Research on Heat kernels and spanning trees

In a graph $G = (V, E)$ with no multiple edges, the combinatorial Laplacian L of G has rows and columns indexed by vertices of G, defined as follows.

$$L(u, v) = \begin{cases} d_v - l_v & \text{if } u = v \\ -1 & \text{if } u \text{ and } v \text{ are adjacent} \\ 0 & \text{otherwise} \end{cases}$$

where l_v denotes the number of loops at v and d_v denotes the degree of v in G.

One of the fundamental theorems in combinatorics is the matrix-tree theorem due to Kirchhoff [4] which states that the number of spanning trees in a graph is equal to the determinant of any principal submatrix of the combinatorial Laplacian.

For a graph G, the combinatorial Laplacian has non-negative eigenvalues, $0 = \rho_0 \leq \rho_1 \leq \ldots \rho_{n-1}$. The number of spanning trees, denoted by $\tau(G)$, can be related to the eigenvalues of L (see [1]).

$$\tau(G) = \frac{1}{n} \prod_{i \neq 0} \rho_i.$$

In a graph G, let S denote a finite connected induced subgraph of G. The combinatorial Laplacian L_S restricted to S is just

$$L_S f(v) = \sum_{\substack{u \in S \\ u \sim v}} [f(v) - f(u)].$$

for a function $f : S \to \mathbb{R}$ and a fixed $v \in S$.

Let k denote the maximum degree of G. For $t \geq 0$, the heat kernel h_t of an induced graph S is defined by

$$\begin{aligned} h_t &= \sum_i e^{-\lambda_i t} P_i \\ &= e^{-tL_S/k} \\ &= I - \frac{t}{k} L_S + \frac{t^2}{2!k^2} L_S^2 - \ldots \end{aligned}$$

where

$$\lambda_i = \frac{\rho_i}{k}$$

and P_i denotes the projection into the eigenspace associated with eigenvalue ρ_i of L_S. In particular, $h_0 = I$, the identity matrix, and h_t satisfies the heat equation

$$\frac{\partial h_t}{\partial t} = -\frac{1}{k} L_S h_t.$$

The trace formula in its most general form is

$$\sum_x h_t(x,x) = \sum_i e^{-\lambda_i t} \tag{1}$$

We define the trace function:

$$Tr\ (h_t) = \sum_i e^{-\lambda_i t}$$

For a connected induced subgraph S, we consider the ζ-function

$$\zeta(s) = \sum_{i \neq 0} \frac{1}{\lambda_i^s}$$

where λ_i ranges over all nonzero eigenvalues of $\frac{1}{k} L_S$.

Therefore we have

$$-\zeta'(0) = \log \prod_{i \neq 0} \lambda_i. \tag{2}$$

where log denotes the natural logarithm.

The number of spanning trees can be related to the zeta function of G by (see [2]):

$$\tau(S) = \frac{k^{|S|-1}}{|S|} e^{-\zeta'(0)}$$

where k is the maximum degree k. We consider

$$Tr^*(h_t) = \sum_{i \neq 0} e^{-\lambda_i t}.$$

Because of the fact that

$$\int_0^\infty e^{-\lambda t} t^{z-1} dt = \frac{\Gamma(z)}{\lambda^z}$$

we have the following:

$$\zeta(s) = \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} Tr^*(h_t) dt \tag{3}$$

We note that we also have the following Mellin inversion formula:

$$Tr^*(h_t) = \frac{1}{2\pi i} \int t^{-s} \Gamma(s) \zeta(s) ds$$

Suppose S is an induced subgraph of the 2-dimensional lattice graph $P^{(2)}$. It was shown in [2] that for a connected induced subgraph S in the 2-dimensional lattice graph, the number of spanning trees $\tau(S)$ of S satisfies:

$$\frac{1}{|S|}(4e^{-\alpha})^{|S|-1} e^{-\beta|\partial S|(1-1/|S|)} \leq \tau(S) \leq \frac{1}{|S|} 4^{|S|-1} e^{-\alpha(|S|+|\partial S|^2/|S|}$$

where α and β are constants (independent of S).

Another result by using the heat kernel techniques is an improvement of the previous result of McKay [5] on the the maximum number of spanning trees over all k-regular graphs G_n on n vertices:

$$c_1 \frac{1}{n} C^n \leq \max \tau(G) \leq c_2 \frac{\log n}{n} C^n$$

where

$$C = \frac{(k-1)^{k-1}}{(k^2-2k)^{k/2-1}}$$

and c_1 and c_2 depend only on k (in some complicated formula). McKay conjectured that the upper bound is the right order for $\max \tau(G_n)$. Indeed, it is shown in [3] that this upper bound is best possible within a constant factor.

$$\tau(G_n) \leq (1+o(1)) \frac{2 \log n}{kn \log k} \left(\frac{(k-1)^{k-1}}{(k^2-2k)^{k/2-1}} \right)^n$$

for a k-regular graph G.

It is desirable to improve the bounds in the preceding inequalities concerning spanning trees. Indeed, it is of interest to investigate how zeta function and the heat kernel relate to various other graph invariants as well.

References

[1] N.L. Biggs, *Algebraic Graph Theory*, (2nd ed.), Cambridge University Press, Cambridge, 1993.

[2] Fan Chung, Spanning trees in subgraphs of lattices. *Comp. Math.*, to appear.

[3] F. R. K. Chung and S.-T. Yau, Coverings, heat kernels and spanning trees, *Electronic Journal of Combinatorics* **6** (1999), #R12.

[4] F. Kirchhoff, Über die Auflösung der Gleichungen, auf welche man bei der Untersuchung der linearen Verteilung galvanischer Ströme geführt wird, *Ann. Phys. Chem.* 72 (1847), 497-508.

[5] B. D. McKay, Spanning trees in regular graphs, *Europ. J. Combinatorics* **4** (1983), 149-160.