Introduction to the Heat Kernel

1 Introduction

In this lecture, we introduce the heat kernel for a graph, the heat kernel PageRank, and the zeta function for a graph. We develop some associated theorems to these functions.

2 Heat Kernel PageRank

Recall the definition of the transition probability matrix $W = D^{-1}A$, so that $W(u,v) = \begin{cases} \frac{1}{d_u} & u \sim v \\ 0 & \text{else} \end{cases}$. Let $L' = I - W = D^{-1/2}LD^{1/2}$, the tilted Laplacian.

Let $f : V \to \mathbb{R}, \alpha \in [0,1]$. Recall that we define PageRank with respect to $\alpha, f$ to be the unique vector $pr_{\alpha,f}$ satisfying $pr_{\alpha,f} = \alpha f + (1-\alpha)pr_{\alpha,f}W$. Solving this equation for $pr_{\alpha,f}$, we obtain

$$pr_{\alpha,f} = f \frac{\alpha I}{I - (1-\alpha)W} = \alpha \sum_{k=0}^{\infty} (1-\alpha)^k fW^k.$$

We can use this generating function type structure to give us information about PageRank. However, this is a geometric sum with ratio $(1-\alpha)W$, so when the eigenvalues of this matrix are large, the sum may not converge, or may converge very slowly. In order to take advantage of the generating function structure without having to worry about convergence issues, we turn to an exponential generating function, called the heat kernel PageRank.

**Definition 1.** Let $f : V \to \mathbb{R}$. For $t \geq 0$, define the heat kernel PageRank to be the function

$$h_{t,f} = e^{-t} \sum_{k \geq 0} \frac{t^k}{k!} fW^k.$$
Notice,
\[ h_{t,f} = f e^{-t} \sum_{k \geq 0} \frac{t^k}{k!} W^k = f e^{-t} e^W = f e^{-tL}. \]

3 Heat Kernel

Before we delve into the study of the heat kernel PageRank, we begin by studying the heat kernel of a graph.

**Definition 2.** Define the heat kernel of a graph \( G \) to be the function \( H_t = e^{-t \mathcal{L}} \), for \( t \geq 0 \).

Notice that the heat kernel PageRank is a variant of the heat kernel, where the Laplacian is replaced by the tilted Laplacian. As these two matrices are related, we first develop theory for \( H_t \), which we will then generalize to \( h_{t,f} \).

Let \( 0 = \lambda_0 \leq \lambda_1 \leq \cdots \leq \lambda_{n-1} \) be the eigenvalues of \( \mathcal{L} \), with associated orthonormal eigenfunctions \( \varphi_0, \varphi_1, \ldots, \varphi_{n-1} \). Let \( P_i = \varphi_i^* \varphi_i \), the projection onto the \( i \)th eigenspace. Then \( \mathcal{L} = \sum_{i=0}^{n-1} \lambda_i P_i \), so we may write

\[
H_t = e^{-t \mathcal{L}} = I - t \mathcal{L} + \frac{t^2}{2!} \mathcal{L}^2 - \frac{t^3}{3!} \mathcal{L}^3 + \ldots
\]

\[
= I - t \sum_{i=0}^{n-1} \lambda_i P_i + \frac{t^2}{2!} \left( \sum_{i=0}^{n-1} \lambda_i P_i \right)^2 - \frac{t^3}{3!} \left( \sum_{i=0}^{n-1} \lambda_i P_i \right)^3 + \ldots.
\]

Now, for \( i \neq j \), we have \( P_i P_j = \varphi_i^* (\varphi_i \varphi_j^*) \varphi_j = 0 \), and \( P_i P_i = \varphi_i^* (\varphi_i \varphi_i^*) \varphi_i = \varphi_i^* \varphi_i \), so we obtain

\[
H_t = I - t \sum_{i=0}^{n-1} \lambda_i P_i + \frac{t^2}{2!} \sum_{i=0}^{n-1} \lambda_i P_i - \frac{t^3}{3!} \sum_{i=0}^{n-1} \lambda_i P_i + \ldots
\]

\[
= \sum_{i=0}^{n-1} e^{-\lambda_i t} P_i.
\]

From this formulation, it is clear to see that \( H_t \) satisfies the heat equation, namely, \( \frac{\partial}{\partial t} H_t = -\mathcal{L} H_t \).

Moreover, \( \text{Tr}(H_t) = \sum_x H_t(x, x) = \sum_i e^{-\lambda_i t} \), the sum of the eigenvalues of \( H_t \).
4 Zeta Function

We define here the zeta function of a graph, and in the next section connect this to \( \mathcal{H}_t \).

**Definition 3.** For a graph with eigenvalues \( 0 = \lambda_0 \leq \lambda_1 \leq \cdots \leq \lambda_{n-1} \), define the zeta function of \( G \) to be \( \zeta(s) = \sum_{\nu \neq 0} \frac{1}{\lambda_\nu^s} \).

Notice, \( \zeta'(s) = \sum_{\nu \neq 0} -\frac{\log \lambda_\nu}{\lambda_\nu^s} \), so that \( \zeta'(0) = -\log \left( \prod_{\nu \neq 0} \lambda_\nu \right) \).

