Resistance distance in the context of association schemes and coherent configurations

R. A. Bailey University of St Andrews



British Combinatorial Conference Lancaster University, 12 July 2022 Mini-Symposium on Designs and Algebraic Structures Joint work with Peter Cameron (University of St Andrews),

and Michael Kagan (Penn State University)

Bailey

resistance distance transform

Suppose that Γ is a (simple, undirected) graph with (finite) vertex-set Ω .

Suppose that Γ is a (simple, undirected) graph with (finite) vertex-set Ω . This defines a partition Π_{Γ} of $\Omega \times \Omega$ into three parts (unless Γ is either complete or null).

diag $(\Omega) = \{(\omega, \omega) : \omega \in \Omega\}$

Suppose that Γ is a (simple, undirected) graph with (finite) vertex-set Ω . This defines a partition Π_{Γ} of $\Omega \times \Omega$ into three parts (unless Γ is either complete or null).

diag(
$$\Omega$$
) = {(ω, ω) : $\omega \in \Omega$ }
{(α, β) : (α, β) is an edge of Γ }

Suppose that Γ is a (simple, undirected) graph with (finite) vertex-set Ω . This defines a partition Π_{Γ} of $\Omega \times \Omega$ into three parts (unless Γ is either complete or null).

$$\begin{aligned} \operatorname{diag}(\Omega) &= \{(\omega, \omega) : \omega \in \Omega\} \\ &\{(\alpha, \beta) : (\alpha, \beta) \text{ is an edge of } \Gamma\} \\ &\{(\alpha, \beta) : \alpha \neq \beta \text{ and } (\alpha, \beta) \text{ is not an edge of } \Gamma\} \end{aligned}$$

Suppose that Γ is a (simple, undirected) graph with (finite) vertex-set Ω . This defines a partition Π_{Γ} of $\Omega \times \Omega$ into three parts (unless Γ is either complete or null).

$$\begin{aligned} \operatorname{diag}(\Omega) &= \{(\omega, \omega) : \omega \in \Omega\} \\ &\{(\alpha, \beta) : (\alpha, \beta) \text{ is an edge of } \Gamma\} \\ &\{(\alpha, \beta) : \alpha \neq \beta \text{ and } (\alpha, \beta) \text{ is not an edge of } \Gamma\} \end{aligned}$$

The corresponding $\Omega \times \Omega$ square matrices (with all entries equal to 1 or 0) are *I*, A_{Γ} and $J - A_{\Gamma} - I$, where *I* is the identity matrix, A_{Γ} is the adjacency matrix of Γ , and *J* is the all-1 matrix.

Suppose that Γ is a (simple, undirected) graph with (finite) vertex-set Ω . This defines a partition Π_{Γ} of $\Omega \times \Omega$ into three parts (unless Γ is either complete or null).

$$\begin{aligned} \operatorname{diag}(\Omega) &= \{(\omega, \omega) : \omega \in \Omega\} \\ &\{(\alpha, \beta) : (\alpha, \beta) \text{ is an edge of } \Gamma\} \\ &\{(\alpha, \beta) : \alpha \neq \beta \text{ and } (\alpha, \beta) \text{ is not an edge of } \Gamma\} \end{aligned}$$

The corresponding $\Omega \times \Omega$ square matrices (with all entries equal to 1 or 0) are *I*, A_{Γ} and $J - A_{\Gamma} - I$, where *I* is the identity matrix, A_{Γ} is the adjacency matrix of Γ , and *J* is the all-1 matrix.

Let \mathcal{A}_{Γ} be the set of real linear combinations of these matrices.

Suppose that Γ is a (simple, undirected) graph with (finite) vertex-set Ω . This defines a partition Π_{Γ} of $\Omega \times \Omega$ into three parts (unless Γ is either complete or null).

$$\begin{array}{ll} \operatorname{diag}(\Omega) &=& \{(\omega, \omega) : \omega \in \Omega\} \\ && \{(\alpha, \beta) : (\alpha, \beta) \text{ is an edge of } \Gamma\} \\ && \{(\alpha, \beta) : \alpha \neq \beta \text{ and } (\alpha, \beta) \text{ is not an edge of } \Gamma\} \end{array}$$

The corresponding $\Omega \times \Omega$ square matrices (with all entries equal to 1 or 0) are *I*, A_{Γ} and $J - A_{\Gamma} - I$, where *I* is the identity matrix, A_{Γ} is the adjacency matrix of Γ , and *J* is the all-1 matrix.

Let \mathcal{A}_{Γ} be the set of real linear combinations of these matrices. Then \mathcal{A}_{Γ} is closed under matrix multiplication if and only if the graph Γ is strongly regular.

Bailey

$$A_W(\alpha,\beta) = \begin{cases} 1 & \text{if } (\alpha,\beta) \in W \\ 0 & \text{otherwise.} \end{cases}$$

Put
$$W^{\top} = \{(\alpha, \beta) : (\beta, \alpha) \in W\}.$$

$$A_W(\alpha,\beta) = \begin{cases} 1 & \text{if } (\alpha,\beta) \in W \\ 0 & \text{otherwise.} \end{cases}$$

Put
$$W^{\top} = \{(\alpha, \beta) : (\beta, \alpha) \in W\}$$
. Then $A_{W^{\top}} = A_W^{\top}$.

$$A_W(\alpha,\beta) = \begin{cases} 1 & \text{if } (\alpha,\beta) \in W \\ 0 & \text{otherwise.} \end{cases}$$

Put
$$W^{\top} = \{(\alpha, \beta) : (\beta, \alpha) \in W\}$$
. Then $A_{W^{\top}} = A_W^{\top}$.

