Resistance Distance

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• Conventional graphical distance between two sites of a graph
  – the minimal sum of edge weights along a path between the two sites
• Not work for some circumstances

Example: chemical bonds

- Fails to indicate this chemical distance is shorter!

• A distance function with the allowance of a mutual influence of multiple pathways is needed.
• A novel distance function based on electrical network theory
  – A fixed resistor is imagined on each edge

\[ D_{ab} = 2, \text{for } G_1 \]
\[ D_{ab} = 2, \text{for } G_2 \]
\[ D_{ab} = 2, \text{for } G_3 \]

The proposed distance function has “multiple-route distance diminishment” feature.
Overview

• Generally, for a battery delivering a current $I$ the voltage will be

$$v_{ab} = I \Omega_{ab}.$$  \hfill (1.2)

• How to compute effective resistance matrix for a finite connected graph?

$G_1$

$$\Omega = 1$$

$G_2$

$$\Omega = 1 / \left(1 + \frac{1}{3}\right) = \frac{3}{4}$$

$G_3$

$$\Omega = 1 / \left(1 + \frac{1}{2}\right) = \frac{2}{3}$$
• Effective resistance – how to compute?
• Resistance is a distance – why?
• Resistance sum rules
• Comparison
• Analogue
• Conclusion
Background ideas:

1. **G-flow**

A G-flow from vertex a to b of a graph G is defined to be a function $i$ on pairs of adjacent sites such that

$$i_{xy} = -i_{yx}$$

and

$$\sum_y i_{xy} = I\delta(x, a) - I\delta(x, b), \quad x \in V(G),$$

Sums over $y \in V(G)$ adjacent to vertex x

Kronecker delta

$$i_{xy}r_{xy} = u_x - u_y, \quad x, y \in E(G),
\quad r_{xy} \equiv r_e \text{ if } e = \{x, y\}$$

Ohm’s law

$$\sum_{x-y}^C i_{xy}r_{xy} = 0 \quad \text{all } C,$$

Kirchhoff’s voltage law

Kirchhoff’s current law
• **Background ideas:**

2. **Admittance (Adjacency) matrix, A**

\[
A_{xy} = (x \mid A \mid y) = \begin{cases} 
1/ r_{xy} & x \sim y \\
0 & \text{otherwise} 
\end{cases} \quad x, y \in V(G). 
\]  

(2.5)

\(|x)\) is an orthonormal basis whose elements are in one-to-one correspondence with the vertices of \(G:\)

\[
\begin{align*}
|x_1) &= \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, & |x_2) &= \begin{bmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{bmatrix}, & \ldots, & |x_n) &= \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{bmatrix}
\end{align*}
\]

3. **Degree matrix, delta**

\[
\Delta_{xy} = (x \mid \Delta \mid y) = \delta(x, y) \sum_{z} 1/ r_{xz},
\]  

(2.6)

Sums over the \(z \in V(G)\) that are adjacent to vertex \(x\)

• **Laplacian matrix, \(\Delta - A\), plays a crucial role.**
• **LEMMA 0**

**LEMMA 0**

The matrix $\Delta - A$ has real eigenvalues, the minimum one of which is zero. If $G$ is connected, this eigenvalue is nondegenerate and the associated eigenvector is (up to a scalar factor)

$$|\psi\rangle \equiv \sum_{x} |x\rangle.$$  

e.g. $|\psi\rangle = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}$

• **Consequences:**

$$(\Delta - A) |\psi\rangle = 0,$$

$\Delta - A$ has no inverse.

• $\Delta - A$ does have an inverse within the subspace orthogonal to $|\psi\rangle$.  

(2.7)
• Pseudo-inverse (generalized inverse)

denoted by $Q/(\Delta - A)$, where $Q$

is the (Hermitean and idempotent) projection

$$Q = 1 - \frac{1}{(\phi | \phi)} |\phi)(\phi|.$$  \hspace{1cm} (2.8)

This “resolvent” matrix $\{Q/(\Delta - A)\}$ satisfies

$$[Q/(\Delta - A)](\Delta - A) = (\Delta - A)[Q/(\Delta - A)] = Q,$$

$$[Q/(\Delta - A)]Q = Q[Q/(\Delta - A)] = [Q/(\Delta - A)]$$  \hspace{1cm} (2.9)

and is called the generalized inverse of $\Delta - A$.  

