

Introduction (Quality measure)

Resolution limit

leaves small communities not identified and hidden inside larger ones



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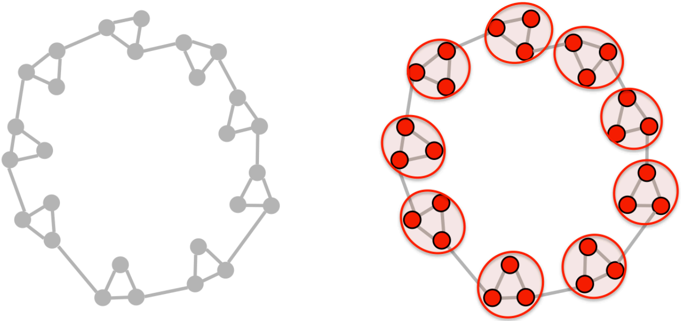

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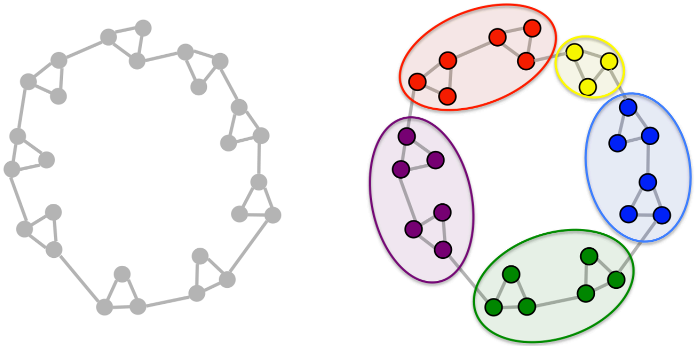

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Introduction (Modularity & Modularity density)

- undirected graph $G = (V, E)$ ($n = |V|$, $m = |E|$)
- $E(C, C') = \{ \{i, j\} \in E \mid i \in C,\ j \in C' \}$ for $C,\ C' \subseteq V$
  (when $C = C'$, we abbreviate it to $E(C)$)
- Π : a partition of the node set V

Modularity

$$\mathsf{M}(\Pi) = \sum_{C \in \Pi} \left(\frac{|E(C)|}{m} - \left(\frac{\sum_{C' \in \Pi} |E(C, C')|}{2m} \right)^2 \right)$$

Modularity density

$$\mathsf{MD}(\Pi) = \sum_{C \in \Pi} \left(\frac{2\,|E(C)| - \sum_{C' \in \Pi} |E(C, C')|}{|C|} \right)$$

Modularity density maximization

$$
\text{(P)} \quad \left| \begin{array}{ll}
\text{max.} & \displaystyle\sum_{p \in T} \left(\frac{2 \sum_{i \in V} \sum_{j \in V} a_{ij} x_{ip} x_{jp} - \sum_{i \in V} d_i x_{ip}}{\sum_{i \in V} x_{ip}} \right) \\
\text{s.t.} & \displaystyle\sum_{p \in T} x_{ip} = 1 \qquad (i \in V) \\
& \displaystyle\sum_{i \in V} x_{ip} \geq 1 \qquad (p \in T) \\
& x_{ip} \in \{0, 1\} \qquad (i \in V, p \in T).
\end{array} \right.
$$

- $T = \{1, \ldots, t\}$: index set of communities (t is unknown a priori)
- $A = (a_{ij})_{i,j \in V}$: adjacency matrix of G
- d_i : degree of node i (i.e., $d_i = \sum_{j \in V} a_{ij}$)
- x_{ip} : decision variable

$$
x_{ip} = \begin{cases} 1 & (i \in C_p) \\ 0 & (i \notin C_p) \end{cases}
$$

Introduction (Overview)

Costa '15

- formulated the problem as Mixed-Integer-Linear-Programming (MILP)
- made use of the *McCormick inequalities*
  $\Rightarrow$ need to solve an auxiliary problem
- solved the instances up to $n = 40$ by branch-and-bound alg.

