A canonical decomposition theory for metrics on a finite set

[1] In this paper a map $d: X \times X \to \mathbb{R}$ will be called a *metric* on X, if it vanishes on the diagonal ($d(x, x) = 0$) and satisfies the triangle inequality ($d(x, y) \leqslant d(x, z) + d(y, z)$), while d is not required to vanish exclusively on the diagonal, that is, $d(x, y) = 0$ does not necessarily imply $x = y$. Sometimes such maps have been called pseudo-metrics. Only by including such "pseudo-metrics" in the set $M(X)$ of metrics on X does this set become a *closed* convex cone in the linear space $\mathbb{R}^{X \times X}$ of all maps from $X \times X$ into $\mathbb{R}$ (topologized with respect to pointwise convergence, say). For further information on the "metric cone" see [3] or [16].

Let X be a set. Non serve finito per ora.

Def. (pseudo-metric)

A function $d : X \times X \to \mathbb{R}$ is a **pseudo-metric** on X if

- $d(x,x) = 0, \quad \forall\, x \in X$
- $d(x,y) \leq d(x,z) + d(y,z), \quad \forall\, x,y,z \in X$

that is, it vanishes on the diagonal $\Delta_X = \{\, (x,y) \in X \times X \mid x = y \,\}$ and it satisfies the triangle inequality.

Def. (metric)

A function $d : X \times X \to \mathbb{R}$ is a **metric** on X if

- $d(x,y) = 0 \iff x = y, \quad \forall\, x,y \in X$
- $d(x,y) \leq d(x,z) + d(y,z), \quad \forall\, x,y,z \in X$

In particular, a metric is a pseudo-metric.

[BD92a] non parla di non-negatività e simmetria
(si possono ricavare da disuguaglianza triangolare + diagonale nulla).

Prop. If $d : X \times X \to \mathbb{R}$ is a pseudo-metric, then

- $d(x,y) = d(y,x), \quad \forall\, x,y \in X$
- $d(x,y) \geq 0, \qquad \forall\, x,y \in X$

that is, it is a symmetric and non-negative function.

Dim. From triangle inequality on x,y,x and on y,x,y

$$d(x,y) \leq \cancel{d(x,x)} + d(y,x)$$

$$d(y,x) \leq \cancel{d(y,y)} + d(x,y)$$

that implies $d(x,y) = d(y,x)$.

From triangle inequality on x,x,y

$$0 = d(x,x) \leq d(x,y) + d(x,y) = 2d(x,y)$$

that implies $d(x,y) \geq 0$.

Let V be a vector space over $\mathbb{R}$.

Def. (convex set)

A subset $C \subseteq V$ is **convex** if $\forall\, v,w \in C$

$$(1-\lambda)v + \lambda w \in C, \qquad \forall\, \lambda \in [0,1]$$

Def. ((linear) cone)

A subset $C \subseteq V$ is a **(linear) cone** if

$$v \in C \implies \lambda v \in C, \qquad \forall\, \lambda \geq 0$$

Not. $\mathbb{R}^{X\times X} := \{ f : X \times X \to \mathbb{R} \mid f \text{ function} \}$

$M(X) := \{ d : X \times X \to \mathbb{R} \mid d \text{ pseudo-metric} \} \subseteq \mathbb{R}^{X\times X}$

Fact $\mathbb{R}^{X\times X}$ is a (real) vector space.

Prop. $M(X)$ is a convex cone.

Dim. Let $d \in M(X)$ pseudo-metric on X and $\lambda \geq 0$. Then

- $d(x,x) = 0 \implies \lambda d(x,x) = 0, \ \forall\, x \in X$
- $d(x,y) \leq d(x,z) + d(y,z) \implies$
  $\lambda d(x,y) \leq \lambda\big(d(x,z) + d(y,z)\big) = \lambda d(x,z) + \lambda d(y,z),$
  $\forall\, x,y,z \in X$

So λd is a pseudo-metric, $\lambda d \in M(X)$, and $M(X)$ is a cone.

To show that $M(X)$ is convex,
we need to show that $\forall\, d_1, d_2 \in M(X)$

$$(1-\lambda)d_1 + \lambda d_2 \in M(X)\,, \qquad \forall\, \lambda \in [0,1]$$

But since $M(X)$ is a cone,

$$(1-\lambda)d_1 \in M(X) \ \text{ and } \ \lambda d_2 \in M(X)$$

so it suffice to show that $M(X)$ is closed under addition.

Let $d_1, d_2 \in M(X)$. Then

- $(d_1 + d_2)(x,x) = \underbrace{d_1(x,x)}_{=0} + \underbrace{d_2(x,x)}_{=0} = 0, \ \forall\, x \in X$
- $(d_1 + d_2)(x,y) = d_1(x,y) + d_2(x,y) \leq$
  $\leq d_1(x,z) + d_1(y,z) + d_2(x,z) + d_2(y,z) =$
  $= d_1(x,z) + d_2(x,z) + d_1(y,z) + d_2(y,z) =$
  $= (d_1 + d_2)(x,z) + (d_1 + d_2)(y,z), \qquad \forall\, x,y,z \in X$

So $d_1 + d_2$ is a pseudo-metric on X.

The set of all metrics is also a non-pointed convex cone (same definition of cone but with $\lambda > 0$): in fact, the zero function is not a metric.

Let us consider $\mathbb{R}^{X \times X}$ with the topology of pointwise convergence τ_p .

Prop. If X is countable*, then $M(X)$ is closed in $(\mathbb{R}^{X \times X}, \tau_p)$.

Dim. Let us show that $M(X)$ is sequentially closed.

Let us consider a convergent sequence of pseudo-metrics

$$d_n \to \bar{d}, \qquad d_n \in M(X), \;\; \forall\, n \in \mathbb{N}$$

and let us show that the limit is also a pseudo-metric,

$$\bar{d} \in M(X)$$

For the characterization of the pointwise convergence,

$$d_n \to \bar{d} \;\; \Leftrightarrow \;\; d_n(\boldsymbol{x}) \to \bar{d}(\boldsymbol{x}), \;\; \forall\, \boldsymbol{x} \in X \times X$$

Now for every $\boldsymbol{x} \in X \times X$,
$\{d_n(\boldsymbol{x})\}_{n \in \mathbb{N}}$ is a real-valued sequence, so $\forall\, x, y, z \in X$

- $d_n(x,x) = 0, \;\; \forall\, n \in \mathbb{N} \implies \lim_{n \to +\infty} d_n(x,x) = \bar{d}(x,x) = 0$
- $d_n(x,y) \le d_n(x,z) + d_n(y,z), \;\; \forall\, n \in \mathbb{N}$, so in the limit $\bar{d}(x,y) \le \bar{d}(x,z) + \bar{d}(y,z)$

This shows that $\bar{d}$ is a pseudo-metric
and $M(X)$ is sequentially closed.

Since X is countable (and so is $X \times X$), the space $\mathbb{R}^{X \times X} = \prod_{\boldsymbol{x} \in X \times X} \mathbb{R}$ is a countable product of first-countable spaces (namely $\mathbb{R}$), so it is first-countable itself.

Now $M(X)$ is sequentially closed in a first-countable space,
so it is closed.

* Here countable means finite or countably infinite (*al più numerabile*).

If X is uncountable, then we cannot conclude that $\mathbb{R}^{X\times X}$ is first-countable.

Oss. In the same hypothesis, the set of metrics is not even sequentially closed in $(\mathbb{R}^{X\times X}, \tau_p)$.

Dim. Let us consider a convergent sequence of metrics such that

$$d_n \to \bar{d} \quad \text{and} \quad d_n(\boldsymbol{x}) = \frac{1}{n}, \ \ n \in \mathbb{N}$$

for some $\boldsymbol{x} \in (X \times X) \setminus \Delta_X$. Then

$$\bar{d}(\boldsymbol{x}) = \lim_{n\to+\infty} d_n(\boldsymbol{x}) = 0$$

but $\boldsymbol{x} \notin \Delta_X$, so $\bar{d}$ is not a metric.

https://en.wikipedia.org/wiki/Metric_space
https://en.wikipedia.org/wiki/Pseudometric_space

https://en.wikipedia.org/wiki/Vector_space
https://en.wikipedia.org/wiki/Convex_set
https://en.wikipedia.org/wiki/Convex_cone

https://en.wikipedia.org/wiki/Pointwise_convergence
https://en.wikipedia.org/wiki/Sequential_space

Sometimes it is useful to think of functions $d : X \times X \to \mathbb{R}$, $(d \in \mathbb{R}^{X\times X})$, as real-valued square matrices $D \in M(|X|, \mathbb{R})$.
In particular, a pseudo-metric corresponds to a symmetric matrix, with 0 on the diagonal, non-negative entries elsewhere and such that the elements satisfy the triangle inequality.

CHAPTER 1: INTRODUCTION

Let us commence by recalling what is known about the structure of the closed convex cone $M(X)$ of (pseudo-)metrics[1] definable on a finite set X,

in case the number $n = \#X$ of elements in X is small. If $X = \{a, b, c\}$ has cardinality 3, then the dimension $\binom{n}{2} = 3$ of the linear space

$$\langle M(X) \rangle = \{d: X \times X \to \mathbb{R} \mid d(x, y) = d(y, x) \text{ and}$$
$$d(x, x) = 0 \text{ for all } x, y \in X\}$$

generated by $M(X)$ equals the number of extreme rays in $M(X)$ which are generated by the three *split metrics* $\delta_{\{a\},\{b,c\}}$, $\delta_{\{b\},\{a,c\}}$, and $\delta_{\{c\},\{a,b\}}$, where for a partition (or *split*) $X = A \cup B$ of X into two disjoint nonempty subsets A, B the associated *split metric* $\delta_{A,B}$ is defined by

$$\delta_{A,B}(x, y) := \begin{cases} 0 & \text{if } \quad x, y \in A \text{ or } x, y \in B, \\ 1 & \text{otherwise.} \end{cases}$$

(Split metrics are also called binary dissimilarities or binary metrics by [14, 15, 20].) Hence, if $\#X = 3$, the cone $M(X)$ is a "simplicial" convex cone generated by the three linearly independent metrics $\delta_{\{a\},\{b,c\}}$, $\delta_{\{b\},\{a,c\}}$, and $\delta_{\{c\},\{a,b\}}$. As a consequence, any metric d defined on X can uniquely be expressed in the form

$$d = \alpha_a \cdot \delta_{\{a\},\{b,c\}} + \alpha_b \cdot \delta_{\{b\},\{a,c\}} + \alpha_c \cdot \delta_{\{c\},\{a,b\}}$$

with nonnegative real numbers α_a, α_b, α_c, namely with

$$\alpha_x := \tfrac{1}{2} \cdot (d(x, y) + d(x, z) - d(y, z))$$

for $\{x, y, z\} = \{a, b, c\}$ (see Fig. 1).

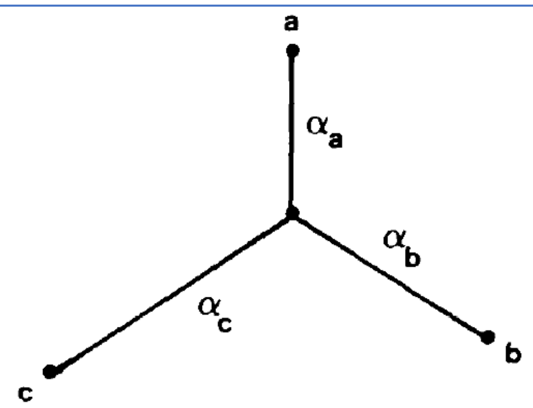


FIG. 1. A generic metric on three points.

Let us consider a real vector space V.

Def. (conic/conical combination)

A point $v \in V$ is a **conical combination** of $v_1, \dots, v_k \in V$ if

$$\exists\, \lambda_1, \dots, \lambda_k \geq 0 \text{ such that } v = \lambda_1 v_1 + \cdots + \lambda_k v_k$$

Def. (extreme/extremal ray)

An **extreme ray** of a cone $C \subseteq V$ is a subset $S \subseteq C$ of the form

$$S = \{\, \lambda r \mid \lambda \geq 0 \,\}$$

for some $r \in C \setminus \{0\}$, such that the elements of S cannot be expressed as conical combinations of elements of $C \setminus S$;

or equivalently, for every $v_1, \dots, v_k \in C$ and $\lambda_1, \dots, \lambda_k \geq 0$

$$\lambda_1 v_1 + \cdots + \lambda_k v_k \in S \implies \exists\, i \in \{1, \dots, k\} : v_i \in S$$

or equivalently, for every $v, w \in C$

$$v + w \in S \implies v \in S \text{ or } w \in S$$

We can identify an extreme ray with the associated vector r.

Def. (simplicial cone)

A cone $C \subseteq V$ is a **simplicial cone** if every complete* set of representatives of the extreme rays is linearly independent;

or equivalently, if

$$\#\{\text{extreme rays}\} = \dim_{\mathbb{R}} \langle C \rangle$$

where $\langle C \rangle$ is the vector subspace spanned by C.

---

* This is to be understood as every vector corresponds to an extreme ray and no two vectors correspond to the same extreme ray.

From now on we will assume X finite of cardinality n.
We may sometimes identify X with $\{1, \dots, n\}$, since they are in bijection.

Def. (split metric / binary metric / binary dissimilarity)

Given a partition (or split) of X into two disjoint non-empty sets A and B, we call **split metric** of $\{A, B\}$ the function $\delta_{A,B} : X \times X \to \mathbb{R}$ defined by

$$\delta_{A,B}(x, y) := \begin{cases} 0\,, & \text{if } x, y \in A \text{ or } x, y \in B \\ 1\,, & \text{otherwise} \end{cases}$$

Not. If $a \in X$, we denote the trivial split metric

$$\delta_a := \delta_{\{a\},(X \setminus \{a\})}$$

Prop. The split metrics are pseudo-metrics.

Dim. Let us fix a split $\{A, B\}$ of X and let us show that $\delta_{A,B} \in M(X)$.
The vanishing on the diagonal is obvious.

Let us show the triangle inequality.