• Effective resistance $\Omega_{ab}$

**LEMMA A**

A physical $G$-flow from vertex $a$ to $b$ of a connected graph $G$ exists, is unique, and is given by

$$i_{xy} = \frac{I}{r_{xy}} (x - y | Q / (\Delta - A) | a - b),$$

where $|a - b| \equiv |a| - |b|).

**THEOREM A**

For a physical $G$-flow from $a$ to $b$,

$$\Omega_{ab} = (a - b | Q / (\Delta - A) | a - b).$$

The result of this theorem may be cast as a more conventional matrix equality if we introduce the diagonal matrix $\nabla$ with elements

$$\nabla_{ab} \equiv \delta_{ab} (a | Q / (\Delta - A) | b).$$

Then a simple rearrangement of the result of the theorem gives
COROLLARY A

A graph $G$ has a resistance matrix

$$\Omega = \nabla |\phi\rangle (\phi \rangle + |\phi\rangle (\phi \rangle |\nabla - 2(\Omega/(\Delta - A))\rangle.\)

As a consequence, all effective resistances are obtained via a matrix inversion. If desired, the generalized inverse $\Omega/(\Delta - A)$ may be computed in terms of an ordinary inverse: by finding the ordinary inverse to $\Delta - A + |\phi\rangle (\phi \rangle$, then subtracting $|\phi\rangle (\phi \rangle |(\phi \rangle |^2$.

For example, for the ("square") graph $G_2$ of fig. 1, we have (for $r = 1$ ohm)

$$\Delta - A = \begin{bmatrix} 2 & -1 & 0 & -1 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ -1 & 0 & -1 & 2 \end{bmatrix},$$

$$\Omega = \begin{bmatrix} 2 & -1 & 0 & -1 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ -1 & 0 & -1 & 2 \end{bmatrix},$$

$$\begin{bmatrix} 5 & -1 & -3 & -1 \\ -1 & 5 & -1 & -3 \\ -3 & -1 & 5 & -1 \\ -1 & -3 & -1 & 5 \end{bmatrix}.$$
• Distance function
  – A mapping $\rho$ from Cartesian product $V(G) \times V(G)$ to the real numbers such that the following axioms are satisfied:

  $$\rho(b, a) \geq 0,$$
  $$\rho(a, b) = 0 \iff a = b,$$
  $$\rho(a, b) = \rho(b, a),$$
  $$\rho(a, x) + \rho(x, b) \geq \rho(a, b), \quad (4.1)$$

  Example:

  $$\Omega = \begin{bmatrix}
  0 & 3/4 & 1 & 3/4 \\
  3/4 & 0 & 3/4 & 1 \\
  1 & 3/4 & 0 & 3/4 \\
  3/4 & 1 & 3/4 & 0
  \end{bmatrix}$$
THEOREM B

The resistance function on a graph is a distance function.

To begin the proof, we note that corollary A and the properties of the operator \( \Delta - A \) as appear in lemma A yield the result that \( \Omega_{ab} \) is symmetric and non-negative with \( \Omega_{ab} = 0 \) iff \( a = b \). The focus of the proof then is the triangle inequality (on the last line of (4.1)). Let \( i \) and \( i' \) be \( G \)-flows from \( a \) to \( x \) and from \( x \) to \( b \) associated with potentials \( u \) and \( u' \), respectively. Then it is easily verified that

\[
j = i + i'
\]

(4.2)
is an \( I \)-flow from \( a \) to \( b \) with associated potential

\[
w = u + u'.
\]

(4.3)
Now,

\[
I\Omega_{ab} = w_a - w_b = (u_a - u_b) + (u'_a - u'_b).
\]

