Kemeny's constant for random walks on graphs

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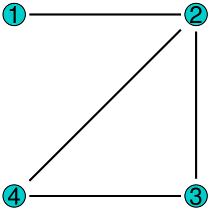
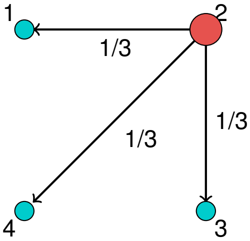
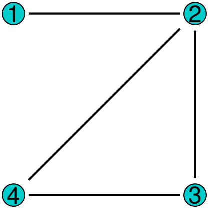
- A random walker traverses the vertices of G, at each step choosing an adjacent vertex to move to uniformly at random. (A random walk on a given graph $G = (V, E)$ is an example of a Markov chain.)





The **mean first passage time** $m_{i,j}$ **from vertex** i **to vertex** j is the expected number of time-steps elapsed before the random walker reaches vertex j, given that it begins at vertex i.



$$\begin{bmatrix} 0 & 1 & 13/3 & 13/3 \\ 7 & 0 & 10/3 & 10/3 \\ 9 & 2 & 0 & 8/3 \\ 9 & 2 & 8/3 & 0 \end{bmatrix}$$

Kemeny's constant $\mathcal{K}(G)$ of a graph G is defined as

$$\mathcal{K}(G) = \sum_{j \neq i} \left(\frac{d_j}{2m} \right) m_{i,j} \quad \forall i \in V(G).$$

It can be recast as follows:

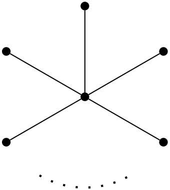
$$\mathcal{K}(G) = \sum_{i} \sum_{j \neq i} \left(\frac{d_i}{2m_G} \right) m_{i,j} \left(\frac{d_j}{2m_G} \right).$$

Kemeny's constant can be interpreted as the expected length of a random trip in the graph G. One can consider it as measuring how well-connected the graph is.

How does graph structure affect Kemeny's constant?

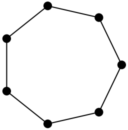
- Sparsity?
- Distances between vertices?

Examples: star, path, cycle, complete graph

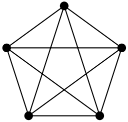


$\mathcal{K}(S_n) = n - \frac{3}{2}$

$\mathcal{K}(P_n) = \frac{1}{3}(n-1)^2 + \frac{1}{6}$



$\mathcal{K}(C_n) = \frac{1}{6}(n-1)(n+1)$



$\mathcal{K}(K_n) = n - 2 + \frac{1}{n}$

Let D be the diagonal matrix of vertex degrees of a connected graph G, and A be its adjacency matrix. It is shown in [Levene and Loizou, 2002] that

$$\mathcal{K}(G) = \sum_{i=2}^{n} \frac{1}{1-\lambda_i},$$

where $1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of the transition matrix $D^{-1}A$.

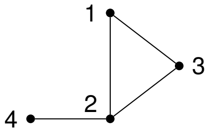
(Note) For r-regular graph, $1, \lambda_2, \ldots, \lambda_n$ can be obtained from adjacency eigenvalues by multiplication of $1/r$. We can obtain $\mathcal{K}(C_n)$ and $\mathcal{K}(K_n)$.

Let F be the matrix given by $F = [f_{i,j}]$ where $f_{i,j}$ is the number of spanning 2-forests of G where one component of the forest contains vertex i, and the other contains j. It is shown in [Kirkland and Zeng, 2016] that

$$\mathcal{K}(G) = \frac{\mathbf{d}^T F \mathbf{d}}{4m\tau},$$

where m is the number of edges, $\mathbf{d}$ is the degree vector of G and τ is the number of spanning trees of G.

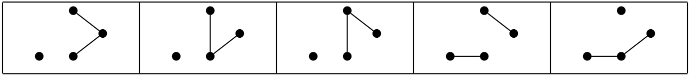
(Example)



G

$f_{1,4} = 5$

$\tau = 3$



(Note) If G is a tree, then F is the distance matrix. We can obtain $\mathcal{K}(S_n)$ and $\mathcal{K}(P_n)$.