- $x, y, z \in A$
$$\underbrace{\delta_{A,B}(x,y)}_{0} \leq \underbrace{\delta_{A,B}(x,z)}_{0} + \underbrace{\delta_{A,B}(y,z)}_{0}$$
- $x, y \in A,\ z \in B$
$$\underbrace{\delta_{A,B}(x,y)}_{0} \leq \underbrace{\delta_{A,B}(x,z)}_{1} + \underbrace{\delta_{A,B}(y,z)}_{1}$$
- $x, z \in A,\ y \in B$
$$\underbrace{\delta_{A,B}(x,y)}_{1} \leq \underbrace{\delta_{A,B}(x,z)}_{0} + \underbrace{\delta_{A,B}(y,z)}_{1}$$
- $x \in A,\ y, z \in B$
$$\underbrace{\delta_{A,B}(x,y)}_{1} \leq \underbrace{\delta_{A,B}(x,z)}_{1} + \underbrace{\delta_{A,B}(y,z)}_{0}$$

Analogous cases switching A and B.

Oss. Given $d \in M(X)$, for every $x, y, z \in X$ we have the following triangle inequalities

$$\begin{cases} d(x,y) \leq d(x,z) + d(y,z) \\ d(x,z) \leq d(x,y) + d(y,z) \\ d(y,z) \leq d(x,y) + d(x,z) \end{cases}$$

If $d(x,y) = 0$, from the last two we get $d(x,z) = d(y,z)$.

Not. For every split $\{A, B\}$ of X, we define

$$\Gamma_{A,B} := \{\, \gamma \in M(X) \mid \gamma(x,y) = 0 \ \text{ if } x,y \in A \text{ or } x,y \in B\}$$

These are the pseudo-metrics that vanish
where the split metric $\delta_{A,B}$ vanishes (the other entries can be anything).

Lemma These pseudo-metrics are multiples of the relative split metric

$$\gamma \in \Gamma_{A,B} \implies \exists \lambda \geq 0 : \gamma = \lambda \delta_{A,B}$$

$$\Gamma_{A,B} = \text{cone}(\delta_{A,B})$$

Dim. Let us fix $a_0 \in A$.
Since $\forall\, b, b' \in B,\ d(b,b') = 0$, we have

$$d(a_0, b) = d(a_0, b'),\ \ \forall\, b, b' \in B$$

Symmetrically, for $b_0 \in B$ we have

$$d(b_0, a) = d(b_0, a'),\ \ \forall\, a, a' \in A$$

Thus $d(a,b) = d(a',b'),\ \ \forall\, a, a' \in A,\ \forall\, b, b' \in B$.

This means that either d vanishes everywhere or, where d does not vanish, it can assume only one value – say λ; and so

$$\gamma = \lambda \delta_{A,B}$$

Prop. The split metrics are extreme rays of $M(X)$.*

Dim. Let us consider a split $\{A, B\}$ and the associated split metric $\delta_{A,B}$. From the previous **Lemma** we have

$$\Gamma_{A,B} = \left\{ \lambda\delta_{A,B} \,\middle|\, \lambda \geq 0 \right\}$$

so we need to show

$$\gamma_1 + \gamma_2 \in \Gamma_{A,B} \implies \gamma_1 \in \Gamma_{A,B} \text{ or } \gamma_2 \in \Gamma_{A,B}$$

Suppose $\gamma_1 + \gamma_2 = \lambda\delta_{A,B}$. Then for every $a, a' \in A$

$$\gamma_1(a, a') + \gamma_2(a, a') = \lambda\delta_{A,B}(a, a') = 0$$

but since γ_1, γ_2 are non-negative, we have

$$\gamma_1(a, a') = \gamma_2(a, a') = 0$$

Idem for every $b, b' \in B$.

Thus γ_1 and γ_2 vanish where $\delta_{A,B}$ vanishes, that is

$$\gamma_1 \in \Gamma_{A,B} \text{ and } \gamma_2 \in \Gamma_{A,B}$$

Oss. The number of split metrics is $2^{n-1} - 1$.

In fact, the set of split metrics is in bijection with the set of splits of X. In creating a split, for every element of X we have two choices: put it in A or put it in B.
We have 2^n possible arrangements. We need to subtract the cases corresponding to $(\emptyset, X)$ and $(X, \emptyset)$, and divide by two, since the split $\{A, B\}$ is the same as $\{B, A\}$.
In the end we get

$$\frac{2^n - 2}{2} = 2^{n-1} - 1$$

---

* For this reason, they may be also called extremal metrics.

Lemma The functions $\varepsilon_{ij} : X \times X \to \mathbb{R}$, $i \neq j \in X$ defined by

$$\varepsilon_{ij}(\boldsymbol{x}) = \begin{cases} 1\,, & \text{if } \boldsymbol{x} = (i,j) \text{ or } \boldsymbol{x} = (j,i) \\ 0\,, & \text{otherwise} \end{cases}$$

can be expressed as linear combinations of the split metrics

$$\{\delta_i\}_{i \in X}$$

Prop. $\langle M(X) \rangle$ is a vector subspace of $\mathbb{R}^{X \times X}$ with the following properties:

- $\langle M(X) \rangle = \left\{ f : X \times X \to \mathbb{R} \;\middle|\; \begin{matrix} f(x,y) = f(y,x), \ \forall\, x,y \in X \\ \wedge\ f(x,x) = 0, \ \forall\, x \in X \end{matrix} \right\}$
- $\dim_{\mathbb{R}} \langle M(X) \rangle = \binom{n}{2}$

Dim. Let us indicate the set of symmetric functions vanishing on the diagonal with $S_0(X)$.
It is clear that $M(X) \subseteq S_0(X)$ and $S_0(X)$ is closed under linear combinations. So $\langle M(X) \rangle \subseteq S_0(X)$.

Notice that $\{\varepsilon_{ij}\}_{i<j}$ is a basis for $S_0(X)$. In fact, the functions in $S_0(X)$ can be represented as symmetric matrices with zeroes on the diagonal; while the function ε_{ij} can be represented as a symmetric matrix with 1 in positions (i,j) and (j,i), and zeroes elsewhere.

This also shows that

$$\dim_{\mathbb{R}} S_0(X) = \#\{\varepsilon_{ij}\}_{i<j} = \binom{n}{2}$$

From the previous **Lemma** we can express the functions $\{\varepsilon_{ij}\}_{i<j}$ as linear combinations of split metrics, thus every function in $S_0(X)$; that is $S_0(X) \subseteq \langle M(X) \rangle$.

Oss. For $n = 2$, say $X = \{a, b\}$, all the pseudo-metrics are multiple of the only split metric $\delta_{\{a\},\{b\}}$;
so $M(X)$ is just a one-dimensional ray.

For $n = 3$, say $X = \{a, b, c\}$, the split metrics

$$\delta_a = \delta_{\{a\},\{b,c\}}, \qquad \delta_b = \delta_{\{b\},\{a,c\}}, \qquad \delta_c = \delta_{\{c\},\{a,b\}}$$

generate the cone $M(X)$.
In fact, let us consider a pseudo-metric $d \in M(X)$;
then we want to show that $\exists\, \lambda, \mu, \nu \geq 0$ such that

$$d = \lambda\delta_a + \mu\delta_b + \nu\delta_c$$

In particular, by evaluating

$$\begin{aligned} d_{ab} &\coloneqq d(a, b) = \\ &= \lambda\delta_{\{a\},\{b,c\}}(a, b) + \mu\delta_{\{b\},\{a,c\}}(a, b) + \nu\delta_{\{c\},\{a,b\}}(a, b) = \\ &= \lambda \cdot 1 + \mu \cdot 1 + \nu \cdot 0 = \\ &= \lambda + \mu \end{aligned}$$

and analogously for the other couples,
we get the following system of equations

$$\begin{cases} d_{ab} = \lambda + \mu \\ d_{ac} = \lambda + \nu \\ d_{bc} = \mu + \nu \end{cases}$$

Solving for λ, μ, ν we get

$$\lambda = \frac{d_{ab} + d_{ac} - d_{bc}}{2}, \qquad \mu = \frac{d_{ab} - d_{ac} + d_{bc}}{2},$$
$$\nu = \frac{-d_{ab} + d_{ac} + d_{bc}}{2}$$

Moreover, from triangle inequality on d, we have $\lambda, \mu, \nu \geq 0$.
This shows that these split metrics are the only extreme rays (every other pseudo-metric is a conical combination of them).

The same calculation also shows that
the split metrics are linearly independent in $\langle M(X)\rangle$. In fact, if

$$\lambda\delta_a + \mu\delta_b + \nu\delta_c = 0$$

where 0 is the identically zero pseudo-metric, then

$$\lambda = 0, \qquad \mu = 0, \qquad \nu = 0$$

In particular, for $n = 3$ the decomposition in split metrics is unique.

Oss. $M(X)$ is a simplicial cone if and only if $n = 2, 3$. In fact,

$$\#\{\text{extreme rays}\} \geq \#\{\text{split metrics}\} = 2^{n-1} - 1$$

and for $n \geq 4$ this number is greater than

$$\dim_{\mathbb{R}}\langle M(X)\rangle = \binom{n}{2} = \frac{n(n-1)}{2}$$

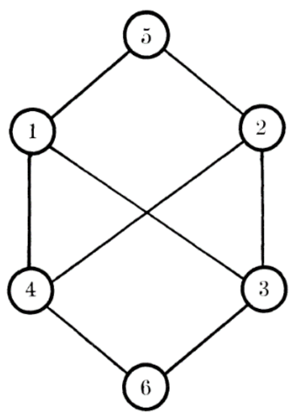
But for $n = 2, 3$ the number of extreme rays coincide with the number of split metrics and

$$n = 2, \qquad 2^{2-1} - 1 = 1 = \binom{2}{2}$$

$$n = 3, \qquad 2^{3-1} - 1 = 3 = \binom{3}{2}$$

Esistono metriche estremali che non sono split?
L'esempio a p. 17 di [Avis80] sembra mostrare nel caso $n = 6$ una metrica (indotta da un grafo) che è estremale ma non split (il grafo è bipartito ma non completo).

Infatti le split metric si possono rappresentare come grafi bipartiti completi.



If $X = \{i, j, k, l\}$ has cardinality 4, then $\langle M(X) \rangle$ has dimension $\binom{n}{2} = 6$, while we have 7 extreme rays of metrics in $M(X)$, corresponding to the $2^{n-1} - 1 = 7$ splits of X. Hence one and the same metric may be expressed in many different ways as a sum of extremal metrics. For instance, if $d: X \times X \to \mathbb{R}$ is defined by

$$d(x, y) := \begin{cases} 2 & \text{if} \quad x \neq y, \\ 0 & \text{if} \quad x = y, \end{cases}$$

then for all $\alpha, \beta \geqslant 0$ with $\alpha + \beta = 1$ one has

$$\begin{aligned} d = \alpha \cdot \delta_{\{i\},\{j,k,l\}} + \alpha \cdot \delta_{\{j\},\{i,k,l\}} + \alpha \cdot \delta_{\{k\},\{i,j,l\}} + \alpha \cdot \delta_{\{l\},\{i,j,k\}} \\ + \beta \cdot \delta_{\{i,j\},\{k,l\}} + \beta \cdot \delta_{\{i,k\},\{j,l\}} + \beta \cdot \delta_{\{i,l\},\{j,k\}}, \end{aligned}$$

and so in particular

$$d = \delta_{\{i\},\{j,k,l\}} + \delta_{\{j\},\{i,k,l\}} + \delta_{\{k\},\{i,j,l\}} + \delta_{\{l\},\{i,j,k\}}$$

as well as

$$d = \delta_{\{i,j\},\{k,l\}} + \delta_{\{i,k\},\{j,l\}} + \delta_{\{i,l\},\{j,k\}}.$$

The counterexample above shows that for $n \geq 4$ the decomposition in split metrics is <u>not</u> necessarily unique.

https://en.wikipedia.org/wiki/Conical_combination
https://www.damtp.cam.ac.uk/user/hf323/M18-OPT/lecture2.pdf
https://people.math.carleton.ca/~kcheung/math/notes/MATH5801/10/10_2_extreme_rays.html

https://www.mat.uniroma2.it/~tvmsscho/Rome-Moscow_School/2012/files/RM12-Cones-Matrices.pdf
https://math.stackexchange.com/questions/4362253/simplicial-polyhedral-cones

It is well known (cf. [23] or [11]) that any metric d on X can *uniquely* be represented by a "network" as depicted in Fig. 2; that is, d has a canonical decomposition as a sum of nonnegative multiples of 6 split metrics, chosen according to the particular structure of d. Indeed, if in case $\{i, j, k, l\} = \{u, v, x, y\}$ and

$$\max\{d(i,j)+d(k,l),\ d(i,k)+d(j,l),\ d(i,l)+d(j,k)\} = d(u,v)+d(x,y),$$

one excludes the split metric $\delta_{\{u,v\},\{x,y\}}$ from participating in the decomposition, one has the unique decomposition

$$\begin{aligned} d = {} & \tfrac{1}{2}\cdot(d(u,x)+d(u,y)-d(x,y))\cdot\delta_{\{u\},\{v,x,y\}} \\ & +\tfrac{1}{2}\cdot(d(v,x)+d(v,y)-d(x,y))\cdot\delta_{\{v\},\{u,x,y\}} \\ & +\tfrac{1}{2}\cdot(d(x,u)+d(x,v)-d(u,v))\cdot\delta_{\{x\},\{u,v,y\}} \\ & +\tfrac{1}{2}\cdot(d(y,u)+d(y,v)-d(u,v))\cdot\delta_{\{y\},\{u,v,x\}} \\ & +\tfrac{1}{2}\cdot(d(u,v)+d(x,y)-d(u,x)-d(v,y))\cdot\delta_{\{u,x\},\{v,y\}} \\ & +\tfrac{1}{2}\cdot(d(u,v)+d(x,y)-d(u,y)-d(v,x))\cdot\delta_{\{u,y\},\{v,x\}}. \end{aligned}$$

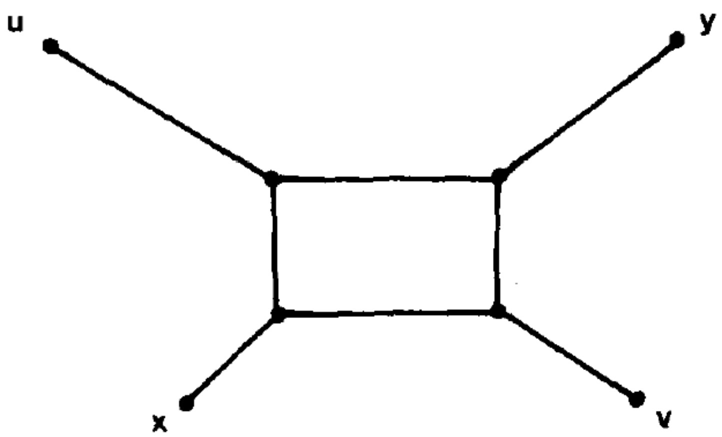


FIG. 2. A generic metric on four points.