Izunaga, Matsui, and Yamamoto

- show that the problem can be modeled as 0-1SDP
  $\Rightarrow$ does not require the number of communities t
- solve a relaxation problem to obtain an upper bound
- develop a heuristics to obtain a lower bound

Mixed-Integer-Linear-Programming (MILP)

MILP formulation

$$
\begin{array}{lll}
\text{max.} & \displaystyle\sum_{p \in T} \alpha_p & \\
\text{s.t.} & \displaystyle\sum_{p \in T} x_{ip} = 1 & (i \in V) \\
& \displaystyle\sum_{i \in V} x_{ip} \geq 1 & (p \in T) \\
& y_{ijp} \leq x_{ip},\ y_{ijp} \leq x_{jp} & (\{i,j\} \in E, p \in T) \\
& \displaystyle\sum_{i \in V} \gamma_{ip} \leq 4 \sum_{\{i,j\} \in E} y_{ijp} - \sum_{i \in V} d_i x_{ip} & (p \in T) \\
& L_\alpha x_{ip} \leq \gamma_{ip} \leq U_\alpha x_{ip} & (i \in V, p \in T) \\
& \alpha_p - U_\alpha(1 - x_{ip}) \leq \gamma_{ip} \leq \alpha_p - L_\alpha(1 - x_{ip}) & (i \in V, p \in T) \\
& x_{ip} \in \{0,1\} & (i \in V, p \in T) \\
& y_{ijp} \in \mathbb{R} & (\{i,j\} \in E, p \in T) \\
& L_\alpha \leq \alpha_p \leq U_\alpha & (p \in T) \\
& \gamma_{ip} \in \mathbb{R} & (i \in V, p \in T).
\end{array}
$$

0-1 semidefinite programming (0-1SDP)

$$\mathcal{S}_n^+ = \{\, Y \in \mathbb{R}^{n\times n} \mid Y^\top = Y,\, \forall \boldsymbol{d} \in \mathbb{R}^n, \boldsymbol{d}^\top Y \boldsymbol{d} \geq 0 \,\}$$
$$\mathcal{N}_n = \{\, Y \in \mathbb{R}^{n\times n} \mid Y^\top = Y,\, \forall i, j,\, y_{ij} \geq 0 \,\}$$
$$A = (a_{ij})_{i,j\in V}$$
$$D = \mathrm{Diag}(d_1, \dots, d_n) \in \mathbb{R}^{n\times n}$$
$$\boldsymbol{e}_k = (1, \dots, 1)^\top \in \mathbb{R}^k$$

Introducing a matrix $X \in \{\, 0, 1 \,\}^{n\times t}$, we have the following problem:

Matrix representation

$$(\mathrm{P}) \quad \begin{array}{|lll} \text{max.} & \mathrm{Tr}((2A - D)Z) \\ \text{s.t.} & X\boldsymbol{e}_t = \boldsymbol{e}_n \\ & X^\top \boldsymbol{e}_n \geq \boldsymbol{e}_t \\ & Z = X(X^\top X)^{-1} X^\top \\ & X \in \{\, 0, 1 \,\}^{n\times t}. \end{array}$$

$$\sum_{p\in T} x_{ip} = 1\,(i \in V) \;\Leftrightarrow\; X\boldsymbol{e}_t = \boldsymbol{e}_n$$

$$\sum_{i\in V} x_{ip} \geq 1\,(p \in T) \;\Leftrightarrow\; X^\top \boldsymbol{e}_n \geq \boldsymbol{e}_t$$

- (X, Z) is feasible for the problem (P)
  $\Rightarrow\ Z\boldsymbol{e}_n = \boldsymbol{e}_n,\ Z^2 = Z,\ Z \in \mathcal{N}_n$

Matrix representation

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0-1SDP formulation

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(\bar{\text{P}})\quad \left|\ \begin{array}{ll} \text{max.} & \text{Tr}((2A - D)Z) \\ \text{s.t.} & Z\boldsymbol{e}_n = \boldsymbol{e}_n \\ & Z^2 = Z \\ & Z \in \mathcal{N}_n. \end{array} \right.
$$

Lemma 1.