Let R be the matrix given by $R = [r_{i,j}]$, where $r_{i,j}$ is the so-called *effective resistance distance* between vertices i and j. It is known that $r_{i,j} = \frac{f_{i,j}}{\tau}$. Hence,

$$\mathcal{K}(G) = \frac{\mathbf{d}^T R \mathbf{d}}{4m}.$$

(Note) The so-called *Kirchhoff index* $\mathrm{Kf}(G)$ is a graph invariant and is defined as $\mathrm{Kf}(G) = \frac{1}{2}\mathbf{1}^T R \mathbf{1}$. If G is r-regular, then $\mathcal{K}(G) = \frac{r}{n}\mathrm{Kf}(G)$.

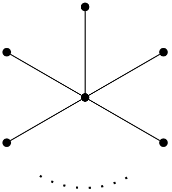
Topic of this talk

- Kemeny's constant is a graph invariant, and it can be regarded as a measure of graph connectivity.
- It is natural to study how graph structure informs a graph invariant.
- We will understand how graph structures influence Kemeny's constant via asymptotic behaviour.

(Notation) Let G_n represent a graph of order n in a sequence or family of graphs.

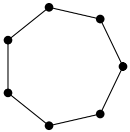
- We write $f(G_n) = O(g(n))$ if $\limsup_{n\to\infty} \frac{f(G_n)}{g(n)}$ is finite.
- We write $f(G_n) = \Omega(g(n))$ if $g(n) = O(f(G_n))$.
- We write $f(G_n) = \Theta(g(n))$ if $f(G_n) = O(g(n))$ and $f(G_n) = \Omega(g(n))$.

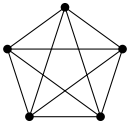
Examples: star, path, cycle, complete graph



$\mathcal{K}(S_n) = n - \frac{3}{2} = \Theta(n)$

$\mathcal{K}(P_n) = \frac{1}{3}(n-1)^2 + \frac{1}{6} = \Theta(n^2)$





$\mathcal{K}(C_n) = \frac{1}{6}(n-1)(n+1) = \Theta(n^2)$

$\mathcal{K}(K_n) = n - 2 + \frac{1}{n} = \Theta(n)$

(Note) For any graph G, $\mathcal{K}(G) \geq \mathcal{K}(K_n)$. Hence, $\mathcal{K}(G_n) = \Omega(n)$.

Proposition (Kim, Madras, Chan, Kempton, Kirkland and Knudson, 2023)

Let G be a connected graph. Then

$$\mathcal{K}(G) < 2m\,\mathrm{diam}(G).$$

(Proof)

- Recall

$$\mathcal{K}(G) = \sum_{j \neq i} \left(\frac{d_j}{2m}\right) m_{i,j} \quad \forall i \in V(G).$$

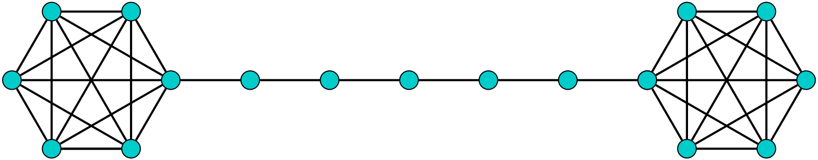
- It is known from [Chandra et al., 1989] that $m_{i,j} + m_{j,i} = 2mr_{i,j}$.
- It follows that

$$\mathcal{K}(G) = \sum_{\substack{j=1 \\ j \neq i}}^{n} \left(\frac{d_j}{2m}\right) m_{i,j} < \sum_{\substack{j=1 \\ j \neq i}}^{n} \left(\frac{d_j}{2m}\right)(m_{i,j} + m_{j,i}) = \sum_{\substack{j=1 \\ j \neq i}}^{n} d_j r_{i,j}$$

- Furthermore, $r_{i,j} \leq \mathrm{diam}(G)$ in [Palacios, 2010]. □

(Note) Since $m = O(n^2)$ and $\mathrm{diam}(G) = O(n)$, we have $\mathcal{K}(G) = O(n^3)$. Moreover, if $\mathrm{diam}(G)$ is fixed, then $\mathcal{K}(G) = O(n^2)$.