Dimostrare la decomposizione.

Per spiegare la roba che viene dopo è meglio aver letto il resto del paper.

This observation is also important in view of the applications of metrics in data analysis, since it allows one to assign well-defined "preference indices" to each of the three possible nondegenerate tree topologies which can be established over X (see Fig. 3) and which correspond to the three nontrivial splits $\{\{i, j\}, \{k, l\}\}$, $\{\{i, k\}, \{j, l\}\}$, and $\{\{i, l\}, \{j, k\}\}$ of X. Namely, the respective preference index is the coefficient of the corresponding split metric in the above canonical decomposition of d, so that the index of the "maximal" and therefore "most unlikely" split $\{u, v\}$, $\{x, y\}$ will always be zero, while the coefficients of the other two splits depend on the difference between the corresponding distance sum and $d(u, v) + d(x, y)$.

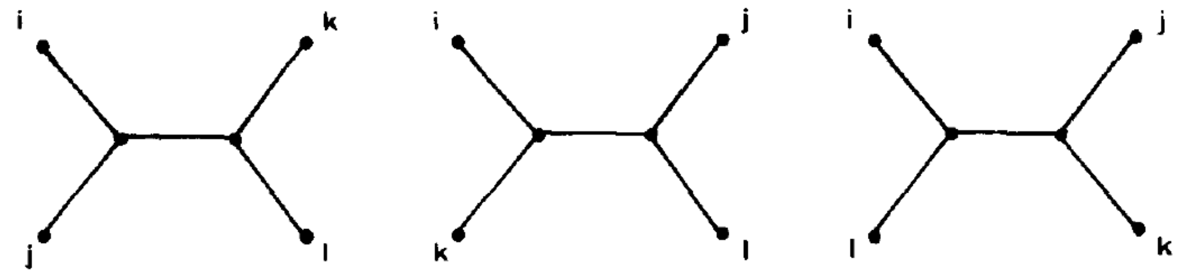
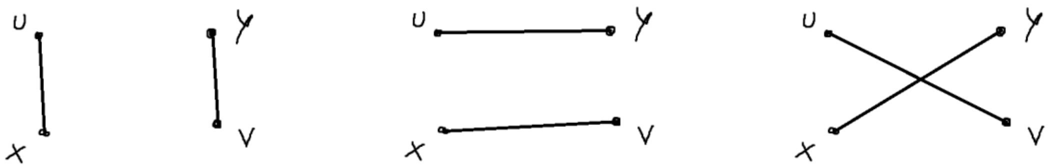
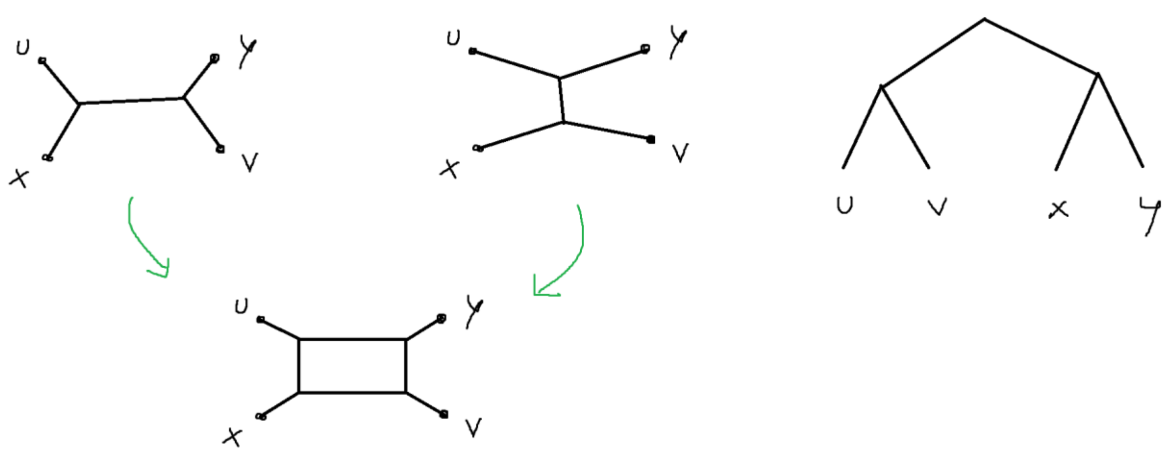


FIG. 3. The nondegenerate tree topologies with four labels.



$ux + vy$ $\qquad$ $uy + vx < uv + xy$

non può essere



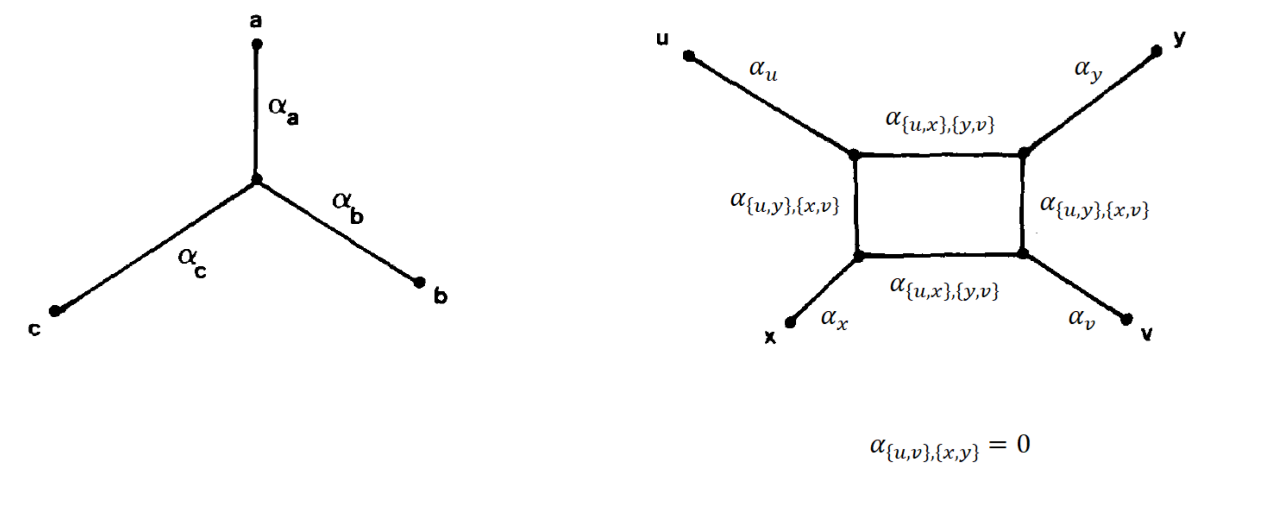
The applications of metrics in hierarchical clustering make it desirable to have similar "canonical" preference indices also in case X has more than four elements. It is the purpose of this paper to provide such indices and to discuss their basic properties. To this end we first observe that a split metric $\delta_{A,B}$ occurs in the above decomposition of d, defined on $X = \{i, j, k, l\}$, with a nonzero coefficient if and only if

$$d(a, a') + d(b, b') < \max\{d(a, b) + d(a', b'), d(a, b') + d(a', b)\}$$

for all $a, a' \in A$ and $b, b' \in B$, that is, if and only if the *isolation index*

$$\alpha_{A,B} = \alpha^d_{A,B} := \tfrac{1}{2} \cdot \min\{\max\{d(a, b) + d(a', b'), d(a, b') + d(a', b), d(a, a') + d(b, b')\} - d(a, a') - d(b, b') \mid a, a' \in A; b, b' \in B\}$$

of A, B with respect to d is positive. In this case the split A, B of X will be called a *d-split*, also if $\# X > 4$. Then for $\# X = 4$ the above decomposition of a metric d on X can be reformulated as $d = \sum \alpha_{A,B} \cdot \delta_{A,B}$, where the sum runs over all (d-)*splits* of X.



Note that for arbitrary X a similar formula holds if d satisfies the so-called *four-point condition*

$$d(a, a') + d(b, b') \leqslant \max\{d(a, b) + d(a', b'), d(a, b') + d(b, a')\}$$

for all $a, a', b, b' \in X$; that is, the two larger ones of the three expressions $d(a, a') + d(b, b')$, $d(a, b) + d(a', b')$, and $d(a, b') + d(a', b)$ are equal for all $a, a', b, b' \in X$. This condition is well known to be characteristic for tree metrics; cf. [10]. Indeed, if d is a tree metric, then a split A, B of X is a d-split if and only if

$$d(a, a') + d(b, b') < d(a, b) + d(a', b') = d(a, b') + d(b, a')$$

for all $a, a' \in A$ and $b, b' \in B$, in which case this split corresponds to a unique edge of length $\alpha_{A,B}$ in the tree representing d (see [9]). Hence the basic results concerning metrics d satisfying the four-point condition can be summarized as follows:

Such a metric can be written in the form

$$d = \sum \alpha^d_{A,B} \cdot \delta_{A,B},$$

where the sum runs through the collection $\mathscr{S}_d$ of all d-splits A, B. Moreover, a family $\mathscr{S}$ of splits is of the form $\mathscr{S} = \mathscr{S}_d$ for some metric d satisfying the four-point condition if and only if any two splits A, B and A', B' in $\mathscr{S}$ are *compatible* in the sense that one of the four intersections $A \cap A'$, $A \cap B'$, $B \cap A'$, $B \cap B'$ is empty, in which case any nonnegative linear combination $d := \sum_{A,B \in \mathscr{S}} \alpha_{A,B} \cdot \delta_{A,B}$ satisfies the four-point condition as well as the equalities $\alpha^d_{A,B} = \alpha_{A,B}$ for all A, B in $\mathscr{S}$ and $\alpha^d_{A,B} = 0$ for all other splits of X.

Fact A pseudo-metric d is a tree metric if and only if it satisfies the four-point condition, that is for every $t, u, v, w \in X$

$$tu + vw \leq \max\{tv + uw, tw + uv\}$$

Fact Let d be a tree metric. Then a split $\{A, B\}$ is a d-split if and only if for every $a, a' \in A$ and $b, b' \in B$

$$aa' + bb' < ab + a'b' = ab' + a'b$$

In this case the split corresponds to a unique edge of length $\alpha_{A,B}$ in the tree representing d.

Prop. If d is a pseudo-metric satisfying the four-point condition, then it can be written as

$$d = \sum_{S \in \mathcal{S}_d(X)} \alpha_S^d \cdot \delta_S$$

Moreover, a collection of splits $\mathcal{S}$ is of the form $\mathcal{S} = \mathcal{S}_d(X)$ where d is a pseudo-metric satisfying the four-point condition, if and only if the splits in $\mathcal{S}$ are compatible.

Dim. The first assertion is a consequence of **Teo**. 2 and **Cor**. 7.

($\Rightarrow$) It is a consequence of **Cor**. 7.

($\Leftarrow$) Since compatible implies weakly compatible, it is a consequence of **Teo**. 3 + **Cor**. 7.

In other words, tree metrics are totally decomposable and a set of splits coincide with the d-splits of some tree metric if and only if they are compatible.

Problems of applying metrics in cluster analysis arise when the metric d which is to be analysed does not satisfy the four-point condition. In such a case it has been suggested by Imrich and Stotskii [17] to search for splits A, B of X such that

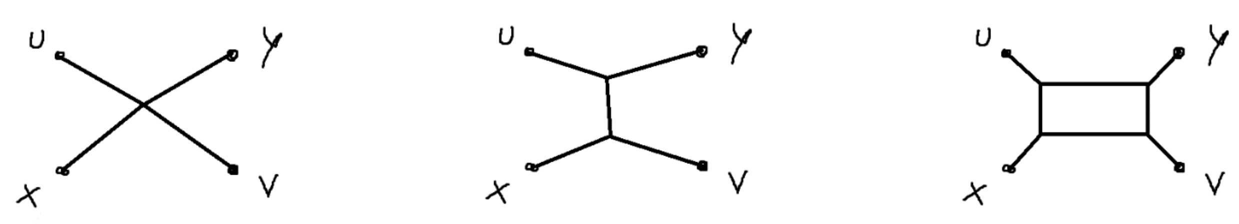
$$d(a, a') + d(b, b') < d(a, b) + d(a', b') = d(a, b') + d(a', b)$$

for all $a, a' \in A$ and $b, b' \in B$. Indeed, if such splits exist, they are very useful to decompose d into a family of simpler metrics (see [12]), and, of course, any two such splits will be compatible, so they will induce a hierarchical structure on X. Unfortunately, this structure is in general far from being "resolved" (using the terminology of [7]); that is, different elements in X will not be distinguishable relative to this structure. If one relaxes the above condition by allowing splits A, B of X for which

$$d(a, a') + d(b, b') < d(a, b) + d(a', b') \qquad \text{for all} \quad a, a' \in A \text{ and } b, b' \in B,$$

one obtains a system of pairwise compatible splits, inducing an even "finer" hierarchical structure on X. But still one would loose much valuable information, as is demonstrated by the above discussion of the case $\# X = 4$ (and similar considerations in case $\# X = 5$) and by many examples from biological taxonomy. Indeed, the set $M_1(X)$ of metrics which can be reconstructed from this information has dimension $2n - 3$, while the set $M(X)$ of all metrics on X has dimension $\binom{n}{2}$, so $M_1(X)$ is a rather complicated subset of measure 0 in $M(X)$.

All this suggests that one relax the above condition even further to the defining condition for d-splits. Still, the main reason for doing so is that the



$$aa' + bb' < ab + a'b' = ab' + a'b$$

$$aa' + bb' < ab + a'b', \;\; ab' + a'b$$
$$aa' + bb' < \min\{ab + a'b', ab' + a'b\}$$

$$aa' + bb' < \max\{ab + a'b', ab' + a'b\}$$

defining condition for d-splits. Still, the main reason for doing so is that the family of d-splits (along with their isolation indices) possesses an amazing wealth of attractive structural features. Among those features we want to emphasize the following ones:

- It is quite clear that $\mathscr{S}_d \subseteq \mathscr{S}_{d'}$ for all metrics $d' \in M(X)$ which are sufficiently close to d and that for a given d-split S the map $d - \varepsilon\delta_S$ is a metric and has isolation index $\alpha_S^d - \varepsilon$ relative to S for all $\varepsilon \leqslant \alpha_S^d$. Certainly much less obvious is the fact that the isolation indices of all other splits remain constant when ε varies in $(-\infty, \alpha_S^d]$. In particular, the *residue* $d_0 := d - \sum_S \alpha_S^d \cdot \delta_S$ of d with respect to its splits is always in $M(X)$ and it is *split-prime*; that is, it has isolation index 0 with respect to every split of X.

