Today

Spectral Methods
- Eigenvalues & Eigenvectors
- Adjacency Matrix
  Laplacian.

CSS.205.1
Toolkit in TCS
- Lecture #20
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Instructor: Prahladh Harsha

Understand Graphs via their spectrum

Graphs
(1) Interaction Graph.
(2) Friendship graph
(3) Protein-protein interaction
(4) Circuit

— Look at the spectrum of the graph
- eigenvalues & eigenvectors
of a related matrix
of the graph.

Matrix (associated w/ graph)

1. Adjacency Matrix
A_G - Col/Rows indexed by vertex

$G = (V, E)$ - unweighted undirected (set)

A_G : $V \times V$ matrix

$$A_G(u,v) = \begin{cases} 1 & \text{if } \{u,v\} \in E \\ 0 & \text{otherwise.} \end{cases}$$

Linear Algebraic Viewpoints of Matrices

(1) Operator: $T: \mathbb{R}^V \to \mathbb{R}^V$

$\varphi \mapsto T\varphi$

(2) Quadratic Form:

Inner Product : Vector space $\mathbb{R}^V$

$\langle \, , \, \rangle : \underbrace{\mathbb{R}^V \times \mathbb{R}^V \to \mathbb{R}}_{\text{bilinear}}$

bilinear $(\langle ax_1 + bx_2, y\rangle = a\langle x_1, y\rangle + b\langle x_2, y\rangle)$

$\langle x, x\rangle = 0 \iff x = 0$

Example: $\underbrace{\langle x, y\rangle = \sum_{u \in V} x(u) \cdot y(u)}_{\text{Standard Dot-product}}$

Standard Dot-product

$\langle x, y\rangle$ - inner product.

Quadratic Form associated w/ matrix M

$Q_M : \mathbb{R}^V \to \mathbb{R}$

$$x \mapsto \langle x, Mx \rangle$$

$$Q_{A_G} = \langle x, Ax \rangle = \sum_{u \in V} x(u) \cdot (Ax)(u)$$

$$= \sum_{u \in V} x(u) \sum_{v \in N(u)} x(v)$$

$$= \sum_{\underbrace{(u,v):\, u \sim v}_{}} x(u)x(v)$$

$\hookrightarrow$ ordered set

(1) Operators: A_G - adjacency matrix

W_G - random walk matrix

$$W_G = D_G^{-1} A_G \qquad D_G = \operatorname{diag}(\deg(u))$$

(2) Quadratic Form: A_G

Laplacian Matrix: $L_G = D_G - A_G$.

Quadratic form associated w/ the Laplacian

$$\langle x, L_G x \rangle = \langle x, D_G x \rangle - \langle x, A_G x \rangle$$

$$\langle x, A_G x \rangle = \sum_{(u,v):\, u \sim v} x(u)x(v)$$

$$\langle x, D_G x \rangle = \sum_{u} x(u)(D_G x)(u) = \sum_{u} d(u) x^2(u)$$

$$\langle x, L_G x\rangle = \sum_u d(u)x^2(u) - \sum_{(u,v):\, u\sim v} x(u)\,x(v)$$

$$= \sum_{\{u,v\}:\, u\sim v} \big(x(u) - x(v)\big)^2$$

$$\langle x, L_G x\rangle = \sum_{\{u,v\}:\, u\sim v} \big(x(u) - x(v)\big)^2$$

<u>Obs:</u> L_G, A_G, D_G - symmetric matrices

L_G - positive semi-definite matrix

<u>Defn:</u> Eigenvalues & Eigen vectors.

M. $n\times n$ matrix.

$\varphi \in \mathbb{C}^n \setminus \{\bar{0}\}$ & $\lambda \in \mathbb{C}$

s.t.

$$M\varphi = \lambda\varphi$$

φ - eigenvector of M

w/ associated eigenvalue λ

$(\lambda I - M)\varphi = 0$ ie, $\lambda I - M$ has a non-trivial kernel

$\det(\lambda I - M) = 0$

Eigen value - roots of $\underbrace{\det(xI - M)}_{\text{characteristic poly of } M} = 0$

Qn: Does A_G, L_G have e-vectors & what are the corresponding e-values?

Inner Product: $\langle\, , \,\rangle : \mathbb{R}^V \times \mathbb{R}^V \to \mathbb{R}$.

Adjoint of a matrix (w/ inner product).

$Adj(M) = M^*$ is such that

$$\langle x, My \rangle = \langle M^* x, y \rangle$$

(Standard dot product:

$\langle x, y \rangle = x^T y$

$\langle x, My \rangle = x^T My = x^T (M^T)^T y = (M^T x)^T y$

$= \langle M^T x, y \rangle$

For dot-product; $M^* = M^T$.

