Kemeny's constant for Markov chains and random walks on graphs

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Ontario Tech University

Algebraic Graph Theory Seminar: November 6th

Overview of the talk

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- What kinds of generalizations can we make of $\mathcal{K}(G)$?

Outline

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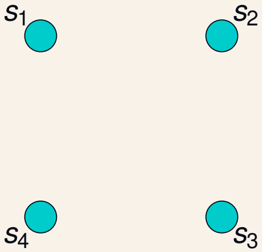
Markov chains

- A Markov chain (finite, discrete-time, time-homogeneous) can be thought of as a system transitioning between states over some finite state space $\{s_1, s_2, \ldots, s_n\}$ in discrete time-steps.



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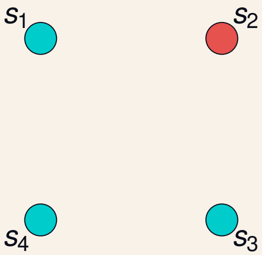

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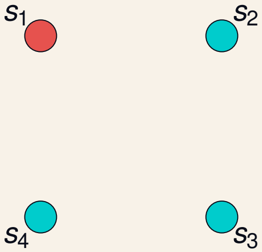

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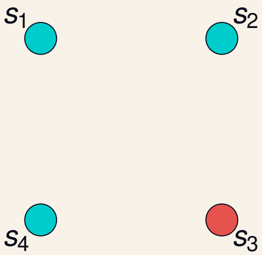
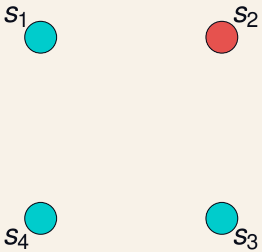


Markov chains

- For each pair of states s_i and s_j, there is some transition probability $t_{i,j}$ representing the probability that the system moves from s_i to s_j in a single time-step.



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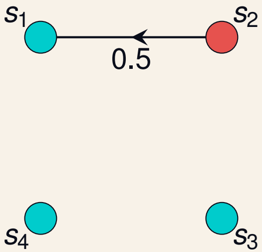

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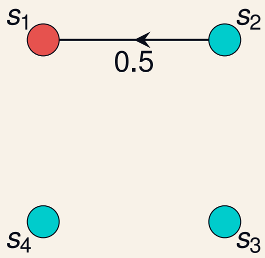
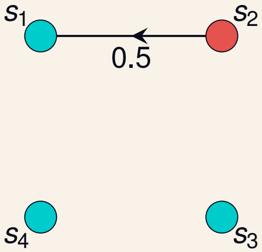


Markov chains

- In this way, the chain is *memoryless*; the movement of the chain depends only on the current state of the system.



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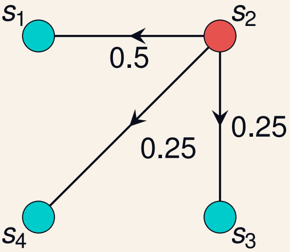

The Transition Matrix

- A Markov chain can be represented entirely by its *transition matrix* $T = [t_{i,j}]$, which is necessarily a row-stochastic matrix T; that is, $T\mathbb{1} = \mathbb{1}$.

$$T = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0.5 & 0 & 0.25 & 0.25 \\ 0 & 0.25 & 0 & 0.75 \\ 0 & 0 & 0.25 & 0.75 \end{bmatrix}$$

Long-term behaviour of a Markov chain

- The left eigenvector $w = [w_1 \ w_2 \ \cdots \ w_n]$ corresponding to the eigenvalue 1, such that $w^\top T = w^\top$ and $w_1 + w_2 + \cdots + w_n = 1$, is called the **stationary vector** of the Markov chain.

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- The stationary vector w describes the long-term behaviour of the system—the i^{th} entry w_i gives the long-term probability that the system occupies state s_i.

Long-term behaviour of a Markov chain

For example, the stationary vector of

$$T = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0.5 & 0 & 0.25 & 0.25 \\ 0 & 0.25 & 0 & 0.75 \\ 0 & 0 & 0.25 & 0.75 \end{bmatrix}$$

is

$$w^\top = \begin{bmatrix} \frac{1}{21} & \frac{2}{21} & \frac{4}{21} & \frac{14}{21} \end{bmatrix}$$

Short-term behaviour of a Markov chain

Definition

The **mean first passage time from i to j** is the expected number of time-steps elapsed before the system reaches state j, given that it begins in state i. It is denoted $m_{i,j}$.

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$$m_{i,j} = \begin{cases} e_i^\top (I - T_{(j)})^{-1} \mathbb{1}, & i < j; \\ e_{i-1}^\top (I - T_{(j)})^{-1} \mathbb{1}, & i > j, \end{cases}$$

Short-term behaviour of a Markov chain

For

$$T = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0.5 & 0 & 0.25 & 0.25 \\ 0 & 0.25 & 0 & 0.75 \\ 0 & 0 & 0.25 & 0.75 \end{bmatrix}$$

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$$m_{1,2} = 1$$

Short-term behaviour of a Markov chain

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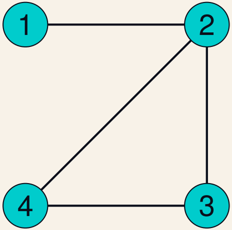
we can calculate

$$\begin{aligned} m_{1,2} &= 1 \\ m_{2,1} &= 20 \end{aligned}$$

Motivating example - Random walks on graphs

Let $\mathcal{G}$ be a simple undirected graph, with adjacency matrix A and vertex degrees $d_1, \ldots, d_n$. Let D be the diagonal matrix $\text{diag}(d_1, \ldots, d_n)$. Then $T = D^{-1}A$ is the probability transition matrix of the random walk on $\mathcal{G}$.