Prop. Let d be a pseudo-metric, S a d-split and $\varepsilon \leq \alpha_S^d$.

Then $d' := d - \varepsilon\delta_S$ is a pseudo-metric,

$\alpha_S^{d'} = \alpha_S^d - \varepsilon$ and $\alpha_T^{d'} = \alpha_T^d$, $\forall\, T \neq S$.

In particular, the residue $d_0 := d - \sum_{S \in S(X)} \alpha_S^d \cdot \delta_S$

is a pseudo-metric and it is split-prime,

that is $\alpha_S^{d_0} = 0$, $\forall\, S \in S(X)$.

Dim. It is a consequence of **Teo**. 2.

- If $\#\mathscr{S}_d = \binom{n}{2}$, then the residue d_0 of d is zero, and there exists a bijection between X and the set $Z_n := \{\zeta \in \mathbb{C} \mid \zeta^n = 1\}$ of all nth roots of unity in the complex plane such that the splits in $\mathscr{S}_d$ correspond precisely to splits of Z_n induced by straight lines through the unit disc. This happens, for instance, when $X = Z_n$ and $d(\zeta, \zeta') := |\zeta - \zeta'|$, in which case the above bijection can be chosen to be the identity. In general, we can deform d homotopically so that eventually X becomes isometric to $(Z_n, |...|)$, keeping the set of splits fixed all the way.

La prima riga è il **Cor**. 5; il resto è conseguenza di (ii) -> (i) del **Teo**. 5 con una riformulazione di circular split. L'ultima frase non viene dimostrata.

- More generally, metrics d with a vanishing split-prime residue

$$d_0 = d - \sum_{S \in \mathscr{S}_d} \alpha_S^d \cdot \delta_S = 0$$

are characterized by the following "*five-point condition*":

$$\alpha^d_{\{t,u\},\{v,w\}} \leqslant \alpha^d_{\{t,x\},\{v,w\}} + \alpha^d_{\{t,u\},\{v,x\}}$$

for all $t, u, v, w, x \in X$ (where $\alpha_{\{a,a'\},\{b,b'\}} := \frac{1}{2} \cdot (\max\{d(a,a') + d(b,b'), d(a,b) + d(a',b'), d(a,b') + d(a',b)\} - d(a,a') - d(b,b'))$). Such metrics will be called *totally (split-)decomposable*.

Questo è (i) => (iv) del **Teo**. 6.

- Finally, the decomposition $d = d_0 + \sum \alpha_S^d \cdot \delta_S$ is closely related to the polytopal structure of the injective hull (alias "tight span") $T(d)$ of (X, d). To be more specific, let $P(d)$ denote the (non-compact) convex polytope in $\mathbb{R}^X$ which consists of all maps $f: X \to \mathbb{R}$ satisfying $d(x, y) \leqslant f(x) + f(y)$ for all $x, y \in X$. Then

$$P(d) = P(d_0) + \sum P(\alpha_S^d \cdot \delta_S), \tag{$*$}$$

and if $d = d_0' + \sum \alpha_S' \cdot \delta_S$ is a further decomposition of d into a split-prime metric d_0 and a sum of nonnegative multiples $\alpha_S' \cdot \delta_S$ of split metrics δ_S, also satisfying

$$P(d) = P(d_0') + \sum P(\alpha_S' \cdot \delta_S),$$

then $d_0' = d_0$ and $\alpha_S' = \alpha_S^d$ for every split S. So, the decomposition we have constructed above can be characterized axiomatically as the unique decomposition into a split-prime metric and a sum of (nonnegative multiples of) split metrics satisfying $(*)$.

Questo è il **Teo**. 8.

2. DECOMPOSITION VIA d-SPLITS

In what follows d is a symmetric function from $X \times X$ to $\mathbb{R}$, where X is a finite set. For the sake of brevity, whenever possible without causing misunderstanding, we will always write uv instead of $d(u, v)$ for $u, v \in X$. To every pair A, B of nonempty subsets of X we associate the *isolation index* $\alpha^d_{A,B}$ (or $\alpha_{A,B}$ for short) with respect to d, defined as follows:

$$\alpha_{A,B} := \tfrac{1}{2} \cdot \min_{\substack{a, a' \in A, \\ b, b' \in B}} (\max\{ab + a'b', a'b + ab', aa' + bb'\} - aa' - bb').$$

Since the quantities over which the minimum is taken in this expression occur frequently in the sequel, we reserve a special symbol for them, namely:

$$\beta_{\{a,a'\},\{b,b'\}} := \tfrac{1}{2} \cdot (\max\{ab + a'b', a'b + ab', aa' + bb'\} - aa' - bb').$$

Then the isolation index $\alpha_{A,B}$ is just the minimum of all $\beta_{\{a,a'\},\{b,b'\}}$ with $a, a' \in A$ and $b, b' \in B$. Note that $\beta_{\{a,a'\},\{b,b'\}} \geqslant 0$ and $\alpha_{A,B} \geqslant 0$ for all a, a', b, $b' \in X$ and $A, B \subseteq X$, and that $\alpha_{A,B} = 0$ whenever $A \cap B \neq \varnothing$. Further, notice that we do not require here that in these expressions a and a' (or b and b') be different. If d is a metric, then the β-indices coincide with the corresponding isolation indices:

$$\alpha_{\{t,u\},\{v,w\}} = \beta_{\{t,u\},\{v,w\}} \quad \text{for all } t, u, v, w \in X \text{ whenever } xy + yz \geqslant xz \text{ and } xx = 0 \text{ for all } x, y, z \in X.$$

Indeed,

$$\begin{aligned} tv + uw - tu - vw &\leqslant tv + tw - vw = 2 \cdot \beta_{\{t\},\{v,w\}} \\ &\leqslant 2 \cdot tv = 2 \cdot \beta_{\{t\},\{v\}}. \end{aligned}$$

Consequently, if d is a metric and $\min\{\#A, \#B\} \geqslant 2$, then $\alpha_{A,B}$ equals $\alpha_{\{a,a'\},\{b,b'\}}$ for some $a \neq a'$ in A and $b \neq b'$ in B.

An unordered pair A, B for which $\alpha_{A,B}$ is positive is called a *partial d-split*. The pair A, B is a *d-split* if, in addition, $A \cup B = X$. In this case both A and B must be *d-convex*; that is, whenever for two points x, y either in A or in B we have $xz + zy = xy$ for some $z \in X$, then this element z is also contained in A or in B, respectively. We say that a partial d-split A, B *extends* another partial d-split A', B' if $A' \subseteq A$ and $B' \subseteq B$. Note that in this case $\alpha_{A',B'} \geqslant \alpha_{A,B}$.

Let $d : X \times X \to \mathbb{R}$ be a symmetric function.

Not. $uv := d(u,v), \ \forall\, u, v \in X$

In the following we will implicitly refer to d.

Def. (isolation index)

Let A, B be non-empty subset of X. Then for every $a, a' \in A$ and $b, b' \in B$

$$\beta_{\{a,a'\},\{b,b'\}} := \frac{1}{2}\left(\max\{ab + a'b', a'b + ab', aa' + bb'\} - aa' - bb' \right)$$

$$\alpha_{A,B} := \min_{\substack{a,a' \in A \\ b,b' \in B}} \beta_{\{a,a'\},\{b,b'\}}$$

We call $\alpha_{A,B} = \alpha^d_{A,B}$ the **isolation index** with respect to d.

Oss. We have $\beta_{\{a,a'\},\{b,b'\}} \geq 0, \ \forall\, a, a' \in A, \ b, b' \in B$
since we are subtracting a term that is inside the maximum:

$$\max\{ab + a'b', a'b + ab', aa' + bb'\} \geq aa' + bb'$$

It follows that also $\alpha_{A,B} \geq 0, \ \forall\, A, B \subseteq X$.

Oss. If A and B intersect, then $\alpha_{A,B} = 0$.

In fact, let $x \in A \cap B$. Then

$$\begin{aligned}\beta_{\{x\},\{x\}} &= \frac{1}{2}\left(\max\{xx + xx, xx + xx, xx + xx\} - xx - xx \right) \\ &= \frac{1}{2}(xx + xx - xx - xx) = 0\end{aligned}$$

and so $\alpha_{A,B} = 0$.

Prop. If d is a pseudo-metric, then $\forall\ t, u, v, w \in X$

$$\alpha_{\{t,u\},\{v,w\}} = \beta_{\{t,u\},\{v,w\}}$$

Dim. By (reverse) triangle inequality and the fact that d vanishes on the diagonal, we observe that

$$\begin{aligned}\beta_{\{t\},\{v,w\}} &= \frac{1}{2}\left(\max\{tv + tw, tv + tw, \cancel{tt} + vw\} - \cancel{tt} - vw \right) \\ &= \frac{1}{2}(tv + tw - vw) \\ &\leq \frac{1}{2}(tv + tv) \\ &= \frac{1}{2}\left(\max\{tv + tv, tv + tv, \cancel{tt} + \cancel{vv}\} - \cancel{tt} - \cancel{vv} \right) \\ &= \beta_{\{t\},\{v\}}\end{aligned}$$

where we used $tv + tw \geq vw$ in the first line
and $tw - vw \leq tv$ in the second one.

With analogous calculations we get

$$\begin{aligned}\beta_{\{t\},\{v,w\}} \leq \beta_{\{t\},\{v\}}, &\quad \beta_{\{t\},\{v,w\}} \leq \beta_{\{t\},\{w\}} \\ \beta_{\{u\},\{v,w\}} \leq \beta_{\{u\},\{v\}}, &\quad \beta_{\{u\},\{v,w\}} \leq \beta_{\{u\},\{w\}} \\ \beta_{\{t,u\},\{v\}} \leq \beta_{\{t\},\{v\}}, &\quad \beta_{\{t,u\},\{v\}} \leq \beta_{\{u\},\{v\}} \\ \beta_{\{t,u\},\{w\}} \leq \beta_{\{t\},\{w\}}, &\quad \beta_{\{t,u\},\{w\}} \leq \beta_{\{u\},\{w\}}\end{aligned}$$

Again by (reverse) triangle inequality

$$\begin{aligned} tv + uw - tu - vw &\leq tv + tw - vw = 2\beta_{\{t\},\{v,w\}} \\ &\leq uv + uw - vw = 2\beta_{\{u\},\{v,w\}} \\ &\leq tv + uv - tu = 2\beta_{\{t,u\},\{v\}} \\ &\leq tw + uw - tu = 2\beta_{\{t,u\},\{w\}} \\ uv + tw - tu - vw &\leq tv + tw - vw = 2\beta_{\{t\},\{v,w\}} \\ &\leq uv + uw - vw = 2\beta_{\{u\},\{v,w\}} \\ &\leq tv + uv - tu = 2\beta_{\{t,u\},\{v\}} \\ &\leq tw + uw - tu = 2\beta_{\{t,u\},\{w\}} \end{aligned}$$

Since

$$\beta_{\{t,u\},\{v,w\}} = \frac{1}{2}\left(\max\{tv + uw, uv + tw, tu + vw\} - tu - vw \right)$$

we have proven that $\beta_{\{t,u\},\{v,w\}}$ is smaller than all other possible β indices for the quartet $\big\{\{t,u\},\{v,w\}\big\}$.

This implies by definition of the isolation index

$$\alpha_{\{t,u\},\{v,w\}} = \beta_{\{t,u\},\{v,w\}}$$

Cor. If d is a pseudo-metric and $\min\{|A|,|B|\} \geq 2$ (that is both A and B have at least 2 elements), then

$$\alpha_{A,B} = \alpha_{\{a,a'\},\{b,b'\}}$$

for some $a \neq a' \in A$ and $b \neq b' \in B$.

Dim. Let $\big\{\{a,a'\},\{b,b'\}\big\}$ be the quartet that minimizes the β index.

Then, for the previous inequalities about β indices and the hypothesis on the number of elements of A and B, we conclude that $a \neq a'$ and $b \neq b'$.

Using the previous **Prop**.

$$\alpha_{A,B} = \beta_{\{a,a'\},\{b,b'\}} = \alpha_{\{a,a'\},\{b,b'\}}$$

Def. (splits and d-splits)

A **partial split** (of X) is a pair $\{A, B\}$ with $A, B \subseteq X$.
A **(total) split** (of X) is partial split $\{A, B\}$ such that $A \cup B = X$.

A partial/total ***d*-split** is a partial/total split $\{A, B\}$ such that $\alpha^d_{A,B} > 0$.
Notice that in this case A and B must be disjoint.

We call a split **trivial** if one of the parts contains only one element.
A partial split of the form $\{\{a, a'\}, \{b, b'\}\}$ is called **quartet**.

We denote the set of all splits of X with $\mathcal{S}(X)$
and the set of all d-splits of X with $\mathcal{S}_d(X)$.

Given $Y \subset X$ and a split $\{A, B\}$ of Y, we have $\alpha^d_{A,B} = \alpha^{d|_{Y\times Y}}_{A,B}$.
For this reason, we may refer to the $d|_{Y\times Y}$-splits as d-split of Y
and indicate them with $\mathcal{S}_d(Y)$.

Def. (d-convex set)

A set $S \subseteq X$ is ***d*-convex** if

$$\forall\, x, y \in S,\ \ \forall\, z \in X, \qquad xz + zy = xy \implies z \in S$$

Prop. If $\{A, B\}$ is a d-split, then A and B are d-convex.

Dim. Let $x, y \in A$ and $z \in X$ such that $xz + zy = xy$.

Since $X = A \cup B$, we have $z \in A$ or $z \in B$.
If by absurd $z \in B$, then

$$\beta_{\{x,y\},\{z\}} = \frac{1}{2}\left(\max\{xz + yz, xz + yz, xy + \cancel{zz}\} - xy - \cancel{zz} \right)$$
$$= \frac{1}{2}(xz + yz - xy) = \frac{1}{2}(xy - xy) = 0$$

that implies $\alpha_{A,B} = 0$. ↯

Then it must be $z \in A$ and so A is d-convex.

Def. (extension of d-splits)

We say that a partial d-split $\{A, B\}$ **extends** another partial d-split $\{A', B'\}$ if $A \supseteq A'$ and $B \supseteq B'$ (or $A \supseteq B'$ and $B \supseteq A'$).
We denote it $\{A, B\} \succcurlyeq \{A', B'\}$.

Notice that $\alpha_{A,B} \leq \alpha_{A',B'}$ (it's a minimum on a larger set).