(4.4)
However, the extreme values of the potential \( u_y \) must be at \( y = a \) and \( x \), since otherwise some other more extreme site would be either a source or a sink. Likewise, \( u'_y \) is extreme at \( y = x \) and \( b \). Thence,

\[
I\Omega_{ab} \leq \{u_a - u_x\} + \{u'_x - u'_b\} = I\Omega_{ax} + I\Omega_{xb}
\]

(4.5)
and the theorem follows.
• **Resistance sum rules**

**Theorem C**

If $G$ is a connected graph and $Z$ is an arbitrary symmetric matrix, then

$$
\sum_{a,b} (b|\Delta - A)Z(\Delta - A)|a)\Omega_{ab} = -2\text{tr}(\Delta - A)Z, \quad \Omega_{ab} = (a - b|Q/(\Delta - A)|a - b).
$$

To prove this, abbreviate $(\Delta - A)Z(\Delta - A)$ to $X$ and use theorem A to obtain

$$
\sum_{a,b} (b|X|a)\Omega_{ab} = 2\sum_{a,b} (b|X|a)\{(a|Q/(\Delta - A)|a) - (a|Q/(\Delta - A)|b)\}. \quad (5.1)
$$

The right-hand side of this equation yields two double-sum terms, the first of which entails a factor

$$
\sum_{b} (b|X|a) = (\phi|(\Delta - A)Z(\Delta - A)|a) = 0, \quad (5.2)
$$

where we have recalled the eigenvector $|\phi\rangle$ of lemma 0. Thence,

$$
\sum_{a,b} (b|X|a)\Omega_{ab} = -2\sum_{a,b} (b|(\Delta - A)Z(\Delta - A)|a)(a|\frac{Q}{\Delta - A}|b)
$$

$$
= -2\text{tr}(\Delta - A)Z(\Delta - A)\frac{Q}{\Delta - A}
$$

$$
= -2\text{tr}(\Delta - A)Z, \quad (5.3)
$$

• **This sum rule avoids the inverse of $\Delta - A$.**
COROLLARY C1

For a connected graph,

\[ \sum_{a,b} (a | A | b) \Omega_{ab} = 2(|V(G)| - 1). \]

A whole sequence of rules is obtained by taking \( Z \) as \((\Delta - A)^n\);

\[ Z = \mathbb{Q} / (\Delta - A) \]

COROLLARY C2

For a connected graph

\[ \sum_{a,b} (a | (\Delta - A)^n | b) \Omega_{ab} = -2 \text{tr}(\Delta - A)^n, \]

with \( n \) a non-negative integer.

For more highly symmetric graphs, these two corollaries yield nearer-neighbor effective resistances:

COROLLARY C3

For \( e \in E(G) \) of an edge-transitive graph

\[ \Omega_e = \frac{|V(G)| - 1}{|E(G)|} r, \]

where \( r \) is the internal resistance common to all edges.

Edge (vertex) transitive graph: every edge (vertex) has the same local environment, so that no edge (vertex) can be distinguished from any other based on the vertices and edges surrounding it.
COROLLARY C4

For a vertex- and edge-transitive graph such that all paths of length 2 are equivalent, the effective resistance between two next-nearest neighbor nnn sites is

\[ \Omega_{nnn} = \frac{2}{d-1} \left( 1 - \frac{2}{|V(G)|} \right) r, \]

where \( d \) is the common vertex degree.

![Symmetric graph](image)

Fig. 4. The cube graph, upon each edge of which one may imagine a resistor \( r \).

As an example, one might consider the cubic graph (of fig. 4) with equal resistors \( r \) on each edge. Then,

\[
\Omega_e = \frac{8-1}{12} r = \frac{7r}{12},
\]

\[
\Omega_{nnn} = \frac{2}{2} \left( 1 - \frac{2}{8} \right) r = \frac{3r}{4}.
\]

(5.4)

Returning to corollary C2 with \( n = 2 \), after some manipulation one can even obtain the remaining resistance of \( 5r/6 \).
Comparison between conventional (CD) and resistance distances (RD)

**Lemma D**

The resistance $\Omega_{ab}$ is a nondecreasing function of the edge resistances. This function is constant only for those edges not lying on any path between $a$ and $b$.