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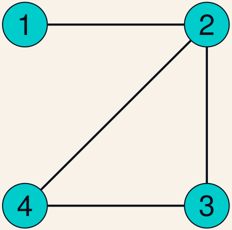

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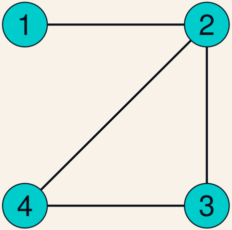

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$$w^\top = \begin{bmatrix} \frac{1}{8} & \frac{3}{8} & \frac{2}{8} & \frac{2}{8} \end{bmatrix}$$

Outline

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Let T be the transition matrix for a Markov chain with n states, with stationary vector w and mean first passage times $m_{i,j}$.

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This is a constant - it doesn't depend on the starting state!

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We can also write

$$\mathcal{K}(T) = \sum_{i=1}^{n} \sum_{\substack{j=1 \\ j \neq i}}^{n} w_i m_{i,j} w_j,$$

and interpret $\mathcal{K}(T)$ as the expected length of a random trip in the Markov chain.

Outline

Finite Markov Chains, Kemeny & Snell (1960)

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- The *fundamental matrix* of a Markov chain with transition matrix T and stationary vector w is

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- Many things can be calculated using Z.
- For example, the matrix of mean first passage times is

$$M = (I - Z + JZ_{dg})W^{-1}.$$

4.4.10 THEOREM. *Let* $c = \sum_i z_{ii}$. *Then* $M\alpha^T = c\xi$.

PROOF.

$$\begin{aligned} M\alpha^T &= (I - Z + EZ_{dg})D\alpha^T \\ &= (I - Z + EZ_{dg})\xi \\ &= \xi(\eta Z_{dg}\xi) = c\xi. \end{aligned}$$

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This statement (translated) says that $Mw = \mathcal{K}(T)\mathbb{1}$; i.e. $\sum_j m_{i,j}w_j = \mathcal{K}(T)$ for all i.

Introduction to Probability with Computing, Snell (1975)

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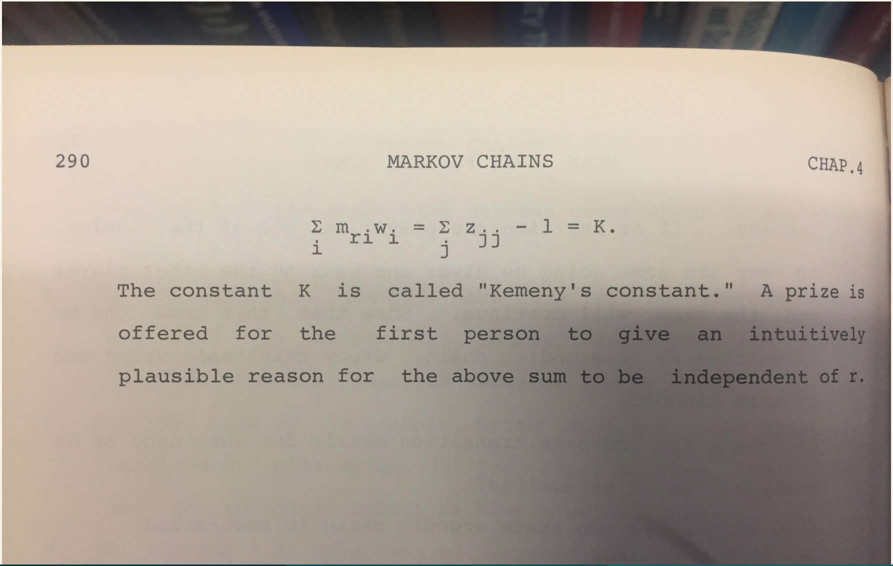

$$\sum_i m_{ri} w_i = \sum_j z_{jj} - 1 = K.$$

The constant K is called "Kemeny's constant." A prize is offered for the first person to give an intuitively plausible reason for the above sum to be independent of r.

Levene & Loizou (2002)

- M. Levene, G. Loizou, 2002. Kemeny's constant and the random surfer. *The American Mathematical Monthly*, 109(8), pp.741-745.

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Theorem

Let T be the transition matrix of a Markov chain, with eigenvalues $1, \lambda_2, \ldots, \lambda_n$. Then

$$\mathcal{K}(T) = \sum_{j=2}^{n} \frac{1}{1-\lambda_j}.$$

Bounds on Kemeny's constant

Proposition

For any Markov chain with transition matrix T,

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- For each j, $|\lambda_j| \leq 1$.
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- What if $\lambda_j = a + bi$?

Proof

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$$\frac{1}{1-\lambda_j} + \frac{1}{1-\bar{\lambda}_j} = \frac{2-(\lambda_j+\bar{\lambda}_j)}{(1-\lambda_j)(1-\bar{\lambda}_j)}$$

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Proof

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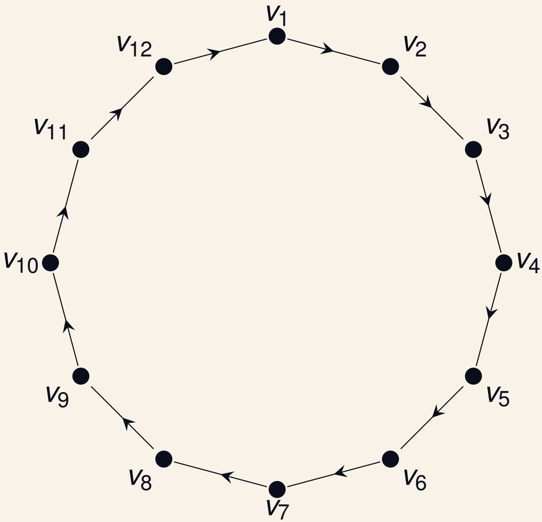
$$\begin{aligned} \frac{1}{1-\lambda_j} + \frac{1}{1-\bar{\lambda}_j} &= \frac{2-(\lambda_j+\bar{\lambda}_j)}{(1-\lambda_j)(1-\bar{\lambda}_j)} \\ &= \frac{2-2a}{1-2a+a^2+b^2} \\ &\geq 1. \end{aligned}$$