Barbell graph



[Breen et al., 2019]: $\mathcal{K}(G) = \frac{1}{54}n^3 + O(n^2)$.

Let $\Delta(G)$ be the maximum degree of G.

Theorem (Kim, Madras, Chan, Kempton, Kirkland and Knudson, 2023)

Let G be a connected graph on n vertices with $\Delta(G) = n - O(1)$. Then, $\mathcal{K}(G) = \Theta(n)$.

Theorem (Kim, Madras, Chan, Kempton, Kirkland and Knudson, 2023)

Let G be a graph on n vertices with $\Delta(G) = n - 1$. Then, $\mathcal{K}(G) < 2(n-1)$.

(Sketch of proof)

- Let i be a vertex of degree $n-1$. Since $r_{i,j} = \frac{1}{\tau} f_{i,j}$,

$$\mathcal{K}(G) < \sum_{\substack{j=1 \\ j \neq i}}^{n} d_j r_{i,j} = \sum_{\substack{j=1 \\ j \neq i}}^{n} \frac{1}{\tau} d_j f_{i,j}.$$

- We claim that $d_j f_{i,j} \leq 2\tau$.

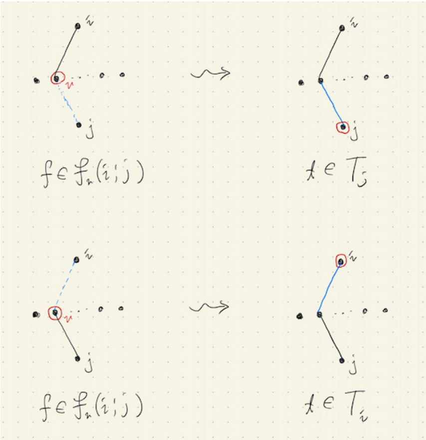
- Let $N(j)$ be the neighbour of j.
- For each $v \in N(j)$, we define $\mathcal{F}_v(i;j)$ to be the set of spanning rooted 2-forests separating i and j by labelling v as a root. Then

$$\left| \bigcup_{v \in N(j)} \mathcal{F}_v(i;j) \right| = \sum_{v \in N(j)} |\mathcal{F}_v(i;j)| = d_j f_{i,j}.$$

- We define $\mathcal{T}_i$ (resp. $\mathcal{T}_j$) to be the set of spanning rooted trees of G with root i (resp. with root j). Then

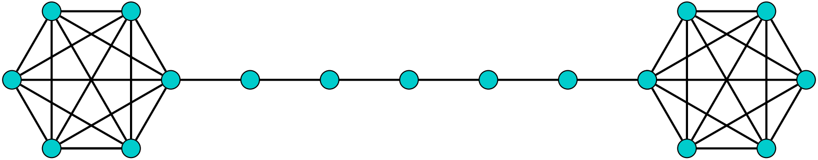
$$|\mathcal{T}_i \cup \mathcal{T}_j| = 2\tau.$$

- It can be proved that the following map from $\bigcup_{v \in N(j)} \mathcal{F}_v(i;j)$ to $\mathcal{T}_i \cup \mathcal{T}_j$ is injective.



