An edge centrality measure based on the Kemeny constant

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The Kemeny constant

$A \in \mathbb{R}^{n \times n}$ adjacency matrix of an undirected, connected, weighted network; $P = D^{-1}A \in \mathbb{R}^{n \times n}_{\geq 0}$ transition matrix of the random walk on it (discrete-time Markov chain). $\text{eig}(P) = \{\lambda_1 = 1, \lambda_2, \ldots, \lambda_n\}$.

**Kemeny constant** [Kemeny,Snell ’60]

$$K(P) = \sum_{i=2}^{n} \frac{1}{1 - \lambda_i}.$$

Probabilistic definition: the mean first passage time from a fixed state $i$ to a state $j$ drawn according the invariant distribution.

Car-based interpretation: Car 1 runs for a long time on a road network and then breaks down. How many steps does car 2 take (on average) to get to the same spot as $A$ with a random walk?

$K(P)$ small $\iff$ $A$ well-connected as a network.
Centralities

We study a centrality measure for roads (edges) based on the Kemeny constant: a road is important if its removal causes a large increase in $K(P)$:

$$c(e) = K(\hat{P}) - K(P).$$

Many other centrality measures are available in literature. [Estrada, book '13]

Main inspirations for us:

- [Estrada, D.Higham, Hatano '09]: communicability betweenness centrality: variation in communicability centrality caused by the removal of an edge.

- [Crisostomi, Kirkland, Shorten '11]: Kemeny constant variation in a Markov chain model of road circulation. Main difference: we do not want to rely on external traffic data, just on the map.
Collaboration with our civil engineering department; research question: is industry location driven by well-connected outskirts?

Large scale maps, e.g., continental Tuscany: 1.56M edges; no traffic data.
Weak ties

**Goal:** highlight weak ties [Granovetter, '73], i.e., crucial edges that separate (strongly-connected) sections of the map. **Example:** bridges.
Challenges

- Deal with negative centralities;
- Deal with cut-edges;
- Make it fast enough for 1.5M road elements.
Negative centralities

Sometimes, the Kemeny constant decreases when removing an edge!

Example $K(\text{left}) \approx 2.54$, $K(\text{right}) = 2.5$.

Not ideal: intuition of “connectedness” says more roads are always better.

This phenomenon is known as Braess paradox [Braess ’68, Kirkland, Zeng ’16].
Analysis

Kemeny constant

\[ K(P) = \sum_{i=2}^{n} \frac{1}{1 - \lambda_i}. \]

\[ \{\lambda_1 = 1, \ldots, \lambda_n\} = \text{eig}(D^{-1}A) = \text{eig}(D^{-1/2}AD^{-1/2}) \]

:= \text{symmetrized adjacency matrix}

The edge removal changes \( W \) in a non-trivial way.

\[
\begin{bmatrix}
0 & 1/2 & 6^{-1/2} & 0 \\
1/2 & 0 & 6^{-1/2} & 1 \\
6^{-1/2} & 6^{-1/2} & 0 & 3^{-1/2} \\
0 & 0 & 3^{-1/2} & 0
\end{bmatrix}
\rightarrow
\begin{bmatrix}
0 & 0 & 3^{-1/2} & 0 \\
0 & 0 & 3^{-1/2} & 0 \\
3^{-1/2} & 3^{-1/2} & 0 & 3^{-1/2} \\
0 & 0 & 3^{-1/2} & 0
\end{bmatrix}
\]
Solution

Idea Replace the removed edge with two loop edges, \[
\begin{bmatrix}
0 & 1 \\
1 & 0
\end{bmatrix}
\rightarrow
\begin{bmatrix}
1 & 0 \\
0 & 1
\end{bmatrix}
\]

This changes the model in an easier-to-predict way:

\[
\begin{bmatrix}
0 & 1/2 & 6^{-1/2} & 0 \\
1/2 & 0 & 6^{-1/2} & 1 \\
6^{-1/2} & 6^{-1/2} & 0 & 3^{-1/2} \\
0 & 0 & 3^{-1/2} & 0
\end{bmatrix}
\rightarrow
\begin{bmatrix}
1/2 & 0 & 6^{-1/2} & 0 \\
0 & 1/2 & 6^{-1/2} & 1 \\
6^{-1/2} & 6^{-1/2} & 0 & 3^{-1/2} \\
0 & 0 & 3^{-1/2} & 0
\end{bmatrix}
\]

\[W \mapsto \hat{W} := W + \frac{1}{\sqrt{d_id_j}}(e_i - e_j)(e_i - e_j)^T.\]

Theorem

With this definition, \(c(e) = k(\hat{P}) - k(P) \geq 0\) after each edge removal.

Proof Standard eigenvalue inequalities for symmetric matrices:

\[
\hat{W} \succeq W \implies \hat{\lambda}_i \geq \lambda_i \implies \sum \frac{1}{1-\hat{\lambda}_i} \geq \frac{1}{1-\lambda_i}.
\]
Cut-edges

(Color scheme: blue edge = higher = important.)

Problem If the removed edge is a cut-edge, $\hat{G}$ is disconnected, $\hat{\lambda}_2 = 1$, and $K(\hat{P}) = +\infty$.

On a road network, cut-edges are often unimportant dead ends, but sometimes they are crucial for connectivity and cannot be ignored/dismissed.
Solution

First idea Change the definition to

\[ K_r(P) = \sum_{i=2}^{n} \frac{1}{1 + r - \lambda_i} . \]

for a small regularization factor \( r > 0 \), e.g., \( r = 10^{-6} \).

