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Resistance Distance

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Overview

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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.**

Overview

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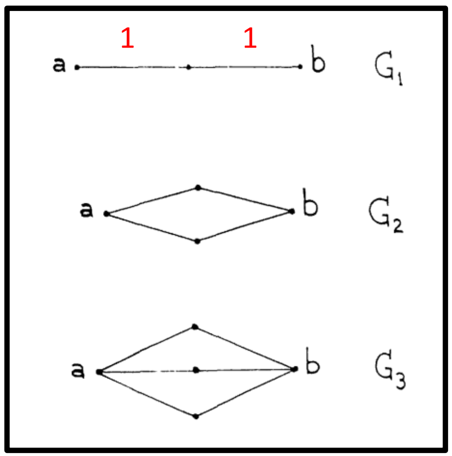
- A novel distance function based on electrical network theory
  - A fixed resistor is imagined on each edge

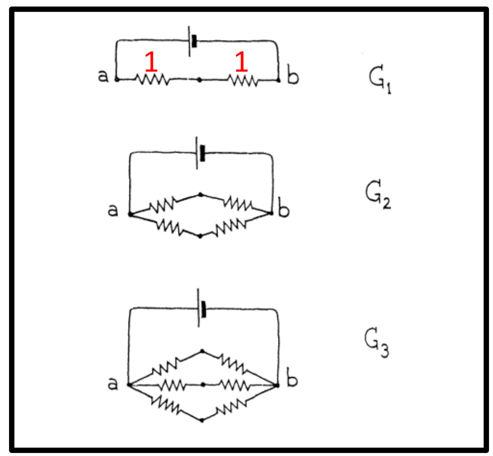


Conventional

$D_{ab} = 2, for\ G_1$

$D_{ab} = 2, for\ G_2$

$D_{ab} = 2, for\ G_3$



Proposed

$\Omega_{ab} = 1 + 1 = 2$ for G_1,

$\Omega_{ab} = 1/(\frac{1}{2} + \frac{1}{2}) = 1$ for G_2,

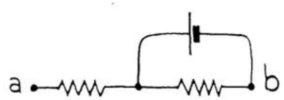
$\Omega_{ab} = 1/(\frac{1}{2} + \frac{1}{2} + \frac{1}{2}) = \frac{2}{3}$ for G_3.

- **The proposed distance function has "multiple-route distance diminishment" feature.**

Overview

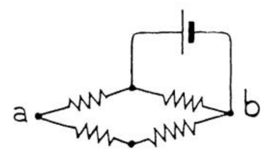
- Generally, for a battery delivering a current I the voltage will be

$$v_{ab} = I\,\Omega_{ab}. \tag{1.2}$$



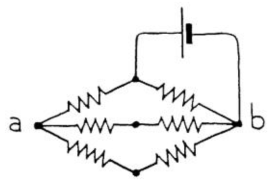
G_1

$$\Omega = 1$$



G_2

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



G_3

$$\Omega = 1/\left(1 + \frac{1}{2}\right) = \frac{2}{3}$$

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

Outline

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- Effective resistance – how to compute?
- Resistance is a distance – why?
- Resistance sum rules
- Comparison
- Analogue
- Conclusion

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- # 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

$$i_{xy} = -i_{yx} \tag{2.1}$$

and

$$\sum_{y}^{\sim x} i_{xy} = I\delta(x,a) - I\delta(x,b) \quad x \in V(G), \tag{2.2}$$

→ Kirchhoff's current law

Sums over y ∈ V(G) adjacent to vertex x

Kronecker delta

$$i_{xy} r_{xy} = v_x - v_y \quad x, y \in E(G), \quad r_{xy} \equiv r_e \text{ if } e = \{x, y\} \tag{2.3}$$

→ Ohm's law

$$\sum_{x \sim y}^{C} i_{xy} r_{xy} = 0 \quad \text{all } C, \tag{2.4}$$

→ Kirchhoff's voltage law

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- Background ideas:

2. Admittance (Adjacency) matrix, A

$$A_{xy} = (x|A|y) = \begin{Bmatrix} 1/r_{xy} & x \sim y \\ 0 & \text{otherwise} \end{Bmatrix} \quad x, y \in V(G). \tag{2.5}$$

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

$$|x_1) = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, |x_2) = \begin{bmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{bmatrix}, \cdots, |x_n) = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{bmatrix}$$

3. Degree matrix, delta

$$\Delta_{xy} = (x|\Delta|y) = \delta(x,y) \sum_{z}^{\sim x} 1/r_{xz}, \tag{2.6}$$

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

- **Laplacian matrix, Δ - A, plays a crucial role.**

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- 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)

$$|\phi) \equiv \sum_x |x). \qquad \text{e.g. } |\emptyset) = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}$$

- **Consequences:**

$$(\Delta - A)|\phi) = 0, \tag{2.7}$$

$\Delta - A$ has no inverse.