If Π is a partition of $\Omega \times \Omega$, let \mathcal{A}_{Π} be the set of real linear combinations of the matrices A_W for all parts W of Π .

$$A_W(\alpha,\beta) = \begin{cases} 1 & \text{if } (\alpha,\beta) \in W \\ 0 & \text{otherwise.} \end{cases}$$

Put
$$W^{\top} = \{(\alpha, \beta) : (\beta, \alpha) \in W\}$$
. Then $A_{W^{\top}} = A_W^{\top}$.

If Π is a partition of $\Omega \times \Omega$, let \mathcal{A}_{Π} be the set of real linear combinations of the matrices A_W for all parts W of Π .

We are going to consider three conditions (and their variants) that Π might satisfy.

(C1) If W is a part of the partition Π , then so is W^{\top} . (Closure under transposition.)

- (C1) If W is a part of the partition Π , then so is W^{\top} . (Closure under transposition.)
- (C2) If *W* is a part of Π , then either $W \subseteq \text{diag}(\Omega)$ or $W \cap \text{diag}(\Omega) = \emptyset$. (The diagonal is special.)

(The corresponding subsets of Ω are called fibres.)

- (C1) If *W* is a part of the partition Π , then so is W^{\top} . (Closure under transposition.)
- (C2) If *W* is a part of Π , then either $W \subseteq \text{diag}(\Omega)$ or $W \cap \text{diag}(\Omega) = \emptyset$.

(The diagonal is special.)

(The corresponding subsets of Ω are called fibres.)

(C3) If *W* and *X* are parts of Π , then $A_W A_X \in \mathcal{A}_{\Pi}$.

(A_{Π} is closed under matrix multiplication.)

- (C1) If *W* is a part of the partition Π , then so is W^{\top} . (Closure under transposition.)
- (C2) If *W* is a part of Π , then either $W \subseteq \text{diag}(\Omega)$ or $W \cap \text{diag}(\Omega) = \emptyset$.

(The diagonal is special.)

(The corresponding subsets of Ω are called fibres.)

(C3) If *W* and *X* are parts of Π , then $A_W A_X \in \mathcal{A}_{\Pi}$.

(A_{Π} is closed under matrix multiplication.)

Variants of these conditions.

(C1+) If *W* is a part of the partition Π , then $W = W^{\top}$.

- (C1) If *W* is a part of the partition Π , then so is W^{\top} . (Closure under transposition.)
- (C2) If *W* is a part of Π , then either $W \subseteq \text{diag}(\Omega)$ or $W \cap \text{diag}(\Omega) = \emptyset$.

(The diagonal is special.)

(The corresponding subsets of Ω are called fibres.)

(C3) If *W* and *X* are parts of Π , then $A_W A_X \in \mathcal{A}_{\Pi}$.

(A_{Π} is closed under matrix multiplication.)

Variants of these conditions.

(C1+) If *W* is a part of the partition Π , then $W = W^{\top}$. (C2+) diag(Ω) is a single class of the partition Π .

- (C1) If *W* is a part of the partition Π , then so is W^{\top} . (Closure under transposition.)
- (C2) If *W* is a part of Π , then either $W \subseteq \text{diag}(\Omega)$ or $W \cap \text{diag}(\Omega) = \emptyset$.

(The diagonal is special.)

(The corresponding subsets of Ω are called fibres.)

(C3) If *W* and *X* are parts of Π , then $A_W A_X \in \mathcal{A}_{\Pi}$.

(A_{Π} is closed under matrix multiplication.)

Variants of these conditions.

- (C1+) If *W* is a part of the partition Π , then $W = W^{\top}$.
- (C2+) diag(Ω) is a single class of the partition Π .
- (C3–) If *W* and *X* are parts of Π , then $A_W A_X + A_X A_W \in \mathcal{A}_{\Pi}$. (\mathcal{A}_{Π} is closed under Jordan multiplication.)

- (C1) If *W* is a part of the partition Π , then so is W^{\top} . (Closure under transposition.)
- (C2) If *W* is a part of Π , then either $W \subseteq \text{diag}(\Omega)$ or $W \cap \text{diag}(\Omega) = \emptyset$.

(The diagonal is special.)

(The corresponding subsets of Ω are called fibres.)

(C3) If *W* and *X* are parts of Π , then $A_W A_X \in \mathcal{A}_{\Pi}$.

(A_{Π} is closed under matrix multiplication.)

Variants of these conditions.

(C1+) If *W* is a part of the partition Π , then $W = W^{\top}$.

(C2+) diag(Ω) is a single class of the partition Π .

(C3–) If *W* and *X* are parts of Π , then $A_W A_X + A_X A_W \in \mathcal{A}_{\Pi}$.

(\mathcal{A}_{Π} is closed under Jordan multiplication.)

 Π is a coherent configuration if (C1), (C2) and (C3) are satisfied.

- (C1) If *W* is a part of the partition Π , then so is W^{\top} . (Closure under transposition.)
- (C2) If *W* is a part of Π , then either $W \subseteq \text{diag}(\Omega)$ or $W \cap \text{diag}(\Omega) = \emptyset$.

(The diagonal is special.)

(The corresponding subsets of Ω are called fibres.)