- So clearly,

$$\mathcal{K}(T) = \sum_{j=2}^{n} \frac{1}{1-\lambda_j} \geq \frac{n-1}{2}.$$

Extremal example - directed cycle



Extremal example - directed cycle

$$T = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & \cdots & 0 \end{bmatrix}.$$

Outline

Methods of computation I

Eigenvalues and related expressions

The transition matrix for a random walk on a graph is $T = D^{-1}A$, so

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We also have the normalized Laplacian:

$$\mathcal{L} = D^{-\frac{1}{2}}(D-A)D^{-\frac{1}{2}}$$

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We also have the normalized Laplacian:

$$\mathcal{L} = D^{-\frac{1}{2}}(D-A)D^{-\frac{1}{2}}$$

- It's not hard to show that $\mathcal{L}$ is similar to $I - D^{-1}A$.
- If $\mathcal{L}$ has eigenvalues $0 = \mu_0 < \mu_1 \leq \cdots \leq \mu_{n-1} \leq 2$, then we can define

$$\mathcal{K}(\mathcal{G}) = \sum_{j=1}^{n-1} \frac{1}{\mu_j}.$$

Methods of computation I

Eigenvalues and related expressions

- If $\mathcal{L}$ is the normalized Laplacian of a graph $\mathcal{G}$, with characteristic polynomial
$$c_n x^n + c_{n-1} x^{n-1} + \dots c_2 x^2 + c_1 x$$

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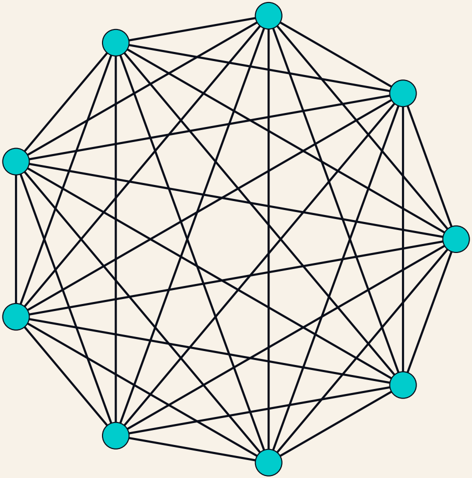
$$c_n x^n + c_{n-1} x^{n-1} + \ldots c_2 x^2 + c_1 x$$
then
$$\mathcal{K}(\mathcal{G}) = -\frac{c_2}{c_1}.$$

Minimum value for $\mathcal{K}(G)$



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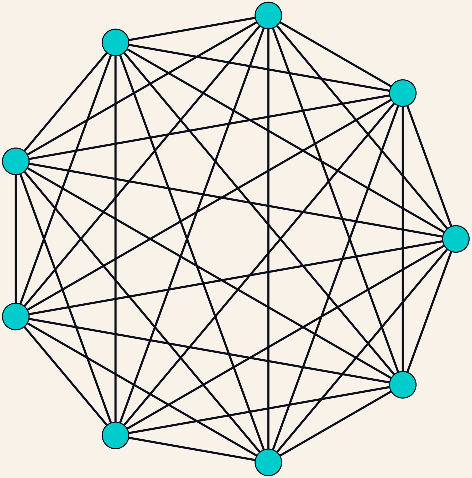
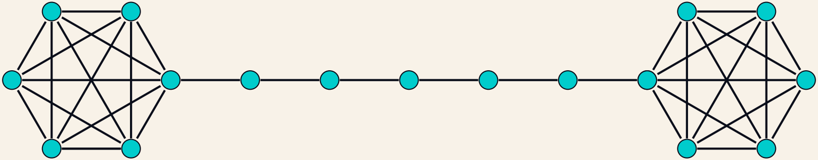


$$\mathcal{K}(K_n) = n - 2 + \frac{1}{n}$$

Maximum value for $\mathcal{K}(G)$

(Conjectured)



$$\mathcal{K}(\mathcal{G}) = \frac{1}{54}n^3 + O(n^2)$$

- Aksoy, Chung, Tait, Tobin (2018): $\frac{1}{\mu_1} = (1 + o(1))\frac{1}{54}n^3$
- Breen, Butler, Day, DeArmond, Lorenzen, Qian, Riesen (2019): $\mathcal{K}(\mathcal{G}) = \frac{1}{54}n^3 + O(n^2)$

(Conjectured by Aldous-Fill to be the extremal graph for both)

Theorem (Kirkland, Zeng, 2014)

Let $\mathcal{G}$ be a simple undirected graph.

- *Let $d = \begin{bmatrix} d_1 & d_2 & \cdots & d_n \end{bmatrix}$ be the degree vector of $\mathcal{G}$.*
- *Let m be the number of edges.*
- *Let τ be the number of spanning trees of $\mathcal{G}$.*
- *Let $f_{i,j}$ be the number of spanning forests of $\mathcal{G}$, consisting of exactly two trees, one containing v_i and one containing v_j.*

Then:

$$\mathcal{K}(\mathcal{G}) = \frac{d^\top F d}{4m\tau} = \frac{1}{4m\tau}\sum_{i,j} d_i d_j f_{i,j}.$$

Formulas for graphs with cut-vertices or bridges

- **A 1-separation formula for the graph Kemeny constant and Braess edges.**
  Nolan Faught, Mark Kempton, Adam Knudson.
  Journal of Mathematical Chemistry 60:1 (2022), 49–69.
- **Kemeny's constant for a graph with bridges.**
  Jane Breen, Emanuele Crisostomi, Sooyeong Kim.
  Discrete Applied Mathematics 322 (2022), 20–35.