For any feasible solution Z of $(\bar{\text{P}})$, we can construct a feasible solution X which satisfies $Z = X(X^\top X)^{-1}X^\top$

$\Rightarrow$ the problem $(\bar{\text{P}})$ is equivalent to (P)

sketch of proof

$Z^2 = Z \Rightarrow Z \succeq 0 \Rightarrow \exists i_1 \in V,\ z_{i_1 i_1} = \max\{z_{ij} \mid i, j \in V\}$.
Let $\mathcal{I}_1 = \{j \in V \mid z_{i_1 j} > 0\}$, then $\forall i, j \in \mathcal{I}_1,\ z_{ij} = 1/|\mathcal{I}_1|$.
By using an appropriate permutation matrix P, we obtain

$$P^\top Z P = \begin{pmatrix} Z_{\mathcal{I}_1} & O \\ O & Z_{\bar{\mathcal{I}}_1} \end{pmatrix}, \quad \text{where } \bar{\mathcal{I}}_1 = V \setminus \mathcal{I}_1.$$

The sub-matrix $Z_{\bar{\mathcal{I}}_1}$ satisfies that $Z_{\bar{\mathcal{I}}_1} \boldsymbol{e} = \boldsymbol{e},\ Z_{\bar{\mathcal{I}}_1}^2 = Z,\ Z_{\bar{\mathcal{I}}_1} \in \mathcal{N}$.
Repeating the process described above, we can convert Z to a block diagonal matrix $P^\top Z P = \mathrm{Diag}(Z_{\bar{\mathcal{I}}_1}, \ldots, Z_{\bar{\mathcal{I}}_t})$.
We construct a matrix $X = (x_{ip})$ such that

$$x_{ip} = \begin{cases} 1 & (i \in \mathcal{I}_p) \\ 0 & (i \notin \mathcal{I}_p) \end{cases},$$

then X is feasible for (P) and $Z = X(X^\top X)^{-1} X^\top$.

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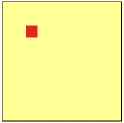

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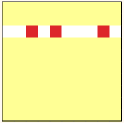

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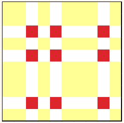

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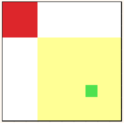

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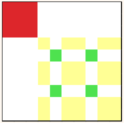

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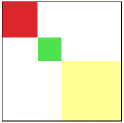

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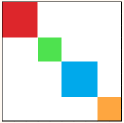

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0-1 semidefinite programming (0-1SDP)

0-1SDP formulation

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- Laplacian: $L = D - A \in \mathcal{S}_n^+$
- $Z^2 = Z$
  $\Rightarrow \forall i,\ \lambda_i \in \{0, 1\}$.
  (λ_i : eigenvalue of Z)

- the objective function is linear with respect to Z
- the idempotence constraint makes the problem difficult
  $\Rightarrow$ relax the constraint $Z^2 = Z$ to a more tractable constraint

$$
D - 2A = \begin{pmatrix} 1 & -2 & 0 \\ -2 & 2 & -2 \\ 0 & -2 & 1 \end{pmatrix} \notin \mathcal{S}_3^+
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Doubly Non-Negative relaxation

- DNN relaxation
  $\Rightarrow$ provides a tight bound for combinatorial optimization problems

0-1SDP formulation

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DNN relaxation

$$(\mathrm{DNN}) \quad \left| \begin{array}{ll} \text{max.} & \mathrm{Tr}((2A-D)Z) \\ \text{s.t.} & Z\boldsymbol{e}_n = \boldsymbol{e}_n \\ & Z \in \mathcal{S}_n^+ \cap \mathcal{N}_n. \end{array} \right.$$

- the interior-point method solves the problem over a symmetric cone efficiently
- we cannot directly apply the interior-point method to solve (DNN) since doubly non-negative cone is not symmetric

$$Z \in \mathcal{S}_n^+ \cap \mathcal{N}_n \Leftrightarrow \begin{pmatrix} Z & O \\ O & \mathrm{Diag}(\mathrm{vec}(Z)) \end{pmatrix} \in \mathcal{S}_{n+n^2}^+$$

Valid inequality

Lemma 2.

The following inequalities are valid for $(\bar{\mathsf{P}})$

$$z_{ii} \geq z_{ij} \quad (i, j \in V).$$

DNN relaxation

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DNN with valid inequalities

$$(\overline{\mathrm{DNN}}) \quad \left| \begin{array}{ll} \text{max.} & \mathrm{Tr}((2A - D)Z) \\ \text{s.t.} & Z\boldsymbol{e}_n = \boldsymbol{e}_n \\ & z_{ii} \geq z_{ij} \ (i, j \in V) \\ & Z \in \mathcal{S}_n^+ \cap \mathcal{N}_n. \end{array} \right.$$

