COMS 4995-2: Advanced Algorithms (Spring'20) Feb 13, 2020

Lecture 7: Spectral Graph Theory

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1 Diffusion Operator

Definition 1. *Given graph G with n nodes, we define the diffusion operator W as the following.*

$$x \in \mathbb{R}^n_+, \quad x_i = Pr(at\ node\ i\ in\ a\ random\ walk\ on\ G)$$

$$W(x) : \mathbb{R}^n \to \mathbb{R}^n, \quad W(x)_i := \sum_{j;(i,j)\in E} \frac{x_j}{degree_j}$$

Example 2.

$$\text{G} = 1\text{—}2\text{—}3\text{—}4\text{—}5, \quad D = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \quad \text{A} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

Suppose we start at node 1, our initial state $x_0 = (0,\ 1,\ 0,\ 0,\ 0)^T$, then we should expect .5 probability of walking to node 0 and 2.

$$W(x_0) = \begin{bmatrix} .5 \\ 0 \\ .5 \\ 0 \\ 0 \end{bmatrix}$$

Definition 3. *A stationary distribution x^* satisfies $W(x^*) = x^*$.*

In our example above, $x^* = (1/8,\ 1/4,\ 1/4,\ 1/4,\ 1/8)^T$. The intuition is that node 1, 5 have degree 1 while nodes 2,3,4 have degree 2, and so $2x^*_1 = 2x^*_5 = x^*_2 = x^*_3 = x^*_4$.

Definition 4. *Another way to define diffusion operator W:*

$$W(x) = A \cdot \underbrace{D^{-1} \cdot x}_{\substack{\text{mass sent to each} \\ \text{neighbor of i}}}, \quad W(x)_j = \sum_{i\in[n]} A_{ij}(D^{-1}x)_i$$

Then the stationary distribution x^* satisifies $AD^{-1}x^* = x^*$.

2 Spectral Decomposition & Theorem for Symmetric M

Definition 5. *v is eigenvector with eigenvalue $\lambda \in \mathbb{R}$ if $Mv = \lambda v$.*

Observation 6. *If λ is an eigenvalue, then $Mv - \lambda v = 0 \Rightarrow (M - \lambda I)v = 0 \Rightarrow det(M - \lambda I) = 0$, where I is the identity matrix. So, solutions to $det(M - \lambda I) = 0$ (where λ is unknown) are the eigenvalues.*

$det(M - \lambda I) = 0$ is degree-n polynomial in $\lambda \Rightarrow$ There are n solutions if counting multiplicities.

Fact 7. *If M is **symmetric**, then all solutions are real (no complex numbers).*

Theorem 8. ***Spectral theorem***

For symmetric matrix M, $\exists$ vectors $v_1, \ldots, v_n$ and eigenvalues $\lambda_1, \ldots, \lambda_n$ s.t.
1) $||v_i||_2 = 1$ 2) $v_i \cdot v_j = 0$ if $i \neq j$ (orthonormal) 3) $Mv_i = \lambda_i v_i$

Remarks:
1) The sorted sequence of eigenvalues, i.e. $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, is unique.
2) The set of eigenvectors $v_1, \ldots, v_n$ is not necessarily unique. E.g., if $\lambda_i = \lambda_{i+1}$, then can replace v_i, v_{i+1} with $\frac{v_i + v_{i+1}}{\sqrt{2}}$, $\frac{v_i - v_{i+1}}{\sqrt{2}}$.
3) $M = \sum_{i=1}^{n} \lambda_i \cdot v_i \cdot v_i^T$, where $v_i \cdot v_i^T$ is the outer product of vector v_i.
4) If $\lambda_1 > \lambda_2 > \cdots > \lambda_n$, i.e., all eigenvalues are strictly different, then the set of eigenvectors $\{v_1, \ldots, v_n\}$ is unique up to taking $\{-v_1, \ldots, -v_n\}$.