**Theorem 1.** Let \( G \) be a connected graph, and let \( \tau(G) \) denote the number of spanning trees of \( G \). Then

\[
\tau(G) = \prod_v \frac{d_v}{d_v} e^{\zeta'(0)}.
\]

**Proof.** Let \( p(x) \) be the characteristic function of \( \mathcal{L} \), so \( p(x) = \det(\mathcal{L} - xI) = \prod_{i=0}^{n-1} (\lambda_i - x) \). Using the second definition, we obtain that the coefficient of the linear term of \( p(x) \) is \(-\sum_{j} \prod_{i \neq j} \lambda_i \).

However, since \( \lambda_0 = 0 \), this product is 0 whenever \( j \neq 0 \), so the coefficient of the linear term of \( p(x) \) is \(-\prod_{i \neq 0} \lambda_i \).

On the other hand, using the first definition of \( p(x) \), we have that

\[
p(x) = \det(\mathcal{L} - xI)
\]

\[
= \det(D^{-1/2}LD^{-1/2} - xD^{-1}D)
\]

\[
= \det(D^{-1}) \det(L - xD),
\]

since the determinant is multiplicative. \( \square \)

Consider \( \det(L - xD) \). Using the combinatorial definition of determinant, where

\[
\det M = \sum_{\sigma \in S_n} \prod_{i=1}^{n} M(i, \sigma_i),
\]

we see that we will get a contribution of a linear term when one element of \([n]\) is fixed by \( \sigma \). Note that if we choose \( \sigma \) to fix \( i \), we obtain a linear term of \(-xd_v \det L_i \), where \( L_i \) denotes the cofactor obtained by deleting the \( i \)th row and column of \( L \). But by Kirchoff’s Matrix-Tree Theorem, this is \(-xd_v \tau(G) \). Therefore, the coefficient of the linear term of \( p(x) \) is given by \( \det(D^{-1}) \sum_v -d_v \tau(G) = \tau(G) \sum_v \frac{d_v}{d_v} \prod_{i \neq 0} \lambda_i \). Therefore, \(-\tau(G) \sum_v \frac{d_v}{d_v} \prod_{i \neq 0} \lambda_i = -\prod_{i \neq 0} \lambda_i \), and thus

\[
\tau(G) = \frac{\sum_v \frac{d_v}{d_v} \prod_{i \neq 0} \lambda_i}{\prod_v \frac{d_v}{d_v} \prod_{i \neq 0} \lambda_i} = \frac{\sum_v \frac{d_v}{d_v} e^{-\zeta'(0)}}{\prod_v \frac{d_v}{d_v} e^{-\zeta'(0)}}.
\]
5 Heat Kernel and Zeta Function

We know from calculus that \( \frac{1}{\Gamma(z)} \int_0^\infty e^{-\rho t} t^{z-1} dt = \rho^{-z} \). Therefore, we have that

\[
\frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} (\text{Tr}(H_t) - 1) dt = \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} \sum_{i \neq 0} e^{-\lambda_i t} dt
\]

\[
= \sum_{i \neq 0} \lambda_i^{-s}
\]

\[
= \zeta(s).
\]

We will use this connection in later classes to establish theorems regarding the number of spanning trees of an induced subgraph of \( G \).

6 Heat Kernel on Subgraphs

Let \( S \subset V \). Define the heat kernel on \( S \) to be

\[
H_t(S) = e^{-tL_S} = \sum_i e^{-t\lambda_{S,i}} P_{S,i},
\]

where \( \lambda_{S,i}, P_{S,i} \) are the eigenvalues and projections onto the associated eigenspaces, respectively.

Notice that if \( f \) is a probability distribution, so that \( f1^* = 1 \), we obtain \( f(I - W)1^* = 1 - fW1^* = 0 \).

Let \( S \subset V \), with \( \text{Vol}S \leq \frac{1}{2} \text{Vol}G \). Define a probability distribution on \( S \) by \( g_S(u) = \left\{ \begin{array}{ll} \frac{d_u}{\text{Vol}S} & u \in S \\ 0 & u \notin S \end{array} \right. \).

Then with respect to this probability distribution, we have

\[
\mathbb{E}(h_{t,u}(S)) = \sum_{u \in S} \frac{d_u}{\text{Vol}S} h_{t,u}(S) = h_{t,g_S}(S).
\]

We will prove the following lemma in the next lecture.

**Lemma 1.** Let \( S \) be as above. Let \( \phi(S) \) denote the Cheeger constant of \( S \). Then

1. \( \frac{\partial}{\partial t} h_{t,g_S}(S) = -\text{Vol}S \sum_{u \sim v} \left( \frac{h_{t/2,g_S}(u)}{d_u} - \frac{h_{t/2,g_S}(v)}{d_v} \right)^2 \leq 0 \).
2. \( \frac{\partial^2}{\partial t^2} h_{t,g_S}(S) \geq 0 \).
3. \( \left| \frac{\partial}{\partial t} h_{t,g_S}(S) \right| \leq \phi(S) \).