What's known?

Here is a list of graph classes for which Kemeny's constant has been studied:

- Trees
- Multipartite graphs
- Barbell-type graphs
- Cycle barbells
- Flower graphs
- Threshold graphs
- Split graphs

Overview of the rest of the talk

Question

What are the interesting questions to ask for extensions of simple, undirected, unweighted graphs?

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- Random walks on **weighted** graphs
  - Many good questions coming from applications

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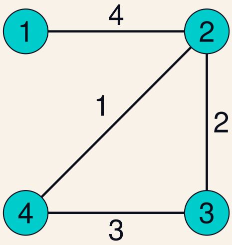
What are the interesting questions to ask for extensions of simple, undirected, unweighted graphs?

- Random walks on **weighted** graphs
  - Many good questions coming from applications
- **Non-backtracking** random walks on graphs
  - tied in with interesting results in mixing times
  - more interesting questions about the influence of graph structure on Kemeny's constant

Outline

What is a weighted random walk?



$$T = \begin{bmatrix} 0 & 1 & 0 & 0 \\ \frac{4}{7} & 0 & \frac{2}{7} & \frac{1}{7} \\ 0 & \frac{2}{5} & 0 & \frac{3}{5} \\ 0 & \frac{1}{4} & \frac{3}{4} & 0 \end{bmatrix}$$

Real-world applications of Kemeny's constant

- Road networks
- Globalization of the economy
- Robotic surveillance
- Social networks and clustering
- Contact networks and disease spread

Robotic surveillance paper

3156 IEEE TRANSACTIONS ON AUTOMATIC CONTROL, VOL. 60, NO. 12, DECEMBER 2015

Robotic Surveillance and Markov Chains With Minimal Weighted Kemeny Constant

Rushabh Patel, *Student Member, IEEE*, Pushkarini Agharkar, *Student Member, IEEE*, and Francesco Bullo, *Fellow, IEEE*

***Abstract*—This article provides analysis and optimization results for the *mean first passage time*, also known as the *Kemeny constant*, of a Markov chain. First, we generalize the notion of the Kemeny constant to environments with heterogeneous travel and service times, denote this generalization as the *weighted Kemeny constant*, and we characterize its properties. Second, for reversible Markov chains, we show that the minimization of the Kemeny constant and its weighted counterpart can be formulated as convex optimization problems and, moreover, as semidefinite programs. Third, we apply these results to the design of stochastic surveillance strategies for quickest detection of anomalies in network environments. We numerically illustrate the proposed design: compared with other well-known Markov chains, the performance of our Kemeny-based strategies are always better and in many cases substantially so.**

***Index Terms*—Fastest mixing Markov chain (FMMC), Kemeny**

vated by the desire to design surveillance strategies with pre-specified stationary distributions, that are easily implementable and inherently unpredictable. In areas of research outside of robotics, the study of the mean first passage time is potentially useful in determining how quickly information propagates in an online network [4] or how quickly an epidemic spreads through a contact network [40].

B. Literature Review

For a random walk associated with a Markov chain, the mean first passage time, also known as the *Kemeny constant*, of the chain is the expected time taken by a random walker to travel from an arbitrary start node to a second randomly-selected

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Summary

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- Consider Kemeny's constant for a random walk on a weighted graph as a measure of the expected length of time to capture the intruder.
- How should the weights of the edges of the graph be chosen so as to minimize Kemeny's constant?

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- Formulate the problem as a convex optimization problem.
- Solve it using semi-definite programming.

Kemeny-based testing for COVID-19

Serife Yilmaz,* Ekaterina Dudkina,‡ Michelangelo Bin,† Emanuele Crisostomi,‡ Pietro Ferraro,*
Roderick Murray-Smith,§ Thomas Parisini,†,¶,‖ Lewi Stone,** Robert Shorten*
*Dyson School of Design Engineering, Imperial College London, London, UK.
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§School of Computing Science, University of Glasgow, Glasgow, Scotland.
¶ Department of Engineering and Architecture, University of Trieste, Trieste, Italy.
‖ KIOS Research and Innovation Center of Excellence, University of Cyprus, Nicosia, Cyprus.
** The George S. Wise Faculty of Life Sciences, Tel Aviv University, Israel.

***Abstract*—Testing, tracking and tracing abilities have been identified as pivotal in helping countries to safely reopen activities after the first wave of the COVID-19 virus. Contact tracing apps give the unprecedented possibility to reconstruct graphs of daily contacts, so the question is who should be tested? As human contact networks are known to exhibit community structure, in this paper we show that the Kemeny constant of a graph can be used to identify and analyze bridges between communities in a graph. Our 'Kemeny indicator' is the change in Kemeny constant when a node or edge is removed from the graph. We show that testing individuals who are associated with large values of the Kemeny indicator can help in efficiently intercepting new virus outbreaks, when they are still in their early stage. Extensive simulations provide promising results in early identification and in blocking possible 'super-spreaders' links that transmit disease between different communities.**

***Index Terms*—Markov chains, Covid-19, Kemeny constant**

rate, and a high compliance of people in using this app, it could significantly help to stop the epidemic as shown in [10]. The benefits of efficient testing are clear. In addition to identifying infected individuals and tracing their contacts, fast diagnostic tests also allow estimation of the degree of spread of the virus in a region.