- Given a graph invariant f, the Nordhaus–Gaddum type problem is to find lower and upper bounds for $f(G) + f(\overline{G})$ and $f(G)f(\overline{G})$, where $\overline{G}$ is the complement of G.
- It provides insights into the interplay between a graph and its complement.
- We consider $f(G) = \mathcal{K}(G)$ for connected G and $\overline{G}$ in order to see how graph structures influence Kemeny's constant.
- Since $\mathcal{K}(G) = O(n^3)$, we have $\mathcal{K}(G) + \mathcal{K}(\overline{G}) = O(n^3)$ and $\mathcal{K}(G)\mathcal{K}(\overline{G}) = O(n^6)$.
- We shall focus on $\mathcal{K}(G)\mathcal{K}(\overline{G})$.
- If $\mathrm{diam}(G) > 3$ then $\mathrm{diam}(\overline{G}) = 2$. Hence $\mathcal{K}(G)\mathcal{K}(\overline{G}) = O(n^5)$.
- Is this sharp?
- We do not know yet.

Barbell graph



There is a vertex of degree $n-3$. Hence $\mathcal{K}(\overline{G}) = \Theta(n)$ and

$$\mathcal{K}(G)\mathcal{K}(\overline{G}) = \Theta(n^4).$$

Theorem (Kim, Madras, Chan, Kempton, Kirkland and Knudson, 2023)

Let U be a real constant such that $0 < U < 1$. Then there is a constant Ψ_U such that for every $n \in \mathbb{N}$ and every graph G on n vertices such that $\Delta(G) \le Un$,

$$\min\left\{\mathcal{K}(G),\, \mathcal{K}(\overline{G})\right\} \;\le\; n\Psi_U\,.$$

(Idea of proof)

- Recall
$$\mathcal{K}(G) \;=\; \sum_{i=2}^{n} \frac{1}{1-\lambda_i},$$
where $\lambda_1 = 1 > \lambda_2 \ge \lambda_3 \ge \ldots \ge \lambda_n$ are the eigenvalues of $D^{-1}A$.
- Then
$$\frac{1}{1-\lambda_2} \;\le\; \mathcal{K}(G) \;\le\; \frac{n}{1-\lambda_2}.$$
- For $S \subseteq V(G)$, let
$$\mathrm{vol}(S) \;:=\; \sum_{v \in S} d_v\,.$$
- When S and T are disjoint subsets of $V(G)$, we define $[S, T]_G$ to be the set of all edges of G.

- The *bottleneck ratio* of the graph G is defined to be

$$\Phi = \Phi(G) = \min_{S \subseteq V:\, 0 < \mathrm{vol}(S) \leq |E(G)|} \frac{|[S, S^c]_G|}{\mathrm{vol}(S)}.$$

- It is known that

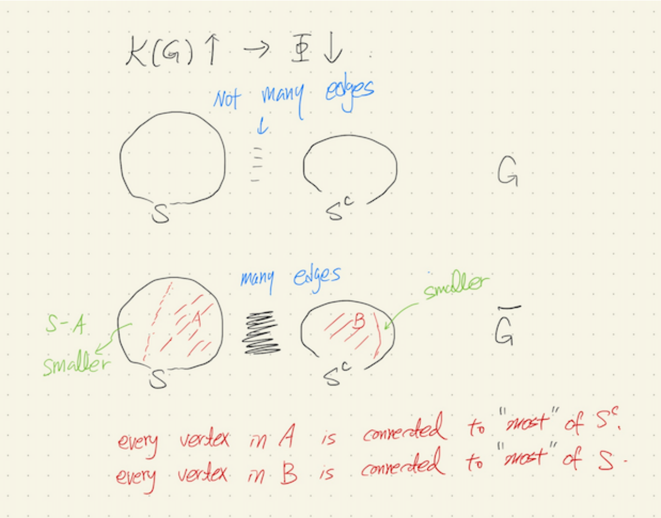
$$\frac{\Phi^2}{2} \leq 1 - \lambda_2 \leq 2\Phi.$$

- Hence,

$$\frac{1}{2\Phi} \leq \mathcal{K}(G) \leq \frac{2n}{\Phi^2}.$$

- Now we claim that if $\mathcal{K}(G)$ is "large", then $\mathcal{K}(\overline{G}) = O(n)$.