- **Δ - A does have an inverse within the subspace orthogonal to $|\emptyset)$.**

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- Pseudo-inverse (generalized inverse)

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

is the (Hermitean and idempotent) *projection*

$$Q = \mathbf{1} - \frac{1}{(\phi\,|\,\phi)}\,|\phi)\,(\phi\,| . \tag{2.8}$$

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

$$\begin{aligned} \{Q/(\Delta - A)\}(\Delta - A) &= (\Delta - A)\{Q/(\Delta - A)\} = Q, \\ \{Q/(\Delta - A)\}\,Q &= Q\{Q/(\Delta - A)\} = \{Q/(\Delta - A)\} \end{aligned} \tag{2.9}$$

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

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- Effective resistance Ω_{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 ∇ with elements

$$\nabla_{ab} \equiv \delta_{ab} (a | Q / (\Delta - A) | b). \tag{3.6}$$

Then a simple rearrangement of the result of the theorem gives

COROLLARY A

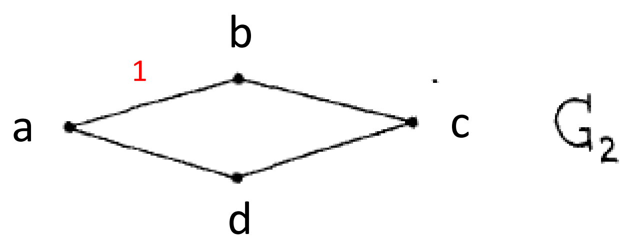
A graph G has a resistance matrix

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

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

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

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



$$\frac{Q}{\Delta - A} = \frac{1}{16}\begin{bmatrix} 5 & -1 & -3 & -1 \\ -1 & 5 & -1 & -3 \\ -3 & -1 & 5 & -1 \\ -1 & -3 & -1 & 5 \end{bmatrix}, \quad (3.7)$$

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

The traditional "series" and "parallel" manipulations (alluded to in section 1) also serve in this special case to yield Ω rather directly.

- Distance function
  - A mapping ρ from Cartesian product V(G)×V(G) to the real numbers such that the following axioms are satisfied:

$$
\begin{aligned}
&\rho(b, a) \geq 0, \\
&\rho(a, b) = 0 \Leftrightarrow a = b, \\
&\rho(a, b) = \rho(b, a), \\
&\rho(a, x) + \rho(x, b) \geq \rho(a, b), \qquad (4.1)
\end{aligned}
$$

Example:

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

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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 Ω_{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 υ and υ', respectively. Then it is easily verified that

$$j \equiv i + i' \tag{4.2}$$

is an I-flow from a to b with associated potential

$$w = \upsilon + \upsilon'. \tag{4.3}$$

Now,

$$I\Omega_{ab} = w_a - w_b = \{\upsilon_a - \upsilon_b\} + \{\upsilon'_a - \upsilon'_b\}. \tag{4.4}$$

However, the extreme values of the potential υ_y must be at $y = a$ and x, since otherwise some other more extreme site would be either a source or a sink. Likewise, υ'_y is extreme at $y = x$ *and* b. Thence,

$$I\Omega_{ab} \leq \{\upsilon_a - \upsilon_x\} + \{\upsilon'_x - \upsilon'_b\} = I\Omega_{ax} + I\Omega_{xb} \tag{4.5}$$

and the theorem follows.

- Resistance sum rules

With all row and column sums zeros?

THEOREM C

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

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

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

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 $|\phi)$ of lemma 0. Thence,

$$\begin{aligned}\sum_{a,b}(b|X|a)\Omega_{ab} &= -2\sum_{a,b}(b|(\Delta-A)Z(\Delta-A)|a)(a|\frac{Q}{\Delta-A}|b)\\ &= -2\,\mathrm{tr}(\Delta-A)Z(\Delta-A)\,\frac{Q}{\Delta-A}\\ &= -2\,\mathrm{tr}(\Delta-A)Z, \quad (5.3)\end{aligned}$$

- **This sum rule avoids the inverse of Δ - A.**

COROLLARY C1

For a connected graph,

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

Z = Q/(Δ - A)

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

COROLLARY C2

For a connected graph

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

$Z = (\Delta - A)^n$

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

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COROLLARY C4 ← Symmetric graph

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.