Accordingly, one proposal is to perform the tracing task by using Bluetooth connectivity to recognize when a prolonged proximity between two smartphones (and thus, their owners) occurs. For instance, the smartphone app that has been recommended by the Italian government stores a contact when a proximity of less or equal than two meters for at least 15 minutes is recorded.[1] Thus, the tracing task is currently designed as a *reactive* process, as it is a reaction to a positive

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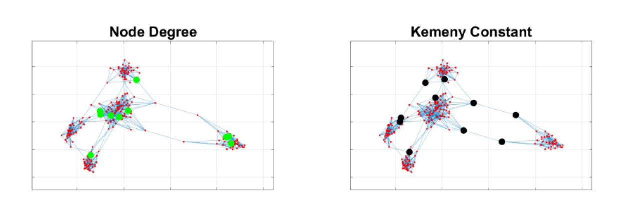
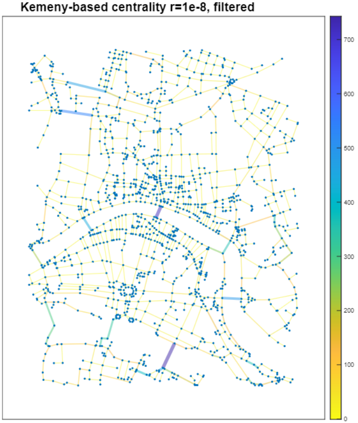
- Which vertex causes the biggest increase in Kemeny's constant after its removal?

Kemeny's constant and COVID-19

- **Kemeny-based testing for COVID-19.** Serife Yilmaz, Ekaterina Dudkina, Michelangelo Bin, Emanuele Crisostomi, Pietro Ferraro, Roderick Murray-Smith, Thomas Parisini, Lewi Stone, Robert Shorten. *PLoS ONE (2020), 15:11.*
- **A comparison of centrality measures and their role in controlling the spread in epidemic networks.** Ekaterina Dudkina, Michelangelo Bin, Jane Breen, Emanuele Crisostomi, Pietro Ferraro, Steve Kirkland, Jakub Maraček, Roderick Murray-Smith, Thomas Parisini, Lewi Stone, Serife Yilmaz, Robert Shorten. *International Journal of Control (2023), in press.*



- **An Edge Centrality Measure Based on the Kemeny Constant.** Diego Altafini, Dario A Bini, Valerio Cutini, Beatrice Meini, Federico Poloni. *SIAM Journal on Matrix Analysis and Applications* 44:2 (2023), 648–669.



Altafini, Bini, Cutini, Meini, Poloni

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- This gives you a centrality 'score' for each road in the network.

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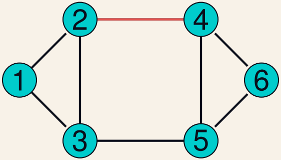
Example



$$A = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{bmatrix} \quad \tilde{A} = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{bmatrix} \quad E = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

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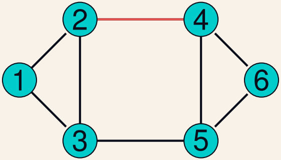

$$T = \begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 & 0 & \frac{1}{3} & 0 \\ 0 & \frac{1}{3} & 0 & 0 & \frac{1}{3} & \frac{1}{3} \\ 0 & 0 & \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} \\ 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 \end{bmatrix} \quad \tilde{T} = \begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 & 0 & \frac{1}{3} & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} \\ 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 \end{bmatrix} \quad E = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{6} & 0 & \frac{1}{6} & -\frac{1}{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{3} & 0 & 0 & \frac{1}{6} & \frac{1}{6} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

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$$V^T = \begin{bmatrix} s_i & 0 \\ 0 & s_j \end{bmatrix} U^T A - a_{i,j} \begin{bmatrix} 0 & (d_i - a_{i,j})^{-1} \\ (d_j - a_{i,j})^{-1} & 0 \end{bmatrix} U^T.$$

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- The main pursuit in this article, though, is finding efficient ways to do this for every edge in the network.

Altafini, Bini, Cutini, Meini, Poloni

Results (continued)

- Judgment call: when deleting an edge $\{i, j\}$, add the lost weight a_{ij} to a loop at i and a loop at j.

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Questions about weighted random walks from applications

- Can we find good expressions and bounds for the difference in Kemeny's constant after removing an edge, or removing a vertex?

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- Can we find good expressions and bounds for the difference in Kemeny's constant after removing an edge, or removing a vertex?
- Under what circumstances does the structure of the graph impose that $\mathcal{K}(G-e) < \mathcal{K}(G)$? (i.e. when is an edge a Braess edge?)

Outline

Kemeny's constant for nonbacktracking random walks

- Noga Alon, Itai Benjamini, Eyal Lubetzky, and Sasha Sodin. Non-backtracking random walks mix faster. *Communications in Contemporary Mathematics* 9, no. 04 (2007): 585-603.

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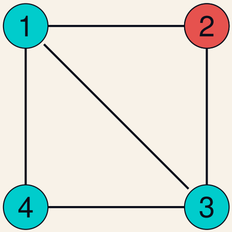
- Do non-backtracking random walks have smaller Kemeny's constant than simple random walks?

- **Kemeny's constant for nonbacktracking random walks.**
  Jane Breen, Nolan Faught, Cory Glover, Mark Kempton, Adam Knudson, Alice Oveson.
  Random Structures & Algorithms 63:2 (2023), 343–363.