Continuing Idea of proof



This structure forces mean first passage to be of order n.

Maximum degree

Theorem (Kim, Madras, Chan, Kempton, Kirkland and Knudson, 2023)

Let U be a real constant such that $0 < U < 1$. Then there is a constant Ψ_U such that for every $n \in \mathbb{N}$ and every graph G on n vertices such that $\Delta(G) \le Un$,

$$\min\left\{\mathcal{K}(G),\, \mathcal{K}(\overline{G})\right\} \;\le\; n\Psi_U\,.$$

Corollary

Let G be a regular graph on n vertices. There exists a constant Ψ_{reg} such that

$$\min\left\{\mathcal{K}(G),\, \mathcal{K}(\overline{G})\right\} \;\le\; n\Psi_{reg}.$$

(Note) We have proved that when maximum degree is $n - \Omega(n)$, or when it is $n - O(1)$, we have $\mathcal{K}(G)\mathcal{K}(\overline{G}) = O(n^4)$.

- Let G be r-regular graph. Recall

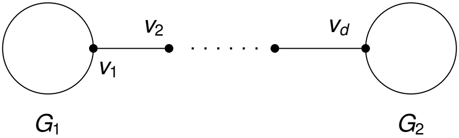
$$\mathcal{K}(G) = \frac{r}{n}\mathrm{Kf}(G).$$

- From [Palacios, 2010], we have $\frac{n(n-1)}{2k} \leq \mathrm{Kf}(G) \leq \frac{3n^3}{k}$.
- Hence,

$$\frac{n-1}{2} \leq \mathcal{K}(G) \leq 3n^2.$$

- That is, $\mathcal{K}(G) = O(n^2)$.
- Since $\min\{\mathcal{K}(G), \mathcal{K}(\overline{G})\} = O(n)$, we have

$$\mathcal{K}(G)\mathcal{K}(\overline{G}) = O(n^3).$$



- Using a formula of Kemeny's constant of graphs with bridges in [Breen, Crisostomi and Kim, 2022], we obtain

$$\mathcal{K}(G) = \Omega\left(\frac{m_{G_1} m_{G_2} d}{m_{G_1} + m_{G_2} + d}\right).$$

- If $d = \Theta(n)$, $m_{G_1} = \Theta(n^2)$ and $m_{G_2} = \Theta(n^2)$, then

$$\mathcal{K}(G) = \Theta(n^3).$$

- Moreover,

$$\mathcal{K}(G)\mathcal{K}(\overline{G}) = \Theta(n^4).$$

Tree for N-G problem

- Let $\mathcal{T}$ be a tree.
- It appears in [Jang, Kim and Song, 2023] that

$$\mathcal{K}(\mathcal{T}) = \frac{2W(\mathcal{T})}{n-1} - n + \frac{1}{2}$$

  where $W(\mathcal{T})$ (called *Wiener index*) is the sum of distances for all pairs of two distinct vertices.
- It is known that $W(\mathcal{T}) = O(n^3)$.
- Hence $\mathcal{K}(\mathcal{T}) = O(n^2)$ and

$$\mathcal{K}(\mathcal{T})\mathcal{K}(\overline{\mathcal{T}}) = O(n^3).$$

See [Brouwer and Haemers, 2012] for a comprehensive monograph on distance regular graphs.

- The spectrum of strongly regular graph G is well-known (see [Godsil and Royle, 2001]). We can find that $\mathcal{K}(G) = O(n)$ and so

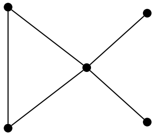
$$\mathcal{K}(G)\mathcal{K}(\overline{G}) = \Theta(n^2).$$

Recall $\mathcal{K}(C_n) = \Theta(n^2)$. How about distance regular graphs with growing diameter?

- The spectrum of distance regular graph with classical parameter is found in [Jurišić and Vidali, 2017].
- We can find that when G is a Hamming graph, $\mathcal{K}(G) = O(n)$.
- In addition, Kemeny's constants for families (C2), (C3), (C3a), (C4), (C4a), (C10), (C11), and (C11a) in [Brouwer and Haemers, 2012, Tables 6.1 and 6.2] are $O(n)$ while their diameters grow as n increases.