The conventional type of *graphical distance* between vertices $a$ and $b$ of $G$ is [2]

$$D_{ab} = \min_{\pi} \sum_{e \in \pi} \frac{1}{r_e},$$  \hspace{1cm} (6.2)

whence the minimum is taken over all paths $\pi$ from $a$ to $b$, and the sum is over all edges of $\pi$. We have:

**Theorem D**

For all distinct pairs of vertices $a, b$ in $G$, $D_{ab} \geq \Omega_{ab}$, with equality iff there is but a single path between $a$ and $b$.

**Corollary D**

The conventional and resistance distances are the same between every pair of vertices of a connected graph iff the graph is a tree.
Analogue theorems:

**Lemma E**

Let \( x \) be a cut-point of a commercial graph, and let \( a \) and \( b \) be points occurring in different components which arise upon deletion of \( x \). Then,

\[
\Omega_{ab} = \Omega_{ax} + \Omega_{xb}.
\]

The proof may be briefly indicated if we consider the assumptive circumstances as indicated in Fig. 5: If vertex \( a \) is the source of current \( I \), then since sink \( b \) is not in the part \( G_a \), all the current from \( a \) must pass through \( x \), so that in the \( G_a \) portion, \( x \) acts as a sink with

\[
v_{ax} = I \Omega_{ax}.
\]  \(\text{(7.1)}\)

Further, since the net current into \( x \) is 0, the current leaving \( x \) into part \( G_b \) must be \( I \), whence one is led to

\[
v_{xb} = I \Omega_{xb}.
\]  \(\text{(7.2)}\)

Addition of these two potential differences gives

\[
v_{ab} = v_{ax} + v_{xb} = I(\Omega_{ax} + \Omega_{xb}).
\]  \(\text{(7.3)}\)

whereupon one obtains the theorem.
• Analogue theorems:

THEOREM E

If $G$ is a connected graph with blocks $G_\alpha$, then

$$\text{cof } \Omega(G) = \prod_\alpha \text{cof } \Omega(G_\alpha),$$

$$\det \Omega(G) = \sum \det \Omega(G_\alpha) \prod_\beta \text{cof } \Omega(G_\beta).$$

The proof exactly follows that for the conventional graphical distance matrix $D(G)$ [10]. The crucial property required (beyond that of being a distance function) is that of lemma E.

Cof: Cofactors of a matrix

$$\text{Cof } A_{ij} \equiv (-1)^{i+j} M_{ij}$$
• Analogue definitions

- **Wiener index**: the sum of the lengths of the shortest paths between all pairs of vertices, which is correlated with the boiling points, density, surface tension, etc.

\[
W = \sum_{a<b} D_{ab},
\]

(8.2)

but for trees \( D_{ab} = \Omega_{ab} \) (as noted in corollary D), so that an extension to other connected graphs could be

\[
W' = \sum_{a<b} \Omega_{ab},
\]

(8.3)

**Theorem F**

For a connected graph with \( N \) vertices,

\[
W' = N \, \text{tr}(Q/(\Delta - A)).
\]

It is a simple matter of algebra to obtain

\[
W' = \frac{1}{2} \sum_{a,b} (a-b|Q/(\Delta - A)|a-b) = N \, \text{tr}(Q/(\Delta - A)) - 2(\phi|Q/(\Delta - A)|\phi).
\]

(8.4)

However, since \( Q/(\Delta - A) \) is null on the \( |\phi\)\)-space one immediately obtains the theorem.
• Conclusion
  – A novel distance function, resistance distance, based on circuit theory has been identified
  – Some first mathematical features of resistance distance has been developed
  – The resistance distance should have chemical relevance because of its “multiple-route distance diminishment” features
Q&A

• Thanks!