Example of non-backtracking random walk



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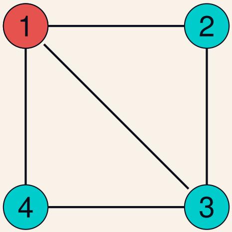

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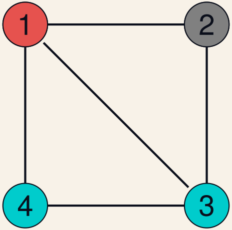

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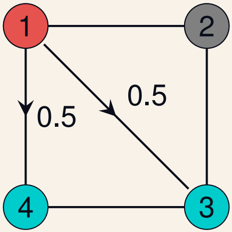

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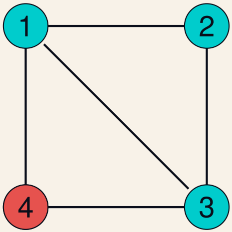

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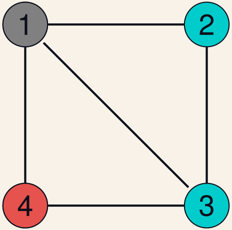

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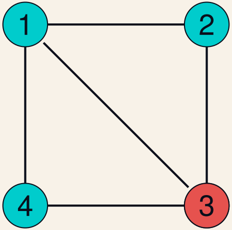

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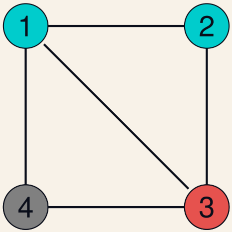
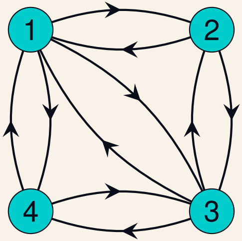


Random walks on the edge-space of a graph



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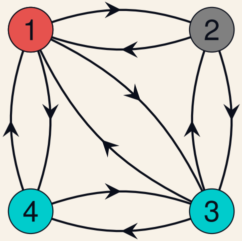

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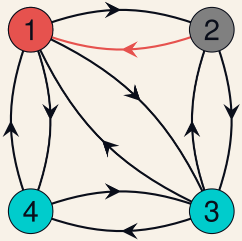

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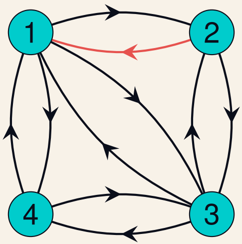

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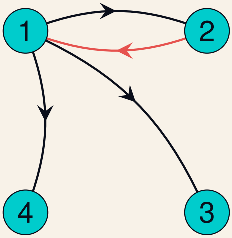

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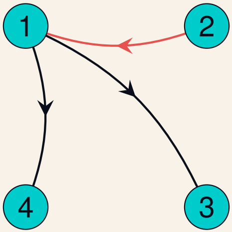

Definition of edge-space random walks

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The transition matrix P_e for the simple random walk on the edge space of G is a $2m \times 2m$ matrix defined entrywise as

$$p^{(e)}_{(i,j),(k,\ell)} = \begin{cases} \frac{1}{\deg(j)}, & \text{if } j = k; \\ 0, & \text{otherwise.} \end{cases}$$

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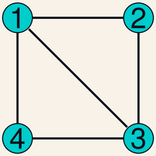
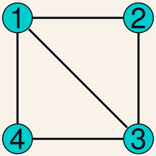
$$p^{(nb)}_{(i,j),(k,\ell)} = \begin{cases} \frac{1}{\deg(j)-1}, & \text{if } j = k \text{ AND } \ell \neq i; \\ 0, & \text{otherwise.} \end{cases}$$

Example



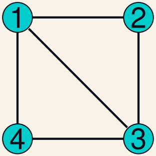
	(1,2)	(1,3)	(1,4)	(2,1)	(2,3)	(3,1)	(3,2)	(3,4)	(4,1)	(4,3)
(1,2)	0	0	0	$\frac{1}{2}$	$\frac{1}{2}$	0	0	0	0	0
(1,3)	0	0	0	0	0	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	0	0
(1,4)	0	0	0	0	0	0	0	0	$\frac{1}{2}$	$\frac{1}{2}$
(2,1)	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	0	0	0	0	0	0	0
(2,3)	0	0	0	0	0	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	0	0
(3,1)	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	0	0	0	0	0	0	0
(3,2)	0	0	0	$\frac{1}{2}$	$\frac{1}{2}$	0	0	0	0	0
(3,4)	0	0	0	0	0	0	0	0	$\frac{1}{2}$	$\frac{1}{2}$
(4,1)	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	0	0	0	0	0	0	0
(4,3)	0	0	0	0	0	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	0	0

Example



	(1,2)	(1,3)	(1,4)	(2,1)	(2,3)	(3,1)	(3,2)	(3,4)	(4,1)	(4,3)
(1,2)	0	0	0	$\frac{1}{2}$	$\frac{1}{2}$	0	0	0	0	0
(1,3)	0	0	0	0	0	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	0	0
(1,4)	0	0	0	0	0	0	0	0	$\frac{1}{2}$	$\frac{1}{2}$
(2,1)	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	0	0	0	0	0	0	0
(2,3)	0	0	0	0	0	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	0	0
(3,1)	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	0	0	0	0	0	0	0
(3,2)	0	0	0	$\frac{1}{2}$	$\frac{1}{2}$	0	0	0	0	0
(3,4)	0	0	0	0	0	0	0	0	$\frac{1}{2}$	$\frac{1}{2}$
(4,1)	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	0	0	0	0	0	0	0
(4,3)	0	0	0	0	0	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	0	0

Example



	(1,2)	(1,3)	(1,4)	(2,1)	(2,3)	(3,1)	(3,2)	(3,4)	(4,1)	(4,3)
(1,2)	0	0	0	0	$\frac{1}{2}$	0	0	0	0	0
(1,3)	0	0	0	0	0	0	$\frac{1}{3}$	$\frac{1}{3}$	0	0
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(2,1)	0	$\frac{1}{3}$	$\frac{1}{3}$	0	0	0	0	0	0	0
(2,3)	0	0	0	0	0	$\frac{1}{3}$	0	$\frac{1}{3}$	0	0
(3,1)	$\frac{1}{3}$	0	$\frac{1}{3}$	0	0	0	0	0	0	0
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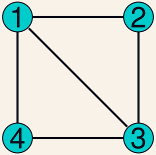