\( \leftrightarrow \) replacing the Laplacian \( L = D - A \) with \( (1 + r)D - A \).

Problem Centrality scores \( c_r(e) = K_r(\hat{P}) - K_r(P) \) of cut-edges become

\( \approx \frac{1}{r} \), artificially high.

Solution

**Filtered Kemeny-based centrality**

\[ \tilde{c}_r(e) = \begin{cases} \frac{1}{r} - c_r(e) & \text{e is a cut-edge,} \\ c_r(e) & \text{otherwise.} \end{cases} \]
Unfiltered vs. filtered

Unfiltered

Filtered

Unfiltered

Filtered

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Sign reversal

Why \( \frac{1}{r} - c_r(e) \) and not the more natural \( c_r(e) - \frac{1}{r} \)?

**Theorem**

If \( e \) is a cut-edge, \( \frac{1}{r} - c_r(e) \geq 0 \).

**Proof** Interlacing inequalities: since \( \hat{W} - W \succeq 0 \) is rank-1 positive semidefinite,

\[
\frac{1}{r} = \hat{\lambda}_2 \geq \lambda_2 \geq \hat{\lambda}_3 \geq \lambda_3 \geq \cdots \geq \hat{\lambda}_n \geq \lambda_n.
\]

Hence

\[
\frac{1}{r} - c_r(e) = \underbrace{\frac{1}{1+r-\lambda_2} - \frac{1}{1+r-\hat{\lambda}_3}}_{\geq 0} + \underbrace{\frac{1}{1+r-\lambda_3} - \frac{1}{1+r-\hat{\lambda}_4}}_{\geq 0} + \cdots + \underbrace{\frac{1}{1+r-\lambda_n}}_{\geq 0}.
\]
Open problem

**Filtered Kemeny-based centrality**

\[
\tilde{c}_r(e) = \begin{cases} 
\frac{1}{r} - c_r(e) & \text{e is a cut-edge}, \\
c_r(e) & \text{otherwise}.
\end{cases}
\]

**Empirical observation**

With this definition, centrality scores of cut-edges have centrality scores comparable with non-cut-edges, and they are sorted correctly in order of importance.

We still do not have a good explanation for this observation!
Getting it done

**Problem** How to reduce the $\mathcal{O}(n^4)$ cost and make it fast enough for large graphs?

**Theorem** [Kemeny '81, Kirkland '10, Wang-Dubbeldam-Van Mieghem '17]

Let $w \in \mathbb{R}^n$ be any vector such that $w^T \mathbf{1} = 1$. Then,

$$K(P) = \text{Trace}(S^{-1}) - 1, \quad S = I - P + \mathbf{1}w^T.$$ 

Since $\hat{P} - P$ and $\hat{S} - S$ is a rank-1 update, we can use the

**Sherman–Morrison formula**

$$(S + uv^T)^{-1} - S^{-1} = \frac{-1}{1 + v^T S^{-1}u} S^{-1}uv^T S^{-1}$$

$$c(e) = K(\hat{P}) - K(P) = \text{Trace} \left( \frac{-1}{1 + v^T S^{-1}u} S^{-1}uv^T S^{-1} \right) = \frac{-u^T S^{-2}v}{1 + v^T S^{-1}u}.$$
Some more routine manipulations:

- Introduce regularization parameter $r$;
- Use again Sherman–Morrison to invert $S_r = (1 + r)I - P + 1w^T$;
- Express it in terms of “regularized Laplacian” $L_r = (1 + r)D - A$;
- Choose $w$ to make the problem symmetric.

**Final formula**

\[
 c(\{i,j\}) = \frac{A_{ij}d^T(x^2)}{1 - A_{ij}(x_i - x_j)}, \quad y = L_r^{-1}(e_i - e_j), \quad x = y - \frac{d^T y}{\gamma} z.
\]

where $d = \text{diag}(D)$, $z = L_r^{-1}d$, $\gamma = d^T z + d^T 1$. 

Practical cost

Final formula

\[ c(\{i,j\}) = \frac{A_{ij}d^T(x^2)}{1 - A_{ij}(x_i - x_j)}, \quad y = L_r^{-1}(e_i - e_j), \quad x = y - \frac{d^Ty}{\gamma}z. \]

where \(d = \text{diag}(D), \quad z = L_r^{-1}d, \quad \gamma = d^Tz + d^T1.\)

1. Precompute Cholesky factorization of \(L_r = (1 + r)D - A\), and \(d, z, \gamma\).

2. To compute \(c(e)\) for each edge (possibly in parallel), solve one linear system with \(L_r\) (using the precomputed factorization) and \(O(n)\) extra operations.

On road networks, often \(n \approx m \approx \text{nnz}(\text{chol}(L_r))\), so all these operations are somewhat cheap — but the cost is still \(O(n^2)\) to compute all centralities.
Experiment: a large-scale network

Mainland Tuscany map: $n = 1.22M, m = 1.56M, \text{nnz}(\text{chol}(L_r)) = 3.36M$.

1. Precomputation and $\text{chol}$: $< 1s$.
2. $\text{parfor}$ centrality computation: 18 hours.

On a machine with 12 3.4GHz Xeon physical cores.
Experiment: the bridges of Pisa

Kemeny-based centrality r=1e-8, filtered

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Conclusions

- The Kemeny constant variation works well to highlight bottlenecks and weak ties.
- Connectivity/positivity issues can be solved.
- Computationally feasible even in large scale.
- Interesting results for our collaborators in civ-eng.


Thanks for your attention!