Our first result, linking the isolation indices of partial d-splits and their extensions to d-splits, paves the way to the basic decomposition theorem we aim at.

THEOREM 1. *Let $d: X \times X \to \mathbb{R}$ be a symmetric function on a set X and let A_0, B_0 be a partial d-split. Then*

$$\sum \{\alpha_{A,B} \mid A, B \text{ is a } d\text{-split extending } A_0, B_0\} \leqslant \alpha_{A_0,B_0}.$$

Proof. First we claim that for all $a_1, a_2 \in A_0$, $b_1, b_2 \in B_0$, and $x \in X - (A_0 \cup B_0)$ we have

$$\alpha_{\{a_1,a_2,x\},\{b_1,b_2\}} + \alpha_{\{a_1,a_2\},\{b_1,b_2,x\}} \leqslant \beta_{\{a_1,a_2\},\{b_1,b_2\}}. \qquad (\star)$$

Suppose this inequality fails for some a_1, a_2, b_1, b_2, x. Then necessarily all three quantities are positive. Let $\{i, j\} = \{1, 2\}$ so that

$$\beta_{\{a_1,x\},\{b_1,b_2\}} = \tfrac{1}{2} \cdot (a_1 b_j + x b_i - a_1 x - b_1 b_2).$$

It follows that

$$\begin{aligned}
&\tfrac{1}{2} \cdot (a_1 b_j + x b_i - a_1 x - b_1 b_2 + \max\{a_1 x + a_2 b_i, a_1 b_i + a_2 x\} - a_1 a_2 - x b_i) \\
&\quad = \beta_{\{a_1,x\},\{b_1,b_2\}} + \beta_{\{a_1,a_2\},\{x,b_i\}} \\
&\quad \geqslant \alpha_{\{a_1,a_2,x\},\{b_1,b_2\}} + \alpha_{\{a_1,a_2\},\{b_1,b_2,x\}} \\
&\quad > \beta_{\{a_1,a_2\},\{b_1,b_2\}} \\
&\quad = \tfrac{1}{2} \cdot (\max\{a_1 b_1 + a_2 b_2, a_1 b_2 + a_2 b_1\} - a_1 a_2 - b_1 b_2).
\end{aligned}$$

Hence

$$a_1 b_j - a_1 x + \max\{a_1 x + a_2 b_i, a_1 b_i + a_2 x\}$$
$$> \max\{a_1 b_1 + a_2 b_2, a_1 b_2 + a_2 b_1\}.$$

This strict inequality can only hold if

$$a_1 x + a_2 b_i < a_1 b_i + a_2 x.$$

Therefore

$$a_1 b_1 + a_1 b_2 - a_1 x + a_2 x = a_1 b_j - a_1 x + a_1 b_i + a_2 x$$
$$> \max\{a_1 b_1 + a_2 b_2, a_1 b_2 + a_2 b_1\},$$

whence

$$a_1 b_k + a_2 x > a_1 x + a_2 b_k \qquad \text{for} \quad k = 1, 2.$$

By symmetry (that is, by interchanging the role of a_1 and a_2) we also obtain the reverse strict inequality. Since this is impossible, our claim (★) is proved.

Next choose $a_1, a_2 \in A_0$ and $b_1, b_2 \in B_0$ such that

$$\alpha_{A_0, B_0} = \beta_{\{a_1, a_2\}, \{b_1, b_2\}}.$$

From (★) we then infer that for every $x \in X - (A_0 \cup B_0)$

$$\alpha_{A_0 \cup \{x\}, B_0} + \alpha_{A_0, B_0 \cup \{x\}} \leqslant \alpha_{\{a_1, a_2, x\}, \{b_1, b_2\}} + \alpha_{\{a_1, a_2\}, \{b_1, b_2, x\}}$$
$$\leqslant \beta_{\{a_1, a_2\}, \{b_1, b_2\}}$$
$$= \alpha_{A_0, B_0}.$$

So, we have established the desired inequality in case that $\#(X - (A_0 \cup B_0)) = 1$. A simple inductive argument on $\#(X - (A_0 \cup B_0))$ finally completes the proof of the theorem:

$$\sum \{\alpha_{A,B} \mid A, B \text{ is a } d\text{-split extending } A_0, B_0\}$$

$$= \sum \{\alpha_{A,B} \mid A, B \text{ is a } d\text{-split extending } A_0 \cup \{x\}, B_0\}$$

$$+ \sum \{\alpha_{A,B} \mid A, B \text{ is a } d\text{-split extending } A_0, B_0 \cup \{x\}\}$$

$$\leqslant \alpha_{A_0 \cup \{x\}, B_0} + \alpha_{A_0, B_0 \cup \{x\}}$$

$$\leqslant \alpha_{A_0, B_0},$$

as claimed. ∎

A particular instance of the preceding theorem is worth mentioning separately:

Corollary 1. *Let A, B be a d-split with respect to a symmetric function $d: X \times X \to \mathbb{R}$. If $a_1, a_2 \in A$ and $b_1, b_2 \in B$ are such that*

$$\alpha_{A,B} = \beta_{\{a_1, a_2\}, \{b_1, b_2\}},$$

then A, B is the unique d-split extending the partial d-split $\{a_1, a_2\}$, $\{b_1, b_2\}$.

Proof. From Theorem 1 we infer

$$\alpha_{A,B} \leqslant \sum \{\alpha_{A',B'} \mid A', B' \text{ is a } d\text{-split extending } \{a_1, a_2\}, \{b_1, b_2\}\}$$

$$\leqslant \alpha_{\{a_1, a_2\}, \{b_1, b_2\}}$$

$$\leqslant \beta_{\{a_1, a_2\}, \{b_1, b_2\}} = \alpha_{A,B}.$$

Hence there is no d-split other than A, B which extends $\{a_1, a_2\}$, $\{b_1, b_2\}$. ∎

Lemma Let $\{A, B\}$ be a partial d-split.
Then for every $a_1, a_2 \in A,\ b_1, b_2 \in B,\ x \in X \setminus (A \cup B)$

$$\alpha_{\{a_1,a_2,x\},\{b_1,b_2\}} + \alpha_{\{a_1,a_2\},\{b_1,b_2,x\}} \leq \beta_{\{a_1,a_2\},\{b_1,b_2\}}$$

Dim. Suppose by absurd that

$$\alpha_{\{a_1,a_2,x\},\{b_1,b_2\}} + \alpha_{\{a_1,a_2\},\{b_1,b_2,x\}} > \beta_{\{a_1,a_2\},\{b_1,b_2\}}$$

Observe that $\beta_{\{a_1,a_2\},\{b_1,b_2\}} > 0$ since $\{A,B\}$ is a d-split, so also

$$\alpha_{\{a_1,a_2,x\},\{b_1,b_2\}} > 0\,, \qquad \alpha_{\{a_1,a_2\},\{b_1,b_2,x\}} > 0$$

From this we have

$$\beta_{\{a_1,x\},\{b_1,b_2\}} \geq \alpha_{\{a_1,a_2,x\},\{b_1,b_2\}} > 0$$

$$\beta_{\{a_1,a_2\},\{x,b_i\}} \geq \alpha_{\{a_1,a_2\},\{b_1,b_2,x\}} > 0, \qquad i = 1,2$$

Let $\{i,j\} = \{1,2\}$ so that

$$\beta_{\{a_1,x\},\{b_1,b_2\}} = \frac{1}{2}(a_1b_j + xb_i - a_1x - b_1b_2)$$

in fact, since $\beta_{\{a_1,x\},\{b_1,b_2\}} > 0$, the maximum

$$\max\{a_1b_1 + xb_2, a_1b_2 + xb_1, a_1x + b_1b_2\}$$

cannot be $a_1x + b_1b_2$.

For the same reason we have

$$\beta_{\{a_1,a_2\},\{x,b_i\}} = \frac{1}{2}(\max\{a_1x + a_2b_i, a_1b_i + a_2x\} - a_1a_2 - xb_i)$$

$$\beta_{\{a_1,a_2\},\{b_1,b_2\}} = \frac{1}{2}(\max\{a_1b_1 + a_2b_2, a_1b_2 + a_2b_1\} - a_1a_2 - b_1b_2)$$

From the previous inequalities we have

$$\beta_{\{a_1,x\},\{b_1,b_2\}} + \beta_{\{a_1,a_2\},\{x,b_i\}} \geq$$
$$\geq \alpha_{\{a_1,a_2,x\},\{b_1,b_2\}} + \alpha_{\{a_1,a_2\},\{b_1,b_2,x\}} > \beta_{\{a_1,a_2\},\{b_1,b_2\}}$$

and by substituting the expressions for the β indices

$$\frac{1}{2}\Big(a_1b_j + \cancel{xb_i} - a_1x - \cancel{b_1b_2}$$
$$+ \max\{a_1x + a_2b_i, a_1b_i + a_2x\} - a_1a_2 - \cancel{xb_i}\Big) >$$
$$> \frac{1}{2}(\max\{a_1b_1 + a_2b_2, a_1b_2 + a_2b_1\} - a_1a_2 - \cancel{b_1b_2})$$

simplifying we obtain

$$a_1 b_j - a_1 x + \max\{a_1 x + a_2 b_i, a_1 b_i + a_2 x\}$$
$$> \max\{a_1 b_1 + a_2 b_2, a_1 b_2 + a_2 b_1\}$$

If by absurd $\max\{a_1 x + a_2 b_i, a_1 b_i + a_2 x\} = a_1 x + a_2 b_i$, the previous inequality would become

$$a_1 b_j - \cancel{a_1 x} + \cancel{a_1 x} + a_2 b_i > \max\{a_1 b_1 + a_2 b_2, a_1 b_2 + a_2 b_1\}$$

but since $a_1 b_j + a_2 b_i$ is a term of the maximum on the right, this is a contradiction. ↯

So we must have $a_1 x + a_2 b_i < a_1 b_i + a_2 x$ and thus

$$a_1 b_j - a_1 x + a_1 b_i + a_2 x = a_1 b_1 + a_1 b_2 - a_1 x + a_2 x$$
$$> \max\{a_1 b_1 + a_2 b_2, a_1 b_2 + a_2 b_1\}$$

For this to be true we need

$$a_1 b_k + a_2 x > a_1 x + a_2 b_k, \qquad k = 1, 2$$

By symmetry, interchanging a_1 and a_2, we obtain the other strict inequality. ↯

Teo. 1 Let $\{A_0, B_0\}$ be a partial d-split. Then

$$\sum \left\{ \alpha_{A,B} \,\middle|\, \{A, B\} \in \mathcal{S}(X)\,,\ \{A, B\} \succcurlyeq \{A_0, B_0\} \right\} \le \alpha_{A_0,B_0}$$

Dim. Let $a_1, a_2 \in A_0$ and $b_1, b_2 \in B_0$ such that

$$\alpha_{A_0,B_0} = \beta_{\{a_1,a_2\},\{b_1,b_2\}}$$

From the previous **Lemma** we have $\forall\, x \in X \setminus (A_0 \cup B_0)$

$$\alpha_{A_0 \cup \{x\},B_0} + \alpha_{A_0,B_0 \cup \{x\}} \le \alpha_{\{a_1,a_2,x\},\{b_1,b_2\}} + \alpha_{\{a_1,a_2\},\{b_1,b_2,x\}}$$
$$\le \beta_{\{a_1,a_2\},\{b_1,b_2\}}$$
$$= \alpha_{A_0,B_0}$$

This proves the theorem in the case $|\, X \setminus (A_0 \cup B_0) \,| = 1$.

We prove the general case by induction on $|\,X \setminus (A_0 \cup B_0)\,|$.
We have already seen the base case.

Let $|\,X \setminus (A_0 \cup B_0)\,| = n > 1$ and $x \in X \setminus (A_0 \cup B_0)$.

Observe that the d-splits extending $\{A_0, B_0\}$ are exactly the union of those extending $\{A_0 \cup \{x\}, B_0\}$ and those extending $\{A_0, B_0 \cup \{x\}\}$.
In fact, since d-splits are partitions, if $\{A, B\}$ extends $\{A_0, B_0\}$ (say WLOG $A \supseteq A_0$ and $B \supseteq B_0$), it must be $x \in A$ or $x \in B$; that is $A \supseteq A_0 \cup \{x\}$ or $B \supseteq B_0 \cup \{x\}$.

Moreover,

$$\left|\,X \setminus \big(\{A_0 \cup \{x\}\} \cup B_0\big)\,\right| = n - 1$$

$$\left|\,X \setminus \big(A_0 \cup \{B_0 \cup \{x\}\}\big)\,\right| = n - 1$$

So we can apply the inductive step:

$$\sum \left\{ \alpha_{A,B} \,\middle|\, \{A, B\} \in \mathcal{S}(X)\,,\ \{A, B\} \succcurlyeq \{A_0, B_0\} \right\} =$$

$$= \sum \left\{ \alpha_{A,B} \,\middle|\, \{A, B\} \in \mathcal{S}(X)\,,\ \{A, B\} \succcurlyeq \{A_0 \cup \{x\}, B_0\} \right\} + \sum \left\{ \alpha_{A,B} \,\middle|\, \{A, B\} \in \mathcal{S}(X)\,,\ \{A, B\} \succcurlyeq \{A_0, B_0 \cup \{x\}\} \right\} \leq$$

$$\leq \alpha_{A_0 \cup \{x\}, B_0} + \alpha_{A_0, B_0 \cup \{x\}} \leq \alpha_{A_0, B_0}$$

Oss. We can substitute splits with d-splits in the sum
(splits that are not d-splits do not contribute).

Cor. 1 Let $\{A, B\}$ a d-split and let $a_1, a_2 \in A$ and $b_1, b_2 \in B$ such that

$$\alpha_{A,B} = \beta_{\{a_1, a_2\}, \{b_1, b_2\}}$$

Then $\{A, B\}$ is the unique d-split that extends $\{\{a_1, a_2\}, \{b_1, b_2\}\}$.

Dim. Observe that $\{\{a_1, a_2\}, \{b_1, b_2\}\}$ is a partial d-split.

In fact, if by absurd

$$\alpha_{\{a_1,a_2\},\{b_1,b_2\}} = \beta_{\{a_1,a_2\},\{b_1,b_2\}} = 0$$

then $\alpha_{A,B} = 0$, but $\{A, B\}$ is a d-split. ↯

By applying **Teo**. 1

$$\begin{aligned} \alpha_{A,B} &\leq \sum \left\{ \alpha_{A',B'} \;\middle|\; \begin{array}{c} \{A', B'\} \in \mathcal{S}_d(X)\,, \\ \{A', B'\} \succcurlyeq \{\{a_1, a_2\}, \{b_1, b_2\}\} \end{array} \right\} \\ &\leq \alpha_{\{a_1,a_2\},\{b_1,b_2\}} \\ &\leq \beta_{\{a_1,a_2\},\{b_1,b_2\}} = \alpha_{A,B} \end{aligned}$$

Since the sum is equal to $\alpha_{A,B}$ and $\{A, B\}$ is a member of the range of the sum, this means that $\{A, B\}$ is the only d-split that extends $\{\{a_1, a_2\}, \{b_1, b_2\}\}$.