(C3) If *W* and *X* are parts of Π , then $A_W A_X \in \mathcal{A}_{\Pi}$.

(A_{Π} is closed under matrix multiplication.)

Variants of these conditions.

(C1+) If *W* is a part of the partition Π , then $W = W^{\top}$.

(C2+) diag(Ω) is a single class of the partition Π .

(C3–) If *W* and *X* are parts of Π , then $A_W A_X + A_X A_W \in \mathcal{A}_{\Pi}$.

(A_{Π} is closed under Jordan multiplication.)

 Π is a coherent configuration if (C1), (C2) and (C3) are satisfied. Π is an association scheme if (C1+), (C2+) and (C3) are satisfied.

- (C1) If W is a part of the partition Π , then so is W^{\top} . (Closure under transposition.)
- (C2) If W is a part of Π , then either $W \subseteq \text{diag}(\Omega)$ or $W \cap \operatorname{diag}(\Omega) = \emptyset.$

(The diagonal is special.)

(The corresponding subsets of Ω are called fibres.)

(C3) If *W* and *X* are parts of Π , then $A_W A_X \in \mathcal{A}_{\Pi}$.

 $(\mathcal{A}_{\Pi} \text{ is closed under matrix multiplication.})$

Variants of these conditions.

(C1+) If *W* is a part of the partition Π , then $W = W^{\top}$.

(C2+) diag(Ω) is a single class of the partition Π .

(C3–) If *W* and *X* are parts of Π , then $A_W A_X + A_X A_W \in \mathcal{A}_{\Pi}$.

 $(\mathcal{A}_{\Pi} \text{ is closed under Jordan multiplication.})$

 Π is a coherent configuration if (C1), (C2) and (C3) are satisfied. Π is an association scheme if (C1+), (C2+) and (C3) are satisfied.

 Π is an Jordan scheme if (C1+), (C2) and (C3-) are satisfied. resistance distance transform

If Φ and Ψ are two partitions of $\Omega \times \Omega$ then $\Phi \preccurlyeq \Psi$ (Φ refines Ψ) if each part of Φ is contained in a single part of Ψ . Also, $\Phi \prec \Psi$ if $\Phi \preccurlyeq \Psi$ and $\Phi \neq \Psi$.

If Φ and Ψ are two partitions of $\Omega \times \Omega$ then $\Phi \preccurlyeq \Psi$ (Φ refines Ψ) if each part of Φ is contained in a single part of Ψ . Also, $\Phi \prec \Psi$ if $\Phi \preccurlyeq \Psi$ and $\Phi \neq \Psi$.

Definition

The infimum, or meet, of partitions Ψ_1 and Ψ_2 is the partition $\Psi_1 \wedge \Psi_2$ each of whose parts is a non-empty intersection of a part of Ψ_1 and a part of Ψ_2 .

If Φ and Ψ are two partitions of $\Omega \times \Omega$ then $\Phi \preccurlyeq \Psi$ (Φ refines Ψ) if each part of Φ is contained in a single part of Ψ . Also, $\Phi \prec \Psi$ if $\Phi \preccurlyeq \Psi$ and $\Phi \neq \Psi$.

Definition

The infimum, or meet, of partitions Ψ_1 and Ψ_2 is the partition $\Psi_1 \wedge \Psi_2$ each of whose parts is a non-empty intersection of a part of Ψ_1 and a part of Ψ_2 . So $\Psi_1 \wedge \Psi_2 \preccurlyeq \Psi_1$ and $\Psi_1 \wedge \Psi_2 \preccurlyeq \Psi_2$;

If Φ and Ψ are two partitions of $\Omega \times \Omega$ then $\Phi \preccurlyeq \Psi$ (Φ refines Ψ) if each part of Φ is contained in a single part of Ψ . Also, $\Phi \prec \Psi$ if $\Phi \preccurlyeq \Psi$ and $\Phi \neq \Psi$.

Definition

The infimum, or meet, of partitions Ψ_1 and Ψ_2 is the partition $\Psi_1 \land \Psi_2$ each of whose parts is a non-empty intersection of a part of Ψ_1 and a part of Ψ_2 . So $\Psi_1 \land \Psi_2 \preccurlyeq \Psi_1$ and $\Psi_1 \land \Psi_2 \preccurlyeq \Psi_2$; and if $\Phi \preccurlyeq \Psi_1$ and $\Phi \preccurlyeq \Psi_2$ then $\Phi \preccurlyeq \Psi_1 \land \Psi_2$.

If Φ and Ψ are two partitions of $\Omega \times \Omega$ then $\Phi \preccurlyeq \Psi$ (Φ refines Ψ) if each part of Φ is contained in a single part of Ψ . Also, $\Phi \prec \Psi$ if $\Phi \preccurlyeq \Psi$ and $\Phi \neq \Psi$.

Definition

The infimum, or meet, of partitions Ψ_1 and Ψ_2 is the partition $\Psi_1 \land \Psi_2$ each of whose parts is a non-empty intersection of a part of Ψ_1 and a part of Ψ_2 . So $\Psi_1 \land \Psi_2 \preccurlyeq \Psi_1$ and $\Psi_1 \land \Psi_2 \preccurlyeq \Psi_2$; and if $\Phi \preccurlyeq \Psi_1$ and $\Phi \preccurlyeq \Psi_2$ then $\Phi \preccurlyeq \Psi_1 \land \Psi_2$.