Example 9. *$M = 0 \Rightarrow \lambda_1, \ldots, \lambda_n = 0$. Any set of n orthonormal vectors is a set of eigenvectors. For example, we can take $e_1, e_2, \ldots, e_n$, or alternatively we can take $\frac{e_1+e_2}{\sqrt{2}}$, $\frac{e_1-e_2}{\sqrt{2}}, e_3, \ldots, e_n$ as a set of eigenvectors.*

Example 10. *$M = I \Rightarrow \lambda_1, \ldots, \lambda_n = 1$. Again, any set of n orthonormal vectors is a set of eigenvectors. So, we can take any basis to be the set of orthogonal eigenvectors.*

If $M = \sum_{i=1}^{n} \lambda_i \cdot v_i \cdot v_i^T$, where $v_i \cdot v_j = 0$ for $i \neq j$, then the λ's and v's are the decomposition given by Spectral Theorem.

$$
\begin{aligned}
M \cdot v_j &= \sum_{i=1}^{n} \lambda_i \cdot v_i \cdot v_i^T \cdot v_j \\
&= \sum_{i=1}^{n} \lambda_i \cdot v_i \cdot \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases} \\
&= \lambda_j \cdot v_j
\end{aligned}
$$

3 Rayleigh Quotients

Definition 11. *For vector $x \neq 0$, $R(x) = \frac{x^T M x}{||x||^2}$.*

Observation 12. $R(v_i) = \lambda_i$

Proof.

$$\begin{aligned} R(v_i) &= \frac{v_i^T \cdot M \cdot v_i}{||v_i||^2} \\ &= \frac{v_i^T \cdot \lambda_i \cdot v_i}{||v_i||^2} \\ &= \lambda_i \end{aligned}$$

□

Theorem 13.

$$\max_{x \neq 0} R(x) = \lambda_1$$

$$\min_{x \neq 0} R(x) = \lambda_n$$

By the above theorem, $v_1 = \operatorname*{argmax}_{x \neq 0} R(x)$.

Proof. Consider $x \neq 0$,

$$R(x) = \frac{x^T \cdot [\sum_{i=1}^n \lambda_i \cdot v_i \cdot v_i^T] \cdot x}{||x||^2}$$

Since $v_1, \ldots, v_n$ is basis $\Rightarrow$ $\exists \underbrace{\alpha_1, \ldots, \alpha_n}_{\text{unique}}$ s.t.

$$1)\ x = \sum_{i=1}^n \alpha_i \cdot v_i \qquad 2)\ ||x||^2 = x^T \cdot x = (\sum_{i=1}^n \alpha_i \cdot v_i)^T (\sum_{j=1}^n \alpha_j \cdot v_j) = \sum_{i=1}^n \alpha_i^2$$

$$\begin{aligned} R(x) &= \frac{x^T \cdot M \cdot x}{||x||^2} \\ &= \frac{x^T \cdot M \cdot \sum_{i=1}^n \alpha_i \cdot v_i}{||x||^2} \\ &= \frac{x^T \cdot \sum_{i=1}^n \alpha_i \cdot \lambda_i \cdot v_i}{||x||^2} \\ &= \frac{\sum_{i,j} (\alpha_j \cdot v_j)^T \cdot \alpha_i \cdot \lambda_i \cdot v_i}{||x||^2} \\ &= \sum_{i=1}^n \lambda_i \cdot \alpha_i^2 \cdot \frac{1}{\sum_{i=1}^n \alpha_i^2} \\ &\leq \max_i \lambda_i = \lambda_1 \end{aligned}$$

The proof for lower bound is precisely the same, by just replacing the maximum with the minimum in the final inequality. □

Theorem 14.

$$\lambda_i = \max_{\substack{x \neq 0 \\ x \perp v_1, \ldots, v_{i-1}}} R(x)$$

Proof for this extension theorem is similar to the previous one.