The building stones in the decomposition we want to study are the split metrics. Notice that we use the term "metric" in the broader sense that the "points" of the space actually constitute those subsets of X whose elements

are pairwise at distance zero. For every pair A, B of disjoint, nonempty subsets of X define the *split metric* $\delta_{A,B}$ on $A \cup B$ by

$$\delta_{A,B}(u, v) := \begin{cases} 0 & \text{if either } u, v \in A \text{ or } u, v \in B, \\ 1 & \text{otherwise.} \end{cases}$$

Then A, B is the unique $\delta_{A,B}$-split, and its isolation index with respect to $\delta_{A,B}$ equals 1. There are functions $d: X \times X \to \mathbb{R}$ which do not admit any d-split; they are called *split-prime*. For instance, the metric d realized by the bipartite graph $K_{2,3}$ (see Fig. 4) is of this kind since for this metric there does not even exist a split into two d-convex disjoint subsets. Actually, up to a scalar, the $K_{2,3}$-metric is the only split-prime metric on five points (see Lemma 1 below).

A symmetric function $d: X \times X \to \mathbb{R}$ is a *dissimilarity function* if $xy \geqslant xx = 0$ for all $x, y \in X$.

Here is our main theorem:

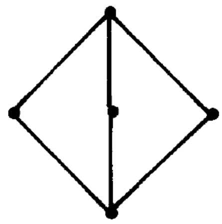


FIG. 4. A split-prime (graph) metric.

Def. Given A, B non-empty disjoint subsets of X, the **split metric** $\delta_{A,B}$ on $A \cup B$ is defined as

$$\delta_{A,B}(u,v) := \begin{cases} 0\,, & \text{if } u,v \in A \text{ or } u,v \in B \\ 1\,, & \text{otherwise} \end{cases}$$

Questa definizione è leggermente diversa da quella data precedentemente perché non si richiede $A \cup B = X$.

Oss. $\{A, B\}$ is the only $\delta_{A,B}$-split and its isolation index is 1.

In fact, let us consider $\{A, B\}$ and another split $\{A', B'\}$, with the following intersections: $A \cap A',\ A \cap B',\ B \cap A',\ B \cap B'$.
Since $A \cup B = A' \cup B' = X$ and $A, B, A', B' \neq \emptyset$,
at least two of these intersection must be non-empty.
We can divide in cases.

If all the intersections are non-empty, we can pick

$$a_1 \in A \cap A', \quad a_2 \in A \cap B', \quad b_1 \in B \cap A', \quad b_2 \in B \cap B'$$

then, with respect to $\delta_{A,B}$, we have

$$\begin{aligned} a_1b_1 + a_2b_2 &= 1 + 1 = 2 \\ a_1b_2 + a_2b_1 &= 1 + 1 = 2 \\ a_1a_2 + b_1b_2 &= 0 + 0 = 0 \end{aligned}$$

$$\beta_{\{a_1,b_1\},\{a_2,b_2\}} = \frac{1}{2}\left(\max \begin{Bmatrix} a_1b_1 + a_2b_2, \\ a_1b_2 + a_2b_1, \\ \cancel{a_1a_2 + b_1b_2} \end{Bmatrix} - a_1b_1 - a_2b_2 \right) = 0$$

so $\alpha_{A',B'} = 0$.

If only three of the intersections are non-empty
– say WLOG $A \cap A'$, $B \cap A'$, $B \cap B'$ – then we can pick

$$a_1 \in A \cap A', \quad b_1 \in B \cap A', \quad b_2 \in B \cap B'$$

then, with respect to $\delta_{A,B}$, we have

$$\begin{aligned} a_1 b_1 + b_2 b_2 &= 1 + 0 = 1 \\ a_1 b_2 + b_1 b_2 &= 1 + 0 = 1 \end{aligned}$$

$$\beta_{\{a_1,b_1\},\{b_2\}} = \frac{1}{2}\left(\max \begin{Bmatrix} a_1 b_1 + b_2 b_2, \\ a_1 b_2 + b_1 b_2 \end{Bmatrix} - a_1 b_1 - b_2 b_2 \right) = 0$$

so $\alpha_{A',B'} = 0$.

If only two intersections are non-empty
– say WLOG $A \cap A'$, $B \cap B'$ – then $\{A, B\} = \{A', B'\}$.
In fact, since $A \cup B = X$ and $A \cap B'$, $B \cap A' = \emptyset$,
then we have $A' \subseteq A$ and $B' \subseteq B$.
But since $A' \cup B' = X$, it must be $A' = A$ and $B' = B$.

Now for every $a_1, a_2 \in A$ and $b_1, b_2 \in B$ (with respect to $\delta_{A,B}$)

$$\begin{aligned} a_1 b_1 + a_2 b_2 &= 1 + 1 = 2 \\ a_1 b_2 + a_2 b_1 &= 1 + 1 = 2 \\ a_1 a_2 + b_1 b_2 &= 0 + 0 = 0 \end{aligned}$$

$$\beta_{\{a_1,a_2\},\{b_1,b_2\}} = \frac{1}{2}\left(\max \begin{Bmatrix} a_1 b_1 + a_2 b_2, \\ a_1 b_2 + a_2 b_1, \\ \cancel{a_1 a_2 + b_1 b_2} \end{Bmatrix} - \cancel{a_1 a_2 - b_1 b_2} \right) = 1$$

so $\alpha_{A,B} = 1$.

Def. (split-prime function)

A function $d : X \times X \to \mathbb{R}$ is **split-prime** if it does not admit any d-split.

$$\mathcal{S}_d(X) = \emptyset$$

Def. (dissimilarity function)

A function $d : X \times X \to \mathbb{R}$ is a **dissimilarity function** if

- $d(x, y) = d(y, x), \quad \forall\, x, y \in X$
- $d(x, x) = 0, \quad \forall\, x \in X$
- $d(x, y) \geq 0, \quad \forall\, x, y \in X$

In practice, it is a pseudo-metric without triangle inequality.

THEOREM 2. *Every symmetric function $d: X \times X \to \mathbb{R}$ on a finite set X can be expressed in the form*

$$d = d_0 + \sum \alpha^d_{A,B} \cdot \delta_{A,B},$$

where d_0 is a split-prime (symmetric) function. More generally, if $\lambda_{A,B}$ ($A, B \subseteq X$) are (not necessarily nonnegative) real numbers such that $\lambda_{A,B} \leqslant \alpha^d_{A,B}$, whenever A, B is a d-split, and $\lambda_{A,B} = 0$ otherwise, then

$$d' := d - \sum \lambda_{A,B} \cdot \delta_{A,B}$$

is a symmetric function such that

$$\alpha^{d'}_{A,B} = \alpha^d_{A,B} - \lambda_{A,B}$$

for all pairs A, B. In addition, if d is a dissimilarity function (or a metric), then d' is also a dissimilarity function (or a metric, respectively).

Proof. It suffices to prove our assertions for

$$d' = \tilde{d} := d - \lambda \cdot \delta_{A_0, B_0},$$

where A_0, B_0 is a d-split and $\lambda \leqslant \alpha^d_{A_0, B_0}$. Evidently, $\tilde{d}$ is a symmetric function. For $u, v \in X$, one has

$$\tilde{d}(u, v) = \begin{cases} uv & \text{if } \{u, v\} \subseteq A_0 \text{ or } \{u, v\} \subseteq B_0, \\ uv - \lambda & \text{otherwise.} \end{cases}$$

If d is a dissimilarity function, then $\tilde{d}(u, u) = 0$ clearly holds, and for $u \in A_0$ and $v \in B_0$ we get

$$\lambda \leqslant \alpha_{A, B} \leqslant \beta_{\{u\}, \{v\}} = uv,$$

whence $\tilde{d}(u, v) = uv - \lambda \geqslant 0$. Now assume that d is a metric. We have to verify the triangle inequality for $\tilde{d}$. Let $u, v, w \in X$, and assume that a majority of u, v, w belongs to A_0. If $u, v, w \in A_0$, then d and $\tilde{d}$ agree on $\{u, v, w\}$. Otherwise, say, $u, v \in A_0$ and $w \in B_0$, in which case we get

$$uw - \lambda \leqslant uv + (vw - \lambda)$$

and, since

$$\lambda \leqslant \alpha_{A_0, B_0} \leqslant \beta_{\{u,v\}, \{w\}} = \tfrac{1}{2} \cdot (uw + vw - uv),$$

also

$$uv \leqslant (uw - \lambda) + (vw - \lambda).$$

This proves that $\tilde{d}$ is a metric whenever d is.

For the remainder of the proof d is an arbitrary symmetric function. While the isolation indices α and β refer to d, we let $\tilde{\alpha}$ and $\tilde{\beta}$ denote the corresponding indices with respect to $\tilde{d}$. Let $\{t, u\}$, $\{v, w\}$ be disjoint subsets of X. We claim that

$$\tilde{\beta}_{\{t,u\}, \{v,w\}} = \beta_{\{t,u\}, \{v,w\}} \qquad (\bigstar\bigstar)$$

unless $\{t, u\}$, $\{v, w\}$ extends to A_0, B_0, in which case we have

$$\tilde{\beta}_{\{t,u\}, \{v,w\}} = \beta_{\{t,u\}, \{v,w\}} - \lambda. \qquad (\bigstar\bigstar\bigstar)$$

If either A_0 or B_0 contains at least three of t, u, v, w, then β and $\tilde{\beta}$ agree for $\{t, u\}$, $\{v, w\}$. If $\{t, u\}$, $\{v, w\}$ is a partial d-split extending to A_0, B_0, then the assertion is easily verified as well. So we may assume that $t, v \in A_0$ and $u, w \in B_0$. Since

$$\begin{aligned}\beta_{\{t,v\},\{u,w\}} &= \tfrac{1}{2} \cdot (\max\{tu + vw, tw + uv\} - tv - uw) \\ &\geqslant \alpha_{A_0, B_0} \geqslant \lambda,\end{aligned}$$

we obtain the inequality

$$tv + uw \leqslant \max\{tu + vw - 2\lambda, tw + uv - 2\lambda\}.$$

Hence

$$\begin{aligned}\tilde{\beta}_{\{t,u\},\{v,w\}} &= \tfrac{1}{2} \cdot (\max\{tu + vw - 2\lambda, tv + uw, tw + uv - 2\lambda\} - tu - vw + 2\lambda) \\ &= \tfrac{1}{2} \cdot (\max\{tu + vw - 2\lambda, tw + uv - 2\lambda\} - tu - vw + 2\lambda) \\ &= \tfrac{1}{2} \cdot (\max\{tu + vw, tw + uv\} - tu - vw) \\ &= \beta_{\{t,u\},\{v,w\}},\end{aligned}$$

as required.

Finally we assert that

$$\tilde{\alpha}_{A,B} = \begin{cases} \alpha_{A,B} - \lambda & \text{if } A, B \text{ equals } A_0, B_0, \\ \alpha_{A,B} & \text{otherwise} \end{cases}$$

for every pair A B of complementary subsets. Clearly $\tilde{\alpha}_{A_0,B_0} = \alpha_{A_0,B_0} - \lambda$ by (★★★). In what follows let A, B be a pair different from A_0, B_0. Then choose $a, a' \in A$ and $b, b' \in B$ such that

$$\alpha_{A,B} = \beta_{\{a,a'\},\{b,b'\}}.$$

Since A_0, B_0 is a d-split, it cannot extend $\{a, a'\}$, $\{b, b'\}$ by Corollary 1 if $\alpha_{A,B} > 0$, and by a trivial reason if $\alpha_{A,B} = 0$. Hence

$$\alpha_{A,B} = \beta_{\{a,a'\},\{b,b'\}} = \tilde{\beta}_{\{a,a'\},\{b,b'\}} \geqslant \tilde{\alpha}_{A,B}$$

by (★★). To prove the reverse inequality assume that $t, u \in A$ and $v, w \in B$. Observe that by (★★)

$$\alpha_{A,B} \leqslant \beta_{\{t,u\},\{v,w\}} = \tilde{\beta}_{\{t,u\},\{v,w\}}$$

if A_0, B_0 does not extend $\{t, u\}$, $\{v, w\}$. Otherwise, if A_0, B_0 extends $\{t, u\}$, $\{v, w\}$, then

$$\begin{aligned}\alpha_{A,B} &\leqslant \alpha_{A,B} + \alpha_{A_0,B_0} - \lambda \\ &\leqslant \alpha_{\{t,u\},\{v,w\}} - \lambda \\ &\leqslant \beta_{\{t,u\},\{v,w\}} - \lambda \\ &= \tilde{\beta}_{\{t,u\},\{v,w\}}\end{aligned}$$

by Theorem 1 and (★★★). So, $\alpha_{A,B} \leqslant \tilde{\alpha}_{A,B}$ holds. This proves the desired equality and completes the proof. ▮

Teo. 2 Let $d : X \times X \to \mathbb{R}$ be a symmetric function.
Let $\lambda_S \in \mathbb{R}$ such that $\lambda_S \leq \alpha_S^d$ if S is a d-split
and $\lambda_S = 0$ otherwise.
Then

$$d' \coloneqq d - \sum_{S \in \mathcal{S}(X)} \lambda_S \cdot \delta_S$$

is a symmetric function such that

$$\alpha_S^{d'} = \alpha_S^d - \lambda_S\,, \qquad \forall\, S \in \mathcal{S}(X)$$

In addition, if d is a dissimilarity function (or a pseudo-metric), then d' is also a dissimilarity function (or a pseudo-metric).

Dim. It suffices to prove the assertions for

$$d' = \tilde{d} \coloneqq d - \lambda \cdot \delta_{A_0,B_0}$$

where $\{A_0, B_0\}$ is a d-split and $\lambda \leq \alpha_{A_0,B_0}^d$.

Then the general case follows by subtracting one split metric at a time (formally induction on the number of non-zero λ's).