	(1,2)	(1,3)	(1,4)	(2,1)	(2,3)	(3,1)	(3,2)	(3,4)	(4,1)	(4,3)
(1,2)	0	0	0	0	1	0	0	0	0	0
(1,3)	0	0	0	0	0	0	$\frac{1}{2}$	$\frac{1}{2}$	0	0
(1,4)	0	0	0	0	0	0	0	0	0	1
(2,1)	0	$\frac{1}{2}$	$\frac{1}{2}$	0	0	0	0	0	0	0
(2,3)	0	0	0	0	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	0
(3,1)	$\frac{1}{2}$	0	$\frac{1}{2}$	0	0	0	0	0	0	0
(3,2)	0	0	0	1	0	0	0	0	0	0
(3,4)	0	0	0	0	0	0	0	0	1	0
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Some notation and notes

- We define $\mathcal{K}(P_e) =: \mathcal{K}_e(G)$, and $\mathcal{K}(P_{nb}) =: \mathcal{K}_{nb}(G)$.
- Non-backtracking Kemeny's constant cannot be defined for graphs with pendent vertices, or for cycles.

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- Non-backtracking Kemeny's constant cannot be defined for graphs with pendent vertices, or for cycles.
- We will only look at graphs with minimum degree two.
- To compare the behaviour of the simple random walk and the non-backtracking walk, it makes more sense to compare $\mathcal{K}_{nb}(G)$ with $\mathcal{K}_e(G)$, not $\mathcal{K}_v(G)$.

Kemeny's constant for P_e

Theorem

Let G be a connected graph with $|V(G)| = n$ *and* $|E(G)| = m$*. Then*

$$\mathcal{K}_e(G) = \mathcal{K}_v(G) + 2m - n.$$

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Proof: Uses a neat matrix factorization.

Matrix factorization

Definition

The *startpoint incidence* operator of G is the $n \times 2m$ matrix T with rows indexed by the vertices and columns indexed by the directed edges, such that

$$T(u,(v,w)) = \begin{cases} 1, & \text{if } u = v; \\ 0, & \text{otherwise.} \end{cases}$$

$$T = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cccccccccc} (1,2) & (1,3) & (1,4) & (2,1) & (2,3) & (3,1) & (3,2) & (3,4) & (4,1) & (4,3) \end{array} \\ \begin{pmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{pmatrix} \end{array}$$

Matrix factorization

Definition

The *endpoint incidence* operator of G is the $2m \times n$ matrix S with rows indexed by the directed edges and columns indexed by the vertices, such that

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$$S^\top = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cccccccccc} (1,2) & (1,3) & (1,4) & (2,1) & (2,3) & (3,1) & (3,2) & (3,4) & (4,1) & (4,3) \end{array} \\ \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \end{array}$$

Matrix factorization

- The edge-space adjacency matrix A_e can be factored

$$A_e = ST.$$

- The ordinary adjacency matrix A can be factored

$$A = TS.$$

- Let τ be the *edge reversal operator* - the $2m \times 2m$ matrix with rows and columns both indexed by E' that switches a directed edge with its opposite.
- Then $A_{nb} = ST - \tau$.
- $P_e = D_e^{-1}(ST)$
- $P_{nb} = (D_e - I)^{-1}(TS - \tau)$.

Kemeny's constant for P_e

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Let G be a connected graph with $|V(G)| = n$ and $|E(G)| = m$. Then

$$\mathcal{K}_e(G) = \mathcal{K}_v(G) + 2m - n.$$

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Proof:

- $P_e = D_e^{-1}ST = (D_e^{-1}S)T$
- The eigenvalues of $(D_e^{-1}S)T$ are those of $T(D_e^{-1}S)$, with enough extra zeros. ($2m - n$ of them)
- $T(D_e^{-1}S) = TSD^{-1} = AD^{-1}$
- $AD^{-1} \sim D^{-1}A = P.$

Therefore the eigenvalues of P_e are the eigenvalues of P with an additional $2m - n$ zero eigenvalues.

- Cory Glover and Mark Kempton. Some spectral properties of the non-backtracking matrix of a graph. *Linear Algebra and its Applications* 618 (2021): 37-57.

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Do nonbacktracking random walks on regular graphs mix faster, and how much faster can it be?

Edge-space random walks on regular graphs

Lemma

Let G be a connected d-regular graph of order n, where $d \geq 3$, with adjacency spectrum $d = \lambda_1 > \lambda_2 \geq \cdots \geq \lambda_n$. Then

$$\mathcal{K}_e(G) = n(d-1) + \sum_{i=2}^{n} \frac{d}{d-\lambda_i}.$$

Edge-space random walks on regular graphs

Theorem

Let G be a connected d-regular graph of order n, where $d \geq 3$. Then

$$\mathcal{K}_{nb}(G) = \frac{(d-2)\mathcal{K}_e(G)}{d} + 2n + \frac{1}{d-2} - \frac{n}{d}.$$

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Proof:

- The spectrum of the non-backtracking transition probability matrix of a d-regular graph is

$$\left\{ \left(\frac{1}{d-1}\right)^{m-n}, \left(\frac{-1}{d-1}\right)^{m-n}, \frac{\lambda_i \pm \sqrt{\lambda_i^2 - 4(d-1)}}{2(d-1)} \right\},$$

How does $\mathcal{K}_{nb}(G)$ compare?