Permutation based on spectrum

Z^* : solution of the relaxation problem

- $1 = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$: eigenvalues of Z^*
- $\boldsymbol{u}_i \in \mathbb{R}^n$: eigenvector corresponding to λ_i

Permuting the rows and columns of Z^* consistent with the decreasing order of values of elements of $\boldsymbol{u}_2$, we have

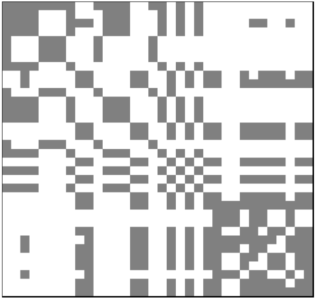

Figure: Original matrix

Permutation based on spectrum

Z^* : solution of the relaxation problem

- $1 = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$: eigenvalues of Z^*
- $\boldsymbol{u}_i \in \mathbb{R}^n$: eigenvector corresponding to λ_i

Permuting the rows and columns of Z^* consistent with the decreasing order of values of elements of $\boldsymbol{u}_2$, we have

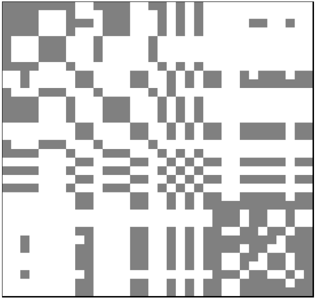

Figure: Original matrix

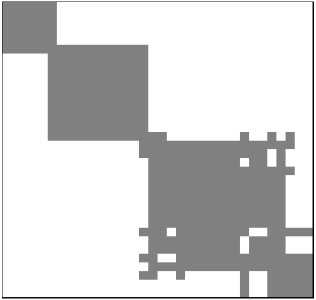

Figure: Permuted matrix

$\overline{V}$: sequence consistent with the decreasing order of $\boldsymbol{u}_2$
(we write $\overline{V} = [1 \ldots n]$ for the sake of simplicity)

- $q(k, \ell) = \dfrac{2 \sum_{i=k}^{\ell} \sum_{j=k}^{\ell} a_{ij} - \sum_{i=k}^{\ell} d_i}{\ell - (k-1)}$ for k, ℓ of $\overline{V}$ with $k \leq \ell$
- $\mu(s)$: the maximum value that is achieved by partitioning of [1. . . s] into several consecutive subsequences
(assume $\mu(0) = 0$ for notational convenience)

Recursive equation

$$\mu(s) = \max\{\, \mu(k) + q(k+1, s) \mid k \in \{\, 0, 1, \ldots, s-1 \,\}\,\}.$$

$\Rightarrow \quad \mu(1) = q(1,1)$
$\mu(2) = \max\{\, q(1,2),\ \mu(1) + q(2,2) \,\}$
$\mu(3) = \max\{\, q(1,3),\ \mu(1) + q(2,3),\ \mu(2) + q(3,3) \,\} \cdots$

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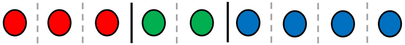

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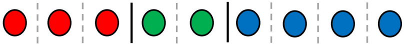

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Computational experiment

- Computational environment
  CPU : Intel Core i7 3.70 GHz
  Memory : 32.0 GB
  SDP Solver : SeDuMi 1.2
  MILP Solver : Gurobi 6.0.0
- The instances we tested :

ID	name	n	m	t	OPT
1	Strike	24	38	4	8.8611
2	Karate	34	78	3	7.8451
3	Mexico	35	117	3	8.7180
4	Sawmill	36	62	4	8.6233
5	Dolphins	62	159	5	12.1252[1]
6	Books	105	441	7	21.9652[1]

[1] the best lower bound reported in Costa et al. '15

Table: Comparison of obtained lower and upper bounds

	(DNN)		($\overline{\text{DNN}}$)		(MILP)	
ID	UB	LB	UB	LB	UB	LB
1	9.5808	8.8611	9.3049	8.8611	8.8611	8.8611
2	8.9548	7.8424	8.4141	7.8451	7.8451	7.8451
3	10.3151	8.5580	9.9570	8.5227	8.7180	8.7180
4	10.5048	7.0486	10.0311	7.3587	8.6223	8.6233
5	15.0218	9.8286	14.3552	11.4610	17.1252	12.1252
6	26.5387	20.2470	24.7749	20.3150	56.8739	21.0815