Definition

The supremum, or join, of partitions Ψ_1 and Ψ_2 is the partition $\Psi_1 \lor \Psi_2$ which satisfies $\Psi_1 \preccurlyeq \Psi_1 \lor \Psi_2$ and $\Psi_2 \preccurlyeq \Psi_1 \lor \Psi_2$ and if $\Psi_1 \preccurlyeq \Phi$ and $\Psi_2 \preccurlyeq \Phi$ then $\Psi_1 \lor \Psi_2 \preccurlyeq \Phi$.

If Φ and Ψ are two partitions of $\Omega \times \Omega$ then $\Phi \preccurlyeq \Psi$ (Φ refines Ψ) if each part of Φ is contained in a single part of Ψ . Also, $\Phi \prec \Psi$ if $\Phi \preccurlyeq \Psi$ and $\Phi \neq \Psi$.

Definition

The infimum, or meet, of partitions Ψ_1 and Ψ_2 is the partition $\Psi_1 \land \Psi_2$ each of whose parts is a non-empty intersection of a part of Ψ_1 and a part of Ψ_2 . So $\Psi_1 \land \Psi_2 \preccurlyeq \Psi_1$ and $\Psi_1 \land \Psi_2 \preccurlyeq \Psi_2$; and if $\Phi \preccurlyeq \Psi_1$ and $\Phi \preccurlyeq \Psi_2$ then $\Phi \preccurlyeq \Psi_1 \land \Psi_2$.

Definition

The supremum, or join, of partitions Ψ_1 and Ψ_2 is the partition $\Psi_1 \lor \Psi_2$ which satisfies $\Psi_1 \preccurlyeq \Psi_1 \lor \Psi_2$ and $\Psi_2 \preccurlyeq \Psi_1 \lor \Psi_2$ and if $\Psi_1 \preccurlyeq \Phi$ and $\Psi_2 \preccurlyeq \Phi$ then $\Psi_1 \lor \Psi_2 \preccurlyeq \Phi$. Draw a graph by putting an edge between two points if they are in the same part of Ψ_1 or the same part of Ψ_2 . Then the parts of $\Psi_1 \lor \Psi_2$ are the connected components of the graph.

Association schemes and coherent configurations

Suppose that Φ and Ψ are both association schemes. Then $\Phi \lor \Psi$ is also an association scheme. In general $\Phi \land \Psi$ is not an association scheme: indeed, there may be no association scheme which refines them both. Suppose that Φ and Ψ are both association schemes. Then $\Phi \lor \Psi$ is also an association scheme. In general $\Phi \land \Psi$ is not an association scheme: indeed, there may be no association scheme which refines them both. On the other hand, if Φ and Ψ are both coherent configurations

then $\Phi \lor \Psi$ and $\Phi \land \Psi$ are both coherent configurations.

Suppose that Φ and Ψ are both association schemes. Then $\Phi \lor \Psi$ is also an association scheme.

In general $\Phi \land \Psi$ is not an association scheme: indeed, there may be no association scheme which refines them both.

On the other hand, if Φ and Ψ are both coherent configurations then $\Phi \lor \Psi$ and $\Phi \land \Psi$ are both coherent configurations.

The trivial partition of $\Omega\times\Omega$ into singletons is a coherent configuration.

Suppose that Φ and Ψ are both association schemes. Then $\Phi \lor \Psi$ is also an association scheme.

In general $\Phi \land \Psi$ is not an association scheme: indeed, there may be no association scheme which refines them both.

On the other hand, if Φ and Ψ are both coherent configurations then $\Phi \lor \Psi$ and $\Phi \land \Psi$ are both coherent configurations.

The trivial partition of $\Omega \times \Omega$ into singletons is a coherent configuration.

Let Π be any partition of $\Omega \times \Omega$. Then the set of coherent configurations which refine Π is non-empty.

Suppose that Φ and Ψ are both association schemes. Then $\Phi \lor \Psi$ is also an association scheme.

In general $\Phi \land \Psi$ is not an association scheme: indeed, there may be no association scheme which refines them both.

On the other hand, if Φ and Ψ are both coherent configurations then $\Phi \lor \Psi$ and $\Phi \land \Psi$ are both coherent configurations.

The trivial partition of $\Omega \times \Omega$ into singletons is a coherent configuration.

Let Π be any partition of $\Omega \times \Omega$. Then the set of coherent configurations which refine Π is non-empty. The supremum of all of these is a coherent configuration $CC(\Pi)$ satisfying

1. $CC(\Pi) \preccurlyeq \Pi;$

2. if Φ is a coherent configuration then $\Phi \preccurlyeq \Pi$ if and only if $\Phi \preccurlyeq CC(\Pi)$.

Put $n = |\Omega|$. Imagine the parts of Π as giving different colours to the n^2 cells of $\Omega \times \Omega$.

Put $n = |\Omega|$. Imagine the parts of Π as giving different colours to the n^2 cells of $\Omega \times \Omega$. Let α , β , γ be elements of Ω .