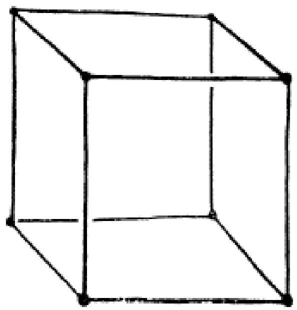

Fig. 4. The cube graph, upon each edge of which one may imagine a resistor r.

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

$$\Omega_e = \frac{8-1}{12} r = \frac{7r}{12},$$
$$\Omega_{nnn} = \frac{2}{2}\left\{1 - \frac{2}{8}\right\} r = \frac{3r}{4}. \qquad (5.4)$$

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 Ω_{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]

$$D_{ab} \equiv \min_{\pi} \sum_{e \in \pi} \frac{1}{r_e}, \qquad (6.2)$$

whence the minimum is taken over all paths π from a to b, and the sum is over all edges of π. 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 commerical 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

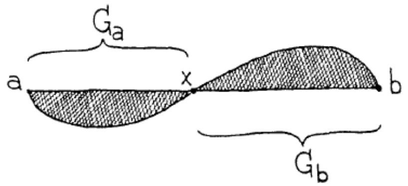

Fig. 5. The general form of the graph assumed for theorem D. Note that x but nothing to the right is included in G_a, whereas x but nothing to the left is included in G_b.

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

$$v_{ax} = I\Omega_{ax}. \tag{7.1}$$

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

$$v_{xb} = I\Omega_{xb}. \tag{7.2}$$

Addition of these two potential differences gives

$$v_{ab} = v_{ax} + v_{xb} = I(\Omega_{ax} + \Omega_{xb}), \tag{7.3}$$

whereupon one obtains the theorem.

- Analogue theorems:

a block of a graph is defined to be a maximal subgraph without cut-points

THEOREM E

If G is a connected graph with blocks G_α, then

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

$$\det \Omega(G) = \sum_{\alpha} \det \Omega(G_\alpha) \prod_{\beta}^{\neq\alpha} \operatorname{cof} \Omega(G_\beta).$$

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

the matrix A	cross out all entries sharing a row or column with entry $a_{2,4}$	the minor $M_{2,4}$
$\begin{bmatrix} 1 & 2 & 3 & 4 \\ 2 & 2 & 2 & 4 \\ 4 & 5 & 6 & 4 \\ 7 & 8 & 9 & 4 \end{bmatrix}$	$\begin{bmatrix} 1 & 2 & 3 & 4 \\ 2 & 2 & 2 & 4 \\ 4 & 5 & 6 & 4 \\ 7 & 8 & 9 & 4 \end{bmatrix}$	$\begin{vmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{vmatrix}$

$$\operatorname{Cof} A_{ij} \equiv (-1)^{i+j} M_{ij}$$

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- 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.

$$W = \sum_{a<b} D_{ab}, \quad (8.2)$$

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

$$W' \equiv \sum_{a<b} \Omega_{ab}, \quad (8.3)$$

THEOREM F

For a connected graph with N vertices,

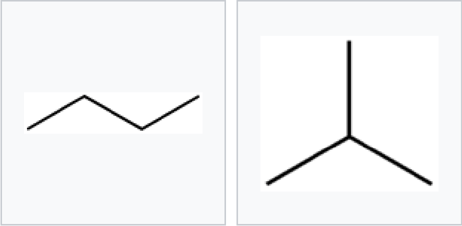
$W' \equiv N \ \mathrm{tr}\{Q/(\Delta - A\}$.

It is a simple matter of algebra to obtain

$$W' = \frac{1}{2}\sum_{a,b}(a-b|Q/(\Delta-A)|a-b) = N \ \mathrm{tr}\{Q/(\Delta-A\} - 2(\phi|Q/(\Delta-A)|\phi). (8.4)$$

However, since $Q/(\Delta - A)$ is null on the $|\phi)$-space one immediately obtains the theorem.

The two isomers of butane



n-Butane Isobutane

$3 \times 1 + 2 \times 2 + 1 \times 3 = 10.$ $3 \times 1 + 3 \times 2 = 9.$

- 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

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- Thanks!