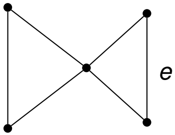
- Kemeny's constant measures how fast a random walker moveces around in a graph.
- Does Kemeny's constant decrease after adding a new edge?
- Recall that $\mathcal{K}(G) = \frac{\mathbf{d}^T R \mathbf{d}}{4m}$ and $\mathrm{Kf}(G) = \frac{1}{2}\mathbf{1}^T R \mathbf{1}$.
- It is known that the addition of a new edge decreases Kirchhoff index.
- It does not hold for Kemeny's constant in general.
- Such an edge is called a *Braess edge*, whose name comes from Braess's paradox in road networks.

Example



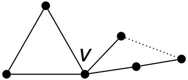
G

$\mathcal{K}(G) = 3.6667$

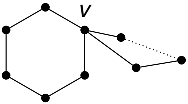


$G \cup e$

$\mathcal{K}(G \cup e) = 4$



−0.4167



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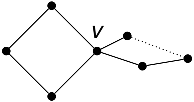
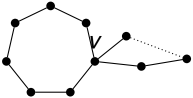


−0.2857



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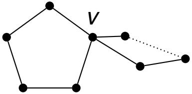

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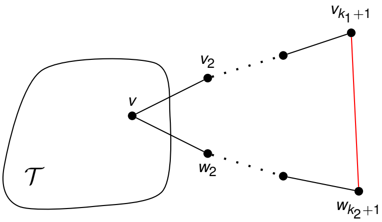


We consider the following sequence $\mathcal{G}^v = (\mathcal{T}_n)^v$ of trees, where $V(\mathcal{T}_1) = \{v\}$ and for each $n \geq 2$, $\mathcal{T}_n$ is obtained from $\mathcal{T}_{n-1}$ by one of the following cases:

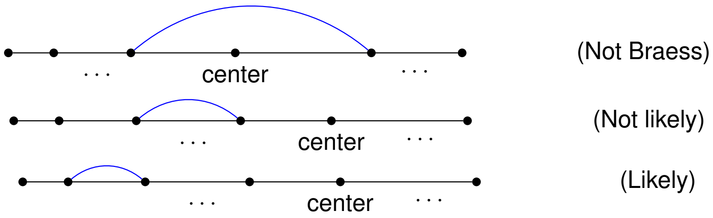
- adding a new pendent vertex to $\mathcal{T}_{n-1}$, or
- subdividing an edge in $\mathcal{T}_{n-1}$ into two edges connecting to a new vertex.

We denote by α_n the eccentricity of v in $\mathcal{T}_n$.

Theorem (Kim, 2022)

Suppose that $\mathcal{G}^v = (\mathcal{T}_n)^v$ is a sequence of trees $\mathcal{T}_n$ such that $\alpha_n = \omega(n^{\frac{2}{3}})$. Given $k_1, k_2 \geq 0$, if $\alpha = \omega(n^{\frac{2}{3}})$, then $\{v_{k_1+1}, v_{w_2+1}\}$ tends to be a Braess edge.

Braess edges on path



- The Braess edges in a path are concentrated towards the endpoints with creating a small cycle.
- An edge connecting points that were originally far apart will tend to decrease travel times of the random walker.
- But, edges close to the endpoints of a path create bottlenecks where the random walker could get stuck for a time.
- In [Jang, Kempton, Kim, Knudson, Madras and Song, 2023], the number of Braess edges for a path of length n is

$$\frac{1}{3} n \ln n - cn + o(n)$$

  for a constant $c \approx .548$.

(Note) In [Kirkland, Li, McAlister and Zhang, 2023], the maximum increment from the addition of a new edge to any tree is approximately $\frac{2}{3}n$.

Thank you for your attention!

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