Put $n = |\Omega|$. Imagine the parts of Π as giving different colours to the n^2 cells of $\Omega \times \Omega$. Let α , β , γ be elements of Ω . If (α, β) is coloured red and (β, γ) is coloured blue then the path (α, β, γ) is coloured by the ordered pair (red, blue). Put $n = |\Omega|$. Imagine the parts of Π as giving different colours to the n^2 cells of $\Omega \times \Omega$. Let α , β , γ be elements of Ω . If (α, β) is coloured red and (β, γ) is coloured blue then the path (α, β, γ) is coloured by the ordered pair (red, blue). There are *n* paths of length two from α to γ (including (α, α, γ) and (α, γ, γ)). If we re-label the pair (α, γ) according to how many such pairs have each ordered pair of colours, then we obtain a new partition of $\Omega \times \Omega$.
Put $n = |\Omega|$. Imagine the parts of Π as giving different colours to the n^2 cells of $\Omega \times \Omega$. Let α , β , γ be elements of Ω . If (α, β) is coloured red and (β, γ) is coloured blue then the path (α, β, γ) is coloured by the ordered pair (red, blue). There are *n* paths of length two from α to γ (including (α, α, γ) and (α, γ, γ)). If we re-label the pair (α, γ) according to how many such pairs have each ordered pair of colours, then we

obtain a new partition of $\Omega \times \Omega$.

We shall call this WL(Π), because this uses the algorithm introduced by Weisfeiler and Leman. It is clear that WL(Π) $\preccurlyeq \Pi$.

Suppose that Π satsifies (C1).

If red is a colour then it has a dual colour red' (which may be the same as red) such that $A_{\text{red}'} = A_{\text{red}}^{\top}$. The reverse of a path coloured (red, blue) from α to β is a path coloured (blue', red') from β to α . Hence WL(Π) also satisfies (C1).

Suppose that Π satsifies (C1).

If red is a colour then it has a dual colour red' (which may be the same as red) such that $A_{\text{red}'} = A_{\text{red}}^{\top}$. The reverse of a path coloured (red, blue) from α to β is a path coloured (blue', red') from β to α . Hence WL(Π) also satisfies (C1).

Suppose that Π satisfies (C2).

If red is a colour which occurs only on diag(Ω) and there is a path of length two from α coloured (red, red) then the path must be (α , α , α). Hence WL(Π) also satisfies (C2).

Suppose that Π satsifies (C1).

If red is a colour then it has a dual colour red' (which may be the same as red) such that $A_{\text{red}'} = A_{\text{red}}^{\top}$. The reverse of a path coloured (red, blue) from α to β is a path coloured (blue', red') from β to α . Hence WL(Π) also satisfies (C1).

Suppose that Π satisfies (C2).

If red is a colour which occurs only on diag(Ω) and there is a path of length two from α coloured (red, red) then the path must be (α , α , α). Hence WL(Π) also satisfies (C2).

In general, the number of (red, blue) paths from α to β is the (α, β) -entry in $A_{\text{red}}A_{\text{blue}}$. Thus if Π satisfies (C3) then WL(Π) = Π . Otherwise, WL(Π) $\prec \Pi$.

Suppose that Π satsifies (C1).

If red is a colour then it has a dual colour red' (which may be the same as red) such that $A_{\text{red}'} = A_{\text{red}}^{\top}$. The reverse of a path coloured (red, blue) from α to β is a path coloured (blue', red') from β to α . Hence WL(Π) also satisfies (C1).

Suppose that Π satisfies (C2).

If red is a colour which occurs only on diag(Ω) and there is a path of length two from α coloured (red, red) then the path must be (α , α , α). Hence WL(Π) also satisfies (C2).

In general, the number of (red, blue) paths from α to β is the (α, β) -entry in $A_{\text{red}}A_{\text{blue}}$. Thus if Π satisfies (C3) then WL(Π) = Π . Otherwise, WL(Π) $\prec \Pi$.

These results show that if Π is a coherent configuration then $\Pi = WL(\Pi)$. On the other hand, if Π satisfies (C1) and (C2) but not (C3) then $WL(\Pi)$ satisfies (C1) and (C2) and $WL(\Pi) \prec \Pi$.

Given a graph Γ , the Weisfeiler–Leman algorithm is applied repeatedly, starting with Π_{Γ} , giving

 $\Pi_{\Gamma} \succcurlyeq WL(\Pi_{\Gamma}) \succcurlyeq WL(WL(\Pi_{\Gamma})) \cdots .$

Given a graph Γ , the Weisfeiler–Leman algorithm is applied repeatedly, starting with Π_{Γ} , giving

 $\Pi_{\Gamma} \succcurlyeq WL(\Pi_{\Gamma}) \succcurlyeq WL(WL(\Pi_{\Gamma})) \cdots .$

Moreover, it is easy to see that if $\Pi_1 \succeq \Pi_2$ then $WL(\Pi_1) \succeq WL(\Pi_2)$. Therefore,

 $\Pi_{\Gamma} \succcurlyeq WL(\Pi_{\Gamma}) \succcurlyeq WL(CC(\Pi_{\Gamma})) = CC(\Pi_{\Gamma}).$

Given a graph Γ , the Weisfeiler–Leman algorithm is applied repeatedly, starting with Π_{Γ} , giving

 $\Pi_{\Gamma} \succcurlyeq WL(\Pi_{\Gamma}) \succcurlyeq WL(WL(\Pi_{\Gamma})) \cdots .$

Moreover, it is easy to see that if $\Pi_1 \succeq \Pi_2$ then $WL(\Pi_1) \succeq WL(\Pi_2)$. Therefore,

 $\Pi_{\Gamma} \succcurlyeq WL(\Pi_{\Gamma}) \succcurlyeq WL(CC(\Pi_{\Gamma})) = CC(\Pi_{\Gamma}).$

Each time that Weisfeiler–Leman is applied, either the resulting partition is strictly finer than the preceding one or the preceding one is $CC(\Pi_{\Gamma})$. Since Π_{Γ} has finitely many classes, the process stabilizes at $CC(\Pi_{\Gamma})$ after finitely many steps.