Table: Comparison of computational time in seconds

ID	(DNN)	($\overline{\text{DNN}}$)	(MILP)
1	1.05	3.54	0.50
2	5.83	36.04	0.74
3	7.64	43.48	7.84
4	7.75	54.21	6.10
5	316.61	1681.81	OT[2]
6	4626.11	60437.45	OT[2]

[2] more than 10,000 seconds

Conclusion

Conclusion

- We proved the equivalence between the modularity density maximization and 0-1SDP
- obtained a tight upper bound by DNN relaxation
- developed a heuristics to obtain a lower bound

However, there is no theoretical validity of using the second largest eigenvector. Here still remains room for further research.

Thank you for your attention.

Conic programming

- $\mathcal{K}$: a nonempty closed convex cone
- $\langle \cdot, \cdot \rangle$: an inner product
- $\mathcal{K}^*$: the dual cone of $\mathcal{K}$, i.e., $\mathcal{K}^* = \{ \boldsymbol{x} \mid \forall \boldsymbol{y} \in \mathcal{K}, \langle \boldsymbol{x}, \boldsymbol{y} \rangle \geq 0 \}$
- $A : \mathbb{R}^n \to \mathbb{R}^m$: a linear operator
- A^* : the adjoint operator of A, i.e., $\langle A\boldsymbol{x}, \boldsymbol{y} \rangle = \langle \boldsymbol{x}, A^*\boldsymbol{y} \rangle$

Primal

$$\left| \begin{array}{ll} \text{min.} & \langle \boldsymbol{c}, \boldsymbol{x} \rangle \\ \text{s.t.} & A\boldsymbol{x} = \boldsymbol{b}, \boldsymbol{x} \in \mathcal{K}. \end{array} \right.$$

Dual

$$\left| \begin{array}{ll} \text{max.} & \langle \boldsymbol{b}, \boldsymbol{y} \rangle \\ \text{s.t.} & \boldsymbol{c} - A^*\boldsymbol{y} \in \mathcal{K}^*. \end{array} \right.$$

Roughly speaking, $\mathcal{K}$ is called a symmetric cone if $\mathcal{K}^* = \mathcal{K}$.

- symmetric cones :
  non-negative orthant $\mathbb{R}^n_+$, semidefinite cone $\mathcal{S}^+_n$, second-order cone, etc.

Conic programming

- Copositive cone $\mathcal{C}_n = \{\, Y \in \mathbb{R}^{n \times n} \mid Y^\top = Y, \forall \boldsymbol{d} \in \mathbb{R}^n_+, \boldsymbol{d}^\top Y \boldsymbol{d} \geq 0 \,\}$
- Completely positive cone $\mathcal{C}_n^* = \text{conv}(\{\, \boldsymbol{y}\boldsymbol{y}^\top \mid \boldsymbol{y} \in \mathbb{R}^n_+ \,\})$
- Doubly non-negative cone $\mathcal{S}_n^+ \cap \mathcal{N}_n$

Properties

- $(\mathcal{S}_n^+ \cap \mathcal{N}_n)^* = \mathcal{S}_n^+ + \mathcal{N}_n$
- $\mathcal{C}_n^* \subseteq \mathcal{S}_n^+ \cap \mathcal{N}_n \subseteq \mathcal{S}_n^+ \subseteq \mathcal{S}_n^+ + \mathcal{N}_n \subseteq \mathcal{C}_n$
- $\mathcal{C}_n^* = \mathcal{S}_n^+ \cap \mathcal{N}_n \subseteq \mathcal{S}_n^+ \subseteq \mathcal{S}_n^+ + \mathcal{N}_n = \mathcal{C}_n$ for $n \leq 4$

Strong results on $\mathcal{C}_n$, $\mathcal{C}_n^*$

- the maximum clique number:

$$\min\{\, \alpha \in \mathbb{N} \mid \alpha(E - A) - E \in \mathcal{C}_n \,\} \text{ where } E = \boldsymbol{e}\boldsymbol{e}^\top.$$

- non-convex quadratic programming:

$$\min\{\, \mathsf{Tr}(QX) \mid \mathsf{Tr}(EX) = 1,\ X \in \mathcal{C}_n^* \,\} \text{ where } E = \boldsymbol{e}\boldsymbol{e}^\top.$$