We use the following notation: $uv = d(u,v),\ \forall\, u,v \in X$

$$\alpha = \alpha^{d},\ \ \beta = \beta^{d}, \qquad \tilde{\alpha} = \alpha^{\tilde{d}},\ \ \tilde{\beta} = \beta^{\tilde{d}}$$

Clearly $\tilde{d}$ is a symmetric function (since d and δ are such).

For every $u,v \in X$ we have

$$\tilde{d}(u,v) = \begin{cases} uv\,, & \text{if } \{u,v\} \subseteq A_0 \text{ or } \{u,v\} \subseteq B_0 \\ uv - \lambda\,, & \text{otherwise} \end{cases}$$

Suppose that d is a dissimilarity function.

Then $\tilde{d}(u,u) = d(u,u) = 0$. For $u \in A_0$ and $v \in B_0$ we have

$$\lambda \le \alpha_{A_0,B_0} \le \beta_{\{u\},\{v\}} = uv$$

thus $\tilde{d}(u,v) = uv - \lambda \ge 0$, so $\tilde{d}$ is a dissimilarity function.

Now suppose that d is a pseudo-metric.
We have to verify the triangle inequality for $\tilde{d}$.

Let $u,v,w \in X$. If they all belong to A_0 or all to B_0,
then d and $\tilde{d}$ agrees on $\{u,v,w\}$ and we are done.
Otherwise, say WLOG $u,v \in A_0$ and $w \in B_0$, then we get

$$\begin{aligned} \lambda \le \alpha_{A_0,B_0} &\le \beta_{\{u,v\},\{w\}} \\ &= \frac{1}{2}\left(\max\{uw + vw, uv + \cancel{ww}\} - uv - \cancel{ww}\right) \\ &= \frac{1}{2}(uw + vw - uv) \end{aligned}$$

where we used the triangle inequality for d, and by rearranging

$$\underbrace{uv}_{\tilde{d}(u,v)} \le \underbrace{(uw - \lambda)}_{\tilde{d}(u,w)} + \underbrace{(vw - \lambda)}_{\tilde{d}(v,w)}$$

For the remainder of the proof d is a symmetric function.

Let $\{t,u\},\{v,w\}$ be disjoint subsets of X.
We claim that

$$\tilde{\beta}_{\{t,u\},\{v,w\}} = \begin{cases} \beta_{\{t,u\},\{v,w\}} - \lambda\,, & \text{if } \{A_0,B_0\} \succcurlyeq \big\{\{t,u\},\{v,w\}\big\} \\ \beta_{\{t,u\},\{v,w\}}\,, & \text{otherwise} \end{cases}$$

Suppose $\{A_0,B_0\} \succcurlyeq \big\{\{t,u\},\{v,w\}\big\}$.
Since $\{A_0,B_0\}$ is a d-split

$$\beta_{\{t,u\},\{v,w\}} = \frac{1}{2}\big(\max\{tv+uw, tw+uv\} - tu - vw\big) > 0$$

$$\lambda \le \alpha_{A_0,B_0} \le \beta_{\{t,u\},\{v,w\}}$$

$$2\lambda \le \max\begin{Bmatrix} tv+uw, \\ tw+uv \end{Bmatrix} - tu - vw$$

$$tu+vw \le \max\begin{Bmatrix} (tv-\lambda)+(uw-\lambda), \\ (tw-\lambda)+(uv-\lambda) \end{Bmatrix}$$

$$\begin{aligned}
\tilde{\beta}_{\{t,u\},\{v,w\}} &= \frac{1}{2}\left(\max\begin{Bmatrix} (tv-\lambda)+(uw-\lambda), \\ (tw-\lambda)+(uv-\lambda), \\ tu+vw \end{Bmatrix} - tu - vw\right) \\
&= \frac{1}{2}\left(\max\begin{Bmatrix} tv+uw, \\ tw+uv \end{Bmatrix} - 2\lambda - tu - vw\right) \\
&= \beta_{\{t,u\},\{v,w\}} - \lambda
\end{aligned}$$

If instead A_0 or B_0 contains at least three of t,u,v,w
– say WLOG $t,u,v \in A_0$ and $w \in B_0$ – then

$$\begin{aligned}
\tilde{\beta}_{\{t,u\},\{v,w\}} &= \frac{1}{2}\left(\max\begin{Bmatrix} tv+(uw-\lambda), \\ (tw-\lambda)+uv, \\ tu+(vw-\lambda) \end{Bmatrix} - tu - (vw-\lambda)\right) \\
&= \frac{1}{2}\left(\max\begin{Bmatrix} tv+uw, \\ tw+uv, \\ tu+vw \end{Bmatrix} \cancel{-\lambda} - tu - (vw \cancel{-\lambda})\right) \\
&= \beta_{\{t,u\},\{v,w\}}
\end{aligned}$$

So we may assume WLOG that $t, v \in A_0$ and $u, w \in B_0$.
Since $\{A_0, B_0\}$ is a d-split

$$\beta_{\{t,v\},\{u,w\}} = \frac{1}{2}\left(\max\{tu + vw, tw + uv\} - tv - uw \right)$$
$$\geq \alpha_{A_0,B_0} \geq \lambda$$

from which, similarly as before, we get the inequality

$$tv + uw \leq \max\{tu + vw - 2\lambda, tw + uv - 2\lambda\}$$

$$\tilde{\beta}_{\{t,u\},\{v,w\}} = \frac{1}{2}\left(\max\begin{Bmatrix} tv + uw, \\ (tw - \lambda) + (uv - \lambda), \\ (tu - \lambda) + (vw - \lambda) \end{Bmatrix} - (tu - \lambda) - (vw - \lambda) \right)$$
$$= \frac{1}{2}\left(\max\begin{Bmatrix} tw + uv, \\ tu + vw \end{Bmatrix} \cancel{-2\lambda} - tu - vw \cancel{+2\lambda} \right)$$
$$= \beta_{\{t,u\},\{v,w\}}$$

Finally, we claim that for every split $\{A, B\}$

$$\tilde{\alpha}_{A,B} = \begin{cases} \alpha_{A,B} - \lambda\,, & \text{if } \{A, B\} = \{A_0, B_0\} \\ \alpha_{A,B}\,, & \text{otherwise} \end{cases}$$

Since $\tilde{\beta}_{\{t,u\},\{v,w\}} = \beta_{\{t,u\},\{v,w\}} - \lambda\,, \quad \forall\, t, u \in A_0,\ \forall\, v, w \in B_0$,
then $\tilde{\alpha}_{A_0,B_0} = \alpha_{A_0,B_0} - \lambda$.

Now let $\{A, B\} \neq \{A_0, B_0\}$.

If $A \cap B \neq \emptyset$, then $\tilde{\alpha}_{A,B} = 0 = \alpha_{A,B}$.
So we can suppose A and B disjoint.

Then choose $a, a' \in A$ and $b, b' \in B$ such that

$$\alpha_{A,B} = \beta_{\{a,a'\},\{b,b'\}}$$

We claim that $\{A_0, B_0\}$ cannot extend $\big\{\{a, a'\}, \{b, b'\}\big\}$.
In fact, if by absurd it is an extension, then there are two cases.

If $\alpha_{A,B} = 0$, then $\beta_{\{a,a'\},\{b,b'\}} = 0$ that implies $\alpha_{A_0,B_0} = 0$.
But $\{A_0, B_0\}$ is a d-split. $\lightning$

If $\alpha_{A,B} > 0$, then $\{A, B\}$ is a d-split extending $\big\{\{a, a'\}, \{b, b'\}\big\}$.
But by **Cor**. 1, such a d-split extension is unique,
so $\{A, B\} = \{A_0, B_0\}$. $\lightning$

Since $\{A_0, B_0\} \not\succcurlyeq \big\{\{a, a'\}, \{b, b'\}\big\}$, we get

$$\alpha_{A,B} = \beta_{\{a,a'\},\{b,b'\}} = \tilde{\beta}_{\{a,a'\},\{b,b'\}} \geq \tilde{\alpha}_{A,B}$$

Now for the same reason, for every $t, u \in A$ and $v, w \in B$

$$\alpha_{A,B} \leq \beta_{\{t,u\},\{v,w\}} = \tilde{\beta}_{\{t,u\},\{v,w\}}$$

if $\{A_0, B_0\}$ does not extend $\big\{\{t, u\}, \{v, w\}\big\}$.

Otherwise, if $\{A_0, B_0\}$ extends $\big\{\{t, u\}, \{v, w\}\big\}$, then

$$\lambda \leq \alpha_{A_0,B_0}$$

$$\begin{aligned} \alpha_{A,B} &\leq \alpha_{A,B} + \alpha_{A_0,B_0} - \lambda \\ &\leq \alpha_{\{t,u\},\{v,w\}} - \lambda \\ &\leq \beta_{\{t,u\},\{v,w\}} - \lambda \\ &= \tilde{\beta}_{\{t,u\},\{v,w\}} \end{aligned}$$

where we used **Teo**. 1.

Since

$$\alpha_{A,B} \leq \tilde{\beta}_{\{t,u\},\{v,w\}}, \qquad \forall\, t, u \in A, \ \ \forall\, v, w \in B$$

then $\alpha_{A,B} \leq \tilde{\alpha}_{A,B}$.

Cor. (**split decomposition** / canonical decomposition)

For any symmetric function $d : X \times X \to \mathbb{R}$ we can write

$$d = d_0 + \sum_{S \in \mathcal{S}(X)} \alpha_S^d \cdot \delta_S$$

where d_0 is a split-prime (symmetric) function.
We call d_0 the **split-prime residue** of d.

Dim. Apply **Teo**. 2 with $\lambda_S = \alpha_S^d$, $\forall\, S \in \mathcal{S}(X)$.

Let $d_0 \coloneqq d - \sum_{S \in \mathcal{S}(X)} \alpha_S^d \cdot \delta_S$.

Then if S is a d-split, $\alpha_S^{d_0} = \alpha_S^d - \alpha_S^d = 0$;
otherwise $\alpha_S^{d_0} = 0 - 0 = 0$.

Oss. We can sum over only the d-splits, since the others do not contribute (they have zero coefficient).

Oss. The residue of a split-prime function coincides with the function itself (there are no splits on which to decompose).

COROLLARY 2. *If $d: X \times X \to \mathbb{R}$ is a metric and $x \in X$, then for any $\lambda \geqslant 0$ and any split A, B not equal to $\{x\}$, $X - \{x\}$, the isolation index $\alpha^{d'}_{A,B}$ with respect to the metric $d' := d + \lambda \cdot \delta_{\{x\}, X - \{x\}}$ coincides with the isolation index $\alpha^d_{A,B}$ with respect to d, and the split-prime residue d'_0 of d' coincides with d_0.*

Proof. Since $d = d' - \lambda \cdot \delta_{\{x\}, X - \{x\}}$, it suffices to observe that for $u, v \in X - \{x\}$ we have

$$\begin{aligned}\beta^{d'}_{\{x,x\},\{u,v\}} &= \tfrac{1}{2} \cdot (\max\{d(x,u) + d(x,v) + 2\lambda,\ d(x,x) + d(u,v)\} \\ &\qquad - d(x,x) - d(u,v)) \\ &= \lambda + \tfrac{1}{2} \cdot (d(u,x) + d(x,v) - d(u,v)) \geqslant \lambda\end{aligned}$$

and therefore $\alpha^{d'}_{\{x\}, X - \{x\}} \geqslant \lambda$. ∎

Corollary 3. *If $d = d_0 + \sum \alpha^d_{A,B} \cdot \delta_{A,B}$ is the canonical decomposition of the symmetric function d, then every partial d_0-split A_0, B_0 is also a partial d-split and every partial d-split A_0, B_0 which does not extend to a (total) d-split is also a partial d_0-split.*

Proof. Put $X_0 := A_0 \cup B_0$ and apply Theorem 2 to the restrictions of d and d_0 to X_0. ∎

Cor. 2 Let $d : X \times X \to \mathbb{R}$ be a pseudo-metric and $x \in X$.
Let $\lambda \geq 0$ and consider

$$d' := d + \lambda \cdot \delta_x$$

Then we have $d'_0 = d_0$ and

$$\begin{cases} \alpha^{d'}_S = \alpha^d_S \,, & \forall\, S \neq \{\{x\}, X \setminus \{x\}\} \\ \alpha^{d'}_{\{x\},X\setminus\{x\}} = \alpha^d_{\{x\},X\setminus\{x\}} + \lambda & \square \end{cases}$$

Dim. Observe that for every $u, v \in X \setminus \{x\}$ we have

$$\begin{aligned} \beta^{d'}_{\{x\},\{u,v\}} &= \frac{1}{2}\left(\max \left\{ \begin{matrix} (xu + \lambda) + (xv + \lambda), \\ \cancel{xx} + uv \end{matrix} \right\} - \cancel{xx} - uv \right) \\ &= \frac{1}{2}(xu + xv + 2\lambda - uv) \\ &= \lambda + \frac{1}{2}(xu + xv - uv) \geq \lambda \end{aligned}$$

where we used the triangle inequality for d.

Therefore $\alpha^{d'}_{\{x\},X\setminus\{x\}} \geq \lambda$ and, since $d = d' - \lambda \cdot \delta_x$, we get the thesis by applying **Teo**. 2.

Moreover, since $\alpha^{d'}_{\{x\},X\setminus\{x\}} = \alpha^d_{\{x\},X\setminus\{x\}} - \lambda$, and

$$\begin{aligned} d'_0 &= d' - \sum \alpha^{d'}_S \cdot \delta_S - \alpha^{d'}_{\{x\},X\setminus\{x\}} \cdot \delta_x = \\ &= (d + \cancel{\lambda \cdot \delta_x}) - \sum \alpha^d_S \cdot \delta_S - \left(\alpha^d_{\{x\},X\setminus\{x\}} \cancel{- \lambda}\right) \cdot \delta_x = d_0 \end{aligned}$$

where the sums range over the splits different from $\{\{x\}, X\setminus\{x\}\}$.

Prop. The split-prime residue of the restriction coincides with the restriction of the split-prime residue

$$(d|_{Y\times Y})_0 = d_0|_{Y\times Y}, \qquad \forall\, Y \subseteq X$$

Moreover, for every partial split $\{A, B\}$ of X we have

$$\alpha_{A,B}^{d_0} = \alpha_{A,B}^{d} - \sum \alpha_{A',B'}^{d}$$

where the sum ranges over all the d-splits that extend $\{A, B\}$.