Although Weisfeiler–Leman stabilizes after finitely many steps, that finite number may still be considered to be "too large".

Although Weisfeiler–Leman stabilizes after finitely many steps, that finite number may still be considered to be "too large". Michael Kagan and Misha Klin proposed an alternative method using resistance distance, which I will now explain.

We can consider the graph Γ as an electrical network with a 1-ohm resistance in each edge. Connect a 1-volt battery between vertices α and β . Current flows in the network, according to these rules.

We can consider the graph Γ as an electrical network with a 1-ohm resistance in each edge. Connect a 1-volt battery between vertices α and β . Current flows in the network, according to these rules.

1. Ohm's Law:

In every edge, voltage drop = current \times resistance = current.

We can consider the graph Γ as an electrical network with a 1-ohm resistance in each edge. Connect a 1-volt battery between vertices α and β . Current flows in the network, according to these rules.

1. Ohm's Law:

In every edge, voltage drop = current \times resistance = current.

2. Kirchhoff's Voltage Law:

The total voltage drop from one vertex to any other vertex is the same no matter which path we take from one to the other.

We can consider the graph Γ as an electrical network with a 1-ohm resistance in each edge. Connect a 1-volt battery between vertices α and β . Current flows in the network, according to these rules.

1. Ohm's Law:

In every edge, voltage drop = current \times resistance = current.

2. Kirchhoff's Voltage Law:

The total voltage drop from one vertex to any other vertex is the same no matter which path we take from one to the other.

3. Kirchhoff's Current Law:

At every vertex which is not connected to the battery, the total current coming in is equal to the total current going out.

We can consider the graph Γ as an electrical network with a 1-ohm resistance in each edge. Connect a 1-volt battery between vertices α and β . Current flows in the network, according to these rules.

1. Ohm's Law:

In every edge, voltage drop = current \times resistance = current.

2. Kirchhoff's Voltage Law:

The total voltage drop from one vertex to any other vertex is the same no matter which path we take from one to the other.

3. Kirchhoff's Current Law:

At every vertex which is not connected to the battery, the total current coming in is equal to the total current going out.

Find the total current *I* from α to β , then use Ohm's Law to define the resistance distance $R_{\alpha\beta}$ between α and β as 1/I.

Bailey





If the distance between α and β is *d*

$$R_{\alpha\beta}=\frac{d(10-d)}{10}.$$

Bailey



If the distance between α and β is *d*

$$R_{\alpha\beta}=\frac{d(10-d)}{10}.$$

Bailey



Using the Laplacian matrix

Definition

The Laplacian matrix *L* of the graph Γ is the $\Omega \times \Omega$ matrix with

$$L_{\alpha\beta} = \begin{cases} \text{ degree of } \alpha & \text{if } \alpha = \beta \\ -1 & \text{if } (\alpha, \beta) \text{ is an edge} \\ 0 & \text{ otherwise.} \end{cases}$$

Using the Laplacian matrix

Definition

The Laplacian matrix *L* of the graph Γ is the $\Omega \times \Omega$ matrix with

$$L_{\alpha\beta} = \begin{cases} \text{ degree of } \alpha & \text{if } \alpha = \beta \\ -1 & \text{if } (\alpha, \beta) \text{ is an edge} \\ 0 & \text{ otherwise.} \end{cases}$$

L is symmetric, with all row-sums zero. If Γ is connected then 0 is an eigenvalue of *L* with multiplicity one and eigenprojector $n^{-1}J$.

Using the Laplacian matrix

Definition

The Laplacian matrix *L* of the graph Γ is the $\Omega \times \Omega$ matrix with

$$L_{\alpha\beta} = \begin{cases} \text{degree of } \alpha & \text{if } \alpha = \beta \\ -1 & \text{if } (\alpha, \beta) \text{ is an edge} \\ 0 & \text{otherwise.} \end{cases}$$

L is symmetric, with all row-sums zero. If Γ is connected then 0 is an eigenvalue of L with multiplicity one and eigenprojector n^{-1} *I*. Hence the Moore–Penrose inverse *M* of *L* is given by

$$M = \left(L + \frac{1}{n}J\right)^{-1} - \frac{1}{n}J$$

and *M* is a polynomial in *L*.

Theorem

The resistance distance $R_{\alpha\beta}$ *between vertices* α *and* β *is*

$$R_{\alpha\beta} = \left(M_{\alpha\alpha} + M_{\beta\beta} - 2M_{\alpha\beta} \right).$$

Bailev

13/21

 Off-diagonal pairs are in the same part if and only if they have the same resistance distance.

- Off-diagonal pairs are in the same part if and only if they have the same resistance distance.
- No pair in diag(Ω) is in any of those parts.

- Off-diagonal pairs are in the same part if and only if they have the same resistance distance.
- No pair in diag(Ω) is in any of those parts.
- Pairs (α, α) and (β, β) are in the same part if and only if $\sum_{\gamma \neq \alpha} 1/R_{\alpha\gamma} = \sum_{\gamma \neq \beta} 1/R_{\beta\gamma}$.

- Off-diagonal pairs are in the same part if and only if they have the same resistance distance.
- No pair in diag(Ω) is in any of those parts.

► Pairs (α , α) and (β , β) are in the same part if and only if $\sum_{\gamma \neq \alpha} 1/R_{\alpha\gamma} = \sum_{\gamma \neq \beta} 1/R_{\beta\gamma}$.