A_G, D_G, L_G - self-adjoint matrices

Spectral Theorem: $M \in \mathbb{R}^{n \times n}$ matrix self-adjoint w.r.t some inner product (ie, $M^* = M$), then there exist n real numbers

$\lambda_1 \le \lambda_2 \le \dots \le \lambda_n \in \mathbb{R}$

& n mutually orthogonal vectors (orthonormal)

$\psi_1 , \psi_2 , \quad \psi_n \in \mathbb{R}^n$

s.t. $M\psi_i = \lambda_i \psi_i$

Obs: (1) e.values - unique (upto multiplicities)

e.vectors - not necessarily

ψ_i & ψ_j share e.value

$$\Downarrow$$

$\psi_i + \psi_j$ - evector

(2) $M = \sum_{i=1}^{n} \lambda_i \varphi_i \varphi_i^* \quad \left(= \sum_{i=1}^{n} \lambda_i \varphi_i \varphi_i^T\right)$

$N = \varphi \psi^T \qquad N v = \varphi \psi^T v$

$= \langle \psi, v \rangle \varphi$

$M = V \Lambda V^*$

where $V = \begin{pmatrix} | & | & & | \\ \varphi_1 & \varphi_2 & \dots & \varphi_n \\ | & | & & | \end{pmatrix}$

$\Lambda = \mathrm{diag}((\lambda_1, \dots \lambda_n)$

Rayleigh Coefficient of a Matrix

$M \in \mathbb{R}^{n \times n}$; $x \in \mathbb{R}^n$

$$R(M,x) = \frac{\langle x, Mx \rangle}{\langle x, x \rangle}$$

Courant-Fischer Characterization of Eigenvalues

$M \in \mathbb{R}^{n \times n}$, $\langle \, , \rangle$ - inner product,

M - self adjoint $(M = M^*)$.

$$\lambda_1 = \min_{x \in \mathbb{R}^n} \frac{\langle x, Mx \rangle}{\langle x, x \rangle} = \min_{x \in \mathbb{R}^n} R(M,x)$$

$$\lambda_n = \max_{x \in \mathbb{R}^n} R(M,x)$$

More generally

$$\lambda_i = \min_{\substack{V \subseteq \mathbb{R}^n \\ \dim V = i}} \max_{x \in V} R(M,x)$$

$$= \max_{\substack{W \subseteq \mathbb{R}^n \\ \dim W = n-i+1}} \min_{x \in W} R(M,x)$$

Adjacency Matrix:

$\mu_1 \geq \mu_2 \ldots \qquad \geq \mu_n$ — eigen values

$\varphi_1 \ldots \qquad \varphi_n$ — eigen vectors

Operator: A:

$$\varphi \longmapsto A\varphi$$

$$(A\varphi)(u) = \sum_{v \in N(u)} \varphi(v)$$

Quadratic Form:

$$\langle \varphi, A\varphi \rangle = \sum_{(u,v):u\sim v} \varphi(u)\varphi(v)$$

Largest Eigenvalue μ_1.

Lemma: $d_{ave} \leq \mu_1 \leq d_{max}$

Pf: $\mu_1 = \max_x R(A,x) \geq R(A, \mathbb{1}^n)$

$$= \frac{\langle \mathbb{1}, A\mathbb{1} \rangle}{\langle \mathbb{1}, \mathbb{1} \rangle} = \frac{\text{sum of deg}}{|V|} \geq d_{ave}$$

(actually $\geq d_{ave}(G_S)$
for any $S \subseteq V$ &
G_S - induced subgraph
of G on S)

Upper Bound: φ_1 - e.vector corresponding to μ_1.

$$A\varphi_1 = \mu_1 \varphi_1$$

$$\mu_1 = \frac{(A\varphi_1)(v)}{\varphi_1(v)} \quad \text{for all } v \in V.$$

$$\mu_1 = \frac{\sum_{u \in N(v)} \varphi_1(u)}{\varphi_1(v)}$$

Fix v to $\operatorname{argmax} \varphi_1(v)$

$$\mu_1 \le \frac{\sum_{u \in N(v)} \varphi_1(v)}{\varphi_1(v)} = \deg(v) \le d_{max}$$

$\boxtimes$

} Obtained by tight inequalities

Lemma: G is connected & $\mu_1 = d_{max}$

$\Downarrow$

G is d_{max}-regular.

Thm [Consequence of Perron-Frobenius theory]

G - connected.

(a) $\mu_1 \ge -\mu_n$

(b) $\mu_1 > \mu_2$

(c) φ_1 - strictly positive (every entry of $\varphi_1 > 0$)

Prop: φ – eigen vector of the adj matrix of a connected graph

φ – non-negative

$\Downarrow$

φ – strictly positive. $\boxtimes$

Pf of Thm:

(c) φ_1 – strictly positive

$x(u) = |\varphi_1(u)|$

$R(A_G, x) \geq R(A_G, \varphi_1)$

x is also an e-vector corresponding to μ_1

& non-negative

Hence, strictly positive

(b) φ_2 – e.vector corresponding to μ_2

$y(u) = |\varphi_2(u)|$

$\mu_2 = R(A_G, \varphi_2) \leq R(A_G, y) \leq \mu_1$

Case (i) $\forall u \in V$, $\varphi_2(u) \neq 0$

$\exists$ an edge (u, v) ; $\varphi_2(u) > 0$; $\varphi_2(v) < 0$

$R(A_G, \varphi_2) < R(A_G, y)$ ✓

Case (2). $\exists\, u \in V,\ \varphi_2(u) = 0$

Suppose for contradiction $\mu_2 = \mu_1$

Hence y is a non-negative e-vector corresponding to μ_1

& $y(u) = 0$ $\Rightarrow\Leftarrow$.

(c). φ_n - e-vector to μ_n

$$z(u) = |\varphi_n(u)|$$

$$|\mu_n| = |R(A, \varphi_n)| \leq R(A, z) \leq \mu_1$$

$\boxtimes$

Thm: G is connected

$\mu_1 = -\mu_n \iff G$ is bipartite