Theorem

Let G be a d-regular graph, $d \geq 3$, which is not K_4, K_5, or $K_{3,3}$. Then

$$\mathcal{K}_e(G) > \mathcal{K}_{nb}(G).$$

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$$1 - \frac{2}{d} < \frac{\mathcal{K}_{nb}(G)}{\mathcal{K}_e(G)} < 1.$$

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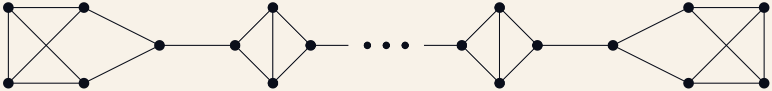

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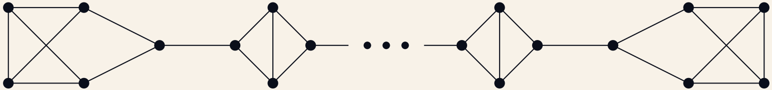

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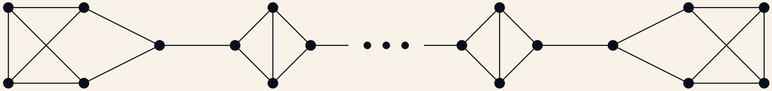

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From these expressions it is then readily seen that $\lim_{n\to\infty} \frac{\mathcal{K}_{nb}(G)}{\mathcal{K}_e(G)} = \frac{1}{3}$.

Improvement on the upper bound

Fix the degree d.

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Theorem

For a family $\{G_k\}$ of d-regular graphs with d fixed, $d \geq 3$, and $|V(G_k)| \to \infty$ as $k \to \infty$, we have

$$\lim_{k\to\infty} \frac{\mathcal{K}_{nb}(G_k)}{\mathcal{K}_e(G_k)} \leq 1 - \frac{1}{d^2}.$$

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Example

- Given a d-regular Ramanujan graph, the ratio of the non-backtracking Kemeny's constant to the edge Kemeny's constant will be close to the upper bound.
- Recall that a graph is a *Ramanujan graph* if its adjacency eigenvalues have $\lambda_2, |\lambda_n| \leq 2\sqrt{d-1}$.

What next?

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- How does $\mathcal{K}_{nb}(G)$ compare with $\mathcal{K}_{e}(G)$?
- Comparing $\mathcal{K}_{nb}(G)$ with $\mathcal{K}_{nb}(H)$ is weird if G and H have a different number of edges.

Cycle barbell graph

These graphs appear to maximise both $\mathcal{K}_{nb}(G)$ and $\mathcal{K}_e(G)$ in an exhaustive search over all graphs of order n with $n+1$ edges, up to $n = 20$.

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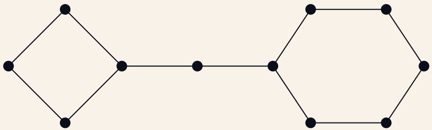

Figure: The graph CB(3,4,6).

Definition

The *cycle barbell* $G = CB(k, a, b) = C_a \oplus P_k \oplus C_b$ is the 1-sum of an a-cycle, a path on k vertices, and a b-cycle. Note $|V(G)| = a + b + k - 2$ and $|E(G)| = a + b + k - 1$.

Expressions for $\mathcal{K}_{nb}$ and $\mathcal{K}_e$ for the cycle barbell

Expressions for $\mathcal{K}_{nb}$ and $\mathcal{K}_e$ for the cycle barbell

For a cycle barbell $G = CB(k, a, b)$, the edge Kemeny's constant is given by

$$\mathcal{K}_e(G) = \frac{1}{a+b+k-1} \cdot \left[\frac{(a+1)(a-1)}{6}(a+2(b+k-1)) + \frac{(b+1)(b-1)}{6}(b+2(a+k-1)) + (a+b)(k-1)^2 + \frac{(k-1)(2k^2-4k+3)}{6} + 2ab(k-1)\right] + a+b+k.$$

and the non-backtracking Kemeny's constant by

$$\mathcal{K}_{nb}(G) = \frac{2(a+b+k-1)^2 + 3(a+b)^2 + 2ab + 4(a+b)(k-1) - (a+b+k-1)}{2(a+b+k-1)}.$$

Extremal graphs

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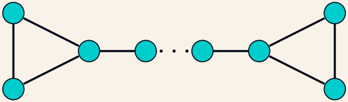
- The graph maximizing $\mathcal{K}_e(G)$ is $CB(n-4,3,3)$:



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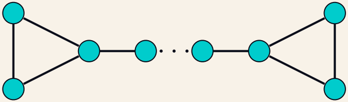
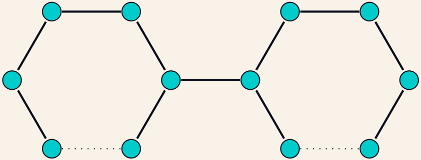


- The graph maximizing $\mathcal{K}_{nb}(G)$ is $CB(2,n/2,n/2)$:



Questions

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For all graphs of sufficiently large order, $\mathcal{K}_{nb}(G) < \mathcal{K}_e(G)$.

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Conjecture

For all graphs of sufficiently large order, $\mathcal{K}_{nb}(G) < \mathcal{K}_e(G)$.

n	# graphs with $\mathcal{K}_{nb}(G) \geq \mathcal{K}_e(G)$
4	2
5	10
6	18
7	7
8	3
9	0
10	0

Questions

- Can we develop more techniques to calculate eigenvalues of P_{nb} or $\mathcal{K}_{nb}(G)$?
- For what graphs are the orders of magnitude of $\mathcal{K}_{nb}(G)$ and $\mathcal{K}_{e}(G)$ the same, and for what graphs they are different? By how much they can differ?
- What is the largest order of magnitude of $\mathcal{K}_{nb}(G)$? All examples here are $O(n^2)$.
- What graph properties lead to large or small simple walk Kemeny's constant versus a large non-backtracking walk Kemeny's constant?
- What about weighted graphs?
- What about applications?

Outline

Thank you!

Go raibh míle maith agaibh!