Then Γ is replaced by the complete graph on Ω with conductance $1/R_{\alpha\beta}$ in each edge (α , β).

- Off-diagonal pairs are in the same part if and only if they have the same resistance distance.
- No pair in diag(Ω) is in any of those parts.

• Pairs (α, α) and (β, β) are in the same part if and only if $\sum_{\gamma \neq \alpha} 1/R_{\alpha\gamma} = \sum_{\gamma \neq \beta} 1/R_{\beta\gamma}$.

Then Γ is replaced by the complete graph on Ω with conductance $1/R_{\alpha\beta}$ in each edge (α , β).

(Think of this as placing $1/R_{\alpha\beta}$ edges between α and β .)

- Off-diagonal pairs are in the same part if and only if they have the same resistance distance.
- No pair in diag(Ω) is in any of those parts.

► Pairs (α , α) and (β , β) are in the same part if and only if $\sum_{\gamma \neq \alpha} 1/R_{\alpha\gamma} = \sum_{\gamma \neq \beta} 1/R_{\beta\gamma}$.

Then Γ is replaced by the complete graph on Ω with conductance $1/R_{\alpha\beta}$ in each edge (α, β) .

(Think of this as placing $1/R_{\alpha\beta}$ edges between α and β .)

Then RDT can be iterated.

Michael Kagan and Misha Klin applied RDT to several highly symmetric graphs Γ .

Michael Kagan and Misha Klin applied RDT to several highly symmetric graphs Γ .

In every case, RDT stabilized at $CC(\Pi_{\Gamma}),$ usually taking far fewer iterations than WL.

Michael Kagan and Misha Klin applied RDT to several highly symmetric graphs Γ .

In every case, RDT stabilized at $CC(\Pi_{\Gamma}),$ usually taking far fewer iterations than WL.

A graph is distance-regular if its distance-classes form an association scheme.

Michael Kagan and Misha Klin applied RDT to several highly symmetric graphs Γ .

In every case, RDT stabilized at $CC(\Pi_{\Gamma})$, usually taking far fewer iterations than WL.

A graph is distance-regular if its distance-classes form an association scheme.

MKMK found that, when applied to a distance-regular graph, RDT stabilizes at that association scheme in a single step.

Michael Kagan and Misha Klin applied RDT to several highly symmetric graphs Γ .

In every case, RDT stabilized at $CC(\Pi_{\Gamma}),$ usually taking far fewer iterations than WL.

A graph is distance-regular if its distance-classes form an association scheme.

MKMK found that, when applied to a distance-regular graph, RDT stabilizes at that association scheme in a single step.

This result agrees with results of Norman Biggs from 1993.

Michael Kagan and Misha Klin applied RDT to several highly symmetric graphs Γ .

In every case, RDT stabilized at $CC(\Pi_{\Gamma}),$ usually taking far fewer iterations than WL.

A graph is distance-regular if its distance-classes form an association scheme.

MKMK found that, when applied to a distance-regular graph, RDT stabilizes at that association scheme in a single step.

This result agrees with results of Norman Biggs from 1993.

Those graphs are rather special. In general, $WL(\Pi_{\Gamma})$ satisfies (C1) but not (C1+), because not all matrices are symmetric.

Michael Kagan and Misha Klin applied RDT to several highly symmetric graphs Γ .

In every case, RDT stabilized at $CC(\Pi_{\Gamma}),$ usually taking far fewer iterations than WL.

A graph is distance-regular if its distance-classes form an association scheme.

MKMK found that, when applied to a distance-regular graph, RDT stabilizes at that association scheme in a single step.

This result agrees with results of Norman Biggs from 1993.

Those graphs are rather special. In general, $WL(\Pi_{\Gamma})$ satisfies (C1) but not (C1+), because not all matrices are symmetric. The result of applying RDT always satisfies (C1+), because the resistance distances $R_{\alpha\beta}$ and $R_{\beta\alpha}$ are equal.
Initial investigations of resistance distance transform

Michael Kagan and Misha Klin applied RDT to several highly symmetric graphs Γ .

In every case, RDT stabilized at $CC(\Pi_{\Gamma})$, usually taking far fewer iterations than WL.

A graph is distance-regular if its distance-classes form an association scheme.

MKMK found that, when applied to a distance-regular graph, RDT stabilizes at that association scheme in a single step.

This result agrees with results of Norman Biggs from 1993.

Those graphs are rather special. In general, $WL(\Pi_{\Gamma})$ satisfies (C1) but not (C1+), because not all matrices are symmetric. The result of applying RDT always satisfies (C1+), because the resistance distances $R_{\alpha\beta}$ and $R_{\beta\alpha}$ are equal.

Does iterated RDT always produce a symmetrized version of iterated WL?

MKMK talked about RDT at a conference in Pilsen in 2018 and one in Yichang in 2019.

- MKMK talked about RDT at a conference in Pilsen in 2018 and one in Yichang in 2019.
- RAB and PJC were at both of these. In Yichang, they gave a short course about Laplacian eigenvalues and their relevance to finding optimal incomplete-block designs.

MKMK talked about RDT at a conference in Pilsen in 2018 and one in Yichang in 2019.

RAB and PJC were at both of these. In Yichang, they gave a short course about Laplacian eigenvalues and their relevance to finding optimal incomplete-block designs. This included the use of resistance distance as a measure of optimality.