Dim. Let $Y \subseteq X$. Restricting the canonical decomposition to Y we get

$$d|_{Y\times Y} = d_0|_{Y\times Y} + \sum_{S\,\in\,\mathcal{S}(X)} \alpha_S^d \cdot \delta_S|_{Y\times Y}$$

Instead, the canonical decomposition of the restriction is

$$d|_{Y\times Y} = (d|_{Y\times Y})_0 + \sum_{S\,\in\,\mathcal{S}(Y)} \alpha_S^d \cdot \delta_S|_{Y\times Y}$$

But the splits of Y are the restriction of the splits of X to Y minus the splits such that one of the parts contains Y.
For such splits, the split metrics restricted to Y become the zero function, so we can ignore their splits in the sum.
Thus the summations in the two decompositions coincide, therefore also the residues.

Consider the case

$$d_0 = d - \alpha_{A_0,B_0}^d \cdot \delta_{A_0,B_0}$$

where $\{A_0, B_0\}$ is a d-split.

We can recycle the proof of **Teo**. 2 with some minor variation.
First we get that for every $\{t,u\},\{v,w\} \subseteq X$ disjoint

$$\beta_{\{t,u\},\{v,w\}}^{d_0} = \begin{cases} \beta_{\{t,u\},\{v,w\}}^{d} - \alpha_{A_0,B_0}^d, & \text{if } \{A_0, B_0\} \succcurlyeq \{\{t,u\},\{v,w\}\} \\ \beta_{\{t,u\},\{v,w\}}^{d}, & \text{otherwise} \end{cases}$$

Suppose that $\{A_0, B_0\}$ extends $\{A, B\}$. Since

$$\beta^{d_0}_{\{t,u\},\{v,w\}} = \beta^{d}_{\{t,u\},\{v,w\}} - \alpha^{d}_{A_0,B_0}, \qquad \forall\, t,u \in A,\ \ \forall\, v,w \in B$$

we get $\alpha^{d_0}_{A,B} = \alpha^{d}_{A,B} - \alpha^{d}_{A_0,B_0}$.

Now suppose that $\{A_0, B_0\}$ does not extend $\{A, B\}$.
Then we prove that $\{A_0, B_0\}$ cannot extend the quartet that realizes $\alpha^{d}_{A,B}$.

In order to apply **Cor**. 1, we need to restrict $\{A_0, B_0\}$ to $A \cup B$

$$\{A_0 \cap A, B_0 \cap B\} \text{ or } \{A_0 \cap B, B_0 \cap A\}$$

Notice that at least one of these is a total split of $A \cup B$, so it must coincide with $\{A, B\}$.

In order to apply **Teo**. 1, we backtrack $\{A_0, B_0\}$ in the tree extension to an ancestor at the same level of $\{A, B\}$ (observe that this must be different from $\{A, B\}$ because $\{A_0, B_0\}$ is not an extension). Then the sum of their indices is less than the sum of the indices of all the partial splits on the same level, that is less than the index of $\{A, B\}$.

Therefore, for every partial split $\{A, B\}$

$$\alpha^{d_0}_{A,B} = \begin{cases} \alpha^{d}_{A,B} - \alpha^{d}_{A_0,B_0}\,, & \text{if } \{A_0, B_0\} \succcurlyeq \{A, B\} \\ \alpha^{d}_{A,B}\,, & \text{otherwise} \end{cases}$$

We conclude by induction as before.

Cor. 3 Let $d : X \times X \to \mathbb{R}$ be a symmetric function.

Then every partial d_0-split is also a partial d-split; and every partial d-split, which does not extend to a (total) d-split, is also a partial d_0-split.

Dim. It is a consequence of the previous **Prop**.

Theorem 2 asserts that any metric d can be expressed in a canonical fashion as a sum of certain split metrics δ_S (where S runs through all d-splits) and a split-prime residue d_0. To go on with the theory we want to develop, the collections of splits which qualify as the collections of all d-splits for some metric d need to be characterized. Clearly, for any symmetric function $d: X \times X \to \mathbb{R}$ and $t, u, v, w \in X$, not all three isolation indices $\alpha_{\{t,u\},\{v,w\}}$, $\alpha_{\{t,v\},\{u,w\}}$, $\alpha_{\{t,w\},\{u,v\}}$ can be positive; that is, the d-splits are "weakly compatible" once we define a collection $\mathcal{S}$ of splits of X to be *weakly compatible* if there are no four points $t, u, v, w \in X$ and three splits $S_1, S_2, S_3 \in \mathcal{S}$ such that S_1 extends the partial split $\{t, u\}$, $\{v, w\}$, while S_2 extends $\{t, v\}$, $\{u, w\}$, and S_3 extends $\{t, w\}$, $\{u, v\}$. The forbidden situation is depicted in Fig. 5, where each split S_i is represented by a line (giving rise to two complementary halfplanes).

Let $d : X \times X \to \mathbb{R}$ be a symmetric function.

Oss. Let $t, u, v, w \in X$.
Then at least one of the following indices must be zero

$$\alpha_{\{t,u\},\{v,w\}}\,, \qquad \alpha_{\{t,v\},\{u,w\}}\,, \qquad \alpha_{\{t,w\},\{u,v\}}$$

In fact, suppose

$$\max\{tu + vw, tv + uw, tw + uv\} = tu + vw$$

then $\beta_{\{t,u\},\{v,w\}} = 0$ and so $\alpha_{\{t,u\},\{v,w\}} = 0$.
The other cases are analogous.

Def. (weakly compatible splits)

Three splits S_1, S_2, S_3 of X are **weakly compatible** if there are no four points $t, u, v, w \in X$ such that

$$S_1 \succcurlyeq \{\{t, u\}, \{v, w\}\}\,, \qquad S_2 \succcurlyeq \{\{t, v\}, \{u, w\}\}\,, \qquad S_3 \succcurlyeq \{\{t, w\}, \{u, v\}\}$$

A set of splits $\mathcal{S}$ of X is **weakly compatible** if its splits are (triplewise) weakly compatible.

Oss. Subsets of weakly compatible sets are weakly compatible.

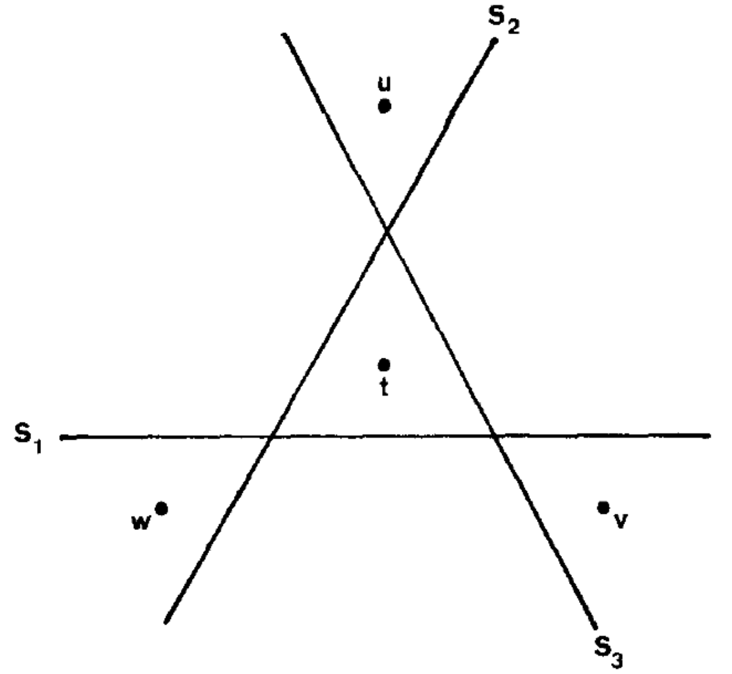


FIG. 5. Three splits that are not weakly compatible.

Prop. The set of all d-splits $\mathcal{S}_d(X)$ is weakly compatible.

Dim. Let $t, u, v, w \in X$. From the previous observation we can suppose WLOG $\alpha_{\{t,u\},\{v,w\}} = 0$.
For every split S that extends $\{\{t,u\},\{v,w\}\}$ we have

$$0 \leq \alpha_S \leq \alpha_{\{t,u\},\{v,w\}} = 0 \quad \Longrightarrow \quad \alpha_S = 0$$

that is S is not a d-split. In other words, there are no d-splits that extend $\{\{t,u\},\{v,w\}\}$.

THEOREM 3. *The d-splits with respect to any symmetric function d on a set X are weakly compatible. Conversely, let $\mathscr{S}$ be any collection of weakly compatible splits of X. For each $S \in \mathscr{S}$ choose some $\lambda_S > 0$ and consider*

$$d := \sum_{S \in \mathscr{S}} \lambda_S \cdot \delta_S.$$

Then $\mathscr{S}$ is the set of all d-splits, and moreover, the isolation index $\alpha_S = \alpha_S^d$ equals λ_S for each $S \in \mathscr{S}$.

Proof. Let the pair A, B be a split from $\mathscr{S}$. Pick $t, u \in A$ and $v, w \in B$ such that

$$\alpha_{\{t,u\},\{v,w\}} = \alpha_{A,B}.$$

By weak compatibility we may assume that there is no split in $\mathscr{S}$ extending, say, $\{t, w\}, \{u, v\}$. Put

$$\mathscr{S}_0 := \{S \in \mathscr{S} \mid S \text{ extends } \{t, u\}, \{v, w\}\},$$

$$\mathscr{S}_1 := \{S \in \mathscr{S} \mid S \text{ extends } \{t, v\}, \{u, w\}\}.$$

All splits in $\mathscr{S} - (\mathscr{S}_0 \cup \mathscr{S}_1)$ equally contribute to each of the three distance sums involving t, u, v, w, so that

$$\begin{aligned}
\alpha_{\{t,u\},\{v,w\}} &= \tfrac{1}{2} \cdot (\max\{tv + uw, tw + uv\} - tu - vw) \\
&= \max\left\{\sum_{S \in \mathscr{S}_0} \lambda_S, \sum_{S \in \mathscr{S}_0 \cup \mathscr{S}_1} \lambda_S\right\} - \sum_{S \in \mathscr{S}_1} \lambda_S \\
&= \sum_{S \in \mathscr{S}_0} \lambda_S \\
&\geqslant \lambda_{A,B} > 0.
\end{aligned}$$

Therefore A, B is a d-split. Now, decompose d according to Theorem 2. Then

$$d = d_0 + \sum_{d\text{-splits } S} \alpha_S \cdot \delta_S$$
$$\geqslant \sum_{S \in \mathscr{S}} \alpha_S \cdot \delta_S$$
$$\geqslant \sum_{S \in \mathscr{S}} \lambda_S \cdot \delta_S = d,$$

whence equality holds throughout. This yields

$$d_0 = 0, \; \alpha_S = \lambda_S \quad \text{for} \quad S \in \mathscr{S}, \quad \text{and} \quad \alpha_S = 0 \text{ otherwise},$$

as claimed. ▮

Teo. 3 Let $\mathcal{S}$ be a set of weakly compatible splits of X.
For each $S \in \mathcal{S}$, let $\lambda_S > 0$ and consider

$$d \coloneqq \sum_{S \in \mathcal{S}} \lambda_S \cdot \delta_S$$

Then $\mathcal{S} = \mathcal{S}_d(X)$ and $\alpha_S = \lambda_S$, $\forall\, S \in \mathcal{S}$.

Dim. Notice that d is a conical combination of split metrics (which are pseudo-metrics), so it is a pseudo-metric.

Let $\{A, B\} \in \mathcal{S}$. Pick $t, u \in A$ and $v, w \in B$ such that

$$\alpha_{\{t,u\},\{v,w\}} = \alpha_{A,B}$$

Consider the sets

$$\mathcal{S}_0 = \left\{ S \in \mathcal{S} \,\middle|\, S \succcurlyeq \{\{t,u\},\{v,w\}\} \right\}$$
$$\mathcal{S}_1 = \left\{ S \in \mathcal{S} \,\middle|\, S \succcurlyeq \{\{t,v\},\{u,w\}\} \right\}$$
$$\mathcal{S}_2 = \left\{ S \in \mathcal{S} \,\middle|\, S \succcurlyeq \{\{t,w\},\{u,v\}\} \right\}$$

If all three sets are non-empty, then there exist three splits that violates the weak compatibility assumption.
So at least one of them is empty, say WLOG $\mathcal{S}_2$.

All splits in $\mathcal{S} \setminus (\mathcal{S}_0 \cup \mathcal{S}_1 \cup \mathcal{S}_2)$ equally contribute to each of the three distances $tu + vw,\ tv + uw,\ tw + uv$;
so we can ignore them in the calculation of the isolation index:

$$
\begin{aligned}
\alpha_{A,B} &= \alpha_{\{t,u\},\{v,w\}} = \beta_{\{t,u\},\{v,w\}} = \\
&= \frac{1}{2} \cdot (\ \max\{tu + vw, tv + uw, tw + uv\} - tu - vw\ ) \\
&= \max\left\{ \sum_{S\, \in\, \mathcal{S}_1 \cup \underbrace{\mathcal{S}_2}_{=\emptyset}} \lambda_S\,,\ \sum_{S\, \in\, \mathcal{S}_0 \cup \underbrace{\mathcal{S}_2}_{=\emptyset}} \lambda_S\,,\ \sum_{S\, \in\, \mathcal{S}_0 \cup \mathcal{S}_1} \lambda_S \right\} - \sum_{S\, \in\, \mathcal{S}_1 \cup \underbrace{\mathcal{S}_2}_{=\emptyset}} \lambda_S \\
&= \sum_{S\, \in\, \mathcal{S}_0 \cup \mathcal{S}_1} \lambda_S - \sum_{S\, \in\, \mathcal{S}_1} \lambda_S \\
&= \sum_{S\, \in\, \mathcal{S}_0} \lambda_S \\
&\geq \lambda_{A,B} > 0
\end{aligned}
$$

So for every $S \in \mathcal{S}$ we have $\alpha_S \geq \lambda_S > 0$
and S is a d-split, therefore $\mathcal{S} \subseteq \mathcal{S}_d(X)$.

Decomposing d as in **Teo**. 2

$$
\begin{aligned}
d &= d_0 + \sum_{S\, \in\, \mathcal{S}_d(X)} \alpha_S \cdot \delta_S \\
&\geq \sum_{S\, \in\, \mathcal{S}} \alpha_S \cdot \delta_S \\
&\geq \sum_{S\, \in\, \mathcal{S}} \lambda_S \cdot \delta_S = d
\end{aligned}
$$

where we used that $d_0 \geq 0$, since it is a pseudo-metric.
So the inequalities hold as equal. Thus

$$
d_0 = 0\,, \qquad \begin{cases} \alpha_S = \lambda_S\,, & \forall\, S \in \mathcal{S} \\ \