MKMK talked about RDT at a conference in Pilsen in 2018 and one in Yichang in 2019.

RAB and PJC were at both of these. In Yichang, they gave a short course about Laplacian eigenvalues and their relevance to finding optimal incomplete-block designs. This included the use of resistance distance as a measure of optimality.

We decided to join forces.

Some small examples: Bad results



Some small examples: Bad results



Some small examples: Bad results



{2,3} is an edge; {4,6} is a non-edge; but $R_{23} = R_{46} = 1$. In this case, the partition defined by resistance distance does not refine the original partition Π_{Γ} .

Bailey

resistance distance transform









edge between 1 and 2. Therefore $R'_{12} = R'_{13}$.



edge between 1 and 2. Therefore $R'_{12} = R'_{13}$. But $R_{12} \neq R_{13}$.



edge between 1 and 2. Therefore $R'_{12} = R'_{13}$. But $R_{12} \neq R_{13}$. Neither of these RDT partitions refines the other.

Bailey

To avoid these problems, MK proposed RDT2, as follows.

To avoid these problems, MK proposed RDT2, as follows. If the partition Π has *r* non-diagonal parts, we associate an indeterminate x_i with the *i*-th part, and regard this as the conductance.

To avoid these problems, MK proposed RDT2, as follows. If the partition Π has *r* non-diagonal parts, we associate an indeterminate x_i with the *i*-th part, and regard this as the conductance.

Put $C = \sum_{i=1}^{r} x_i A_i$, where the sum is over all non-diagonal parts.

To avoid these problems, MK proposed RDT2, as follows. If the partition Π has *r* non-diagonal parts, we associate an indeterminate x_i with the *i*-th part, and regard this as the conductance.

Put $C = \sum_{i=1}^{r} x_i A_i$, where the sum is over all non-diagonal parts. "Laplacianize" this by multiplying by -1 and then changing the diagonal entries so that the row and columns sums are all zero.

To avoid these problems, MK proposed RDT2, as follows. If the partition Π has *r* non-diagonal parts, we associate an indeterminate x_i with the *i*-th part, and regard this as the conductance.

Put $C = \sum_{i=1}^{r} x_i A_i$, where the sum is over all non-diagonal parts. "Laplacianize" this by multiplying by -1 and then changing the diagonal entries so that the row and columns sums are all zero. The Moore–Penrose inverse then gives the resistance distances as rational functions of x_1, \ldots, x_r .

To avoid these problems, MK proposed RDT2, as follows. If the partition Π has *r* non-diagonal parts, we associate an indeterminate x_i with the *i*-th part, and regard this as the conductance.

Put $C = \sum_{i=1}^{r} x_i A_i$, where the sum is over all non-diagonal parts. "Laplacianize" this by multiplying by -1 and then changing the diagonal entries so that the row and columns sums are all zero. The Moore–Penrose inverse then gives the resistance distances as rational functions of x_1, \ldots, x_r .

Now two edges are in the same part of RDT $2(\Pi)$ if and only if their resistance distances are equal as rational functions.

To avoid these problems, MK proposed RDT2, as follows. If the partition Π has *r* non-diagonal parts, we associate an indeterminate x_i with the *i*-th part, and regard this as the conductance.

Put $C = \sum_{i=1}^{r} x_i A_i$, where the sum is over all non-diagonal parts. "Laplacianize" this by multiplying by -1 and then changing the diagonal entries so that the row and columns sums are all zero. The Moore–Penrose inverse then gives the resistance distances as rational functions of x_1, \ldots, x_r .

Now two edges are in the same part of RDT $2(\Pi)$ if and only if their resistance distances are equal as rational functions.

Relabelling the parts simply permutes the indeterminates, so it does not change RDT $2(\Pi)$. In particular, a graph and its complement give the same RDT 2.

To avoid these problems, MK proposed RDT2, as follows. If the partition Π has *r* non-diagonal parts, we associate an indeterminate x_i with the *i*-th part, and regard this as the conductance.

Put $C = \sum_{i=1}^{r} x_i A_i$, where the sum is over all non-diagonal parts. "Laplacianize" this by multiplying by -1 and then changing the diagonal entries so that the row and columns sums are all zero. The Moore–Penrose inverse then gives the resistance distances as rational functions of x_1, \ldots, x_r .

Now two edges are in the same part of RDT $2(\Pi)$ if and only if their resistance distances are equal as rational functions.

Relabelling the parts simply permutes the indeterminates, so it does not change RDT $2(\Pi)$. In particular, a graph and its complement give the same RDT 2.

We have not found an example where edges with different indeterminates get the same resistance distance, but we have not yet proved that this <u>does not happen</u>.

Bailey

Theorem If Π is an association scheme, then RDT $2(\Pi) = \Pi$.

Theorem If Π is an association scheme, then RDT $2(\Pi) = \Pi$.

Theorem

If Γ is the graph corresponding to a non-diagonal part in an association scheme, and RDT2 is applied repeatedly, then it stabilizes at the association scheme which is the supremum of all association schemes which have Γ as such a graph.

1. Does repeated RDT2 always stabilize?

- 1. Does repeated RDT2 always stabilize?
- 2. If so, does it do so in fewer steps than Weisfeiler-Leman?

- 1. Does repeated RDT2 always stabilize?
- 2. If so, does it do so in fewer steps than Weisfeiler-Leman?
- 3. If $CC(\Pi)$ does not satisfy (C1+), does RDT2 stabilize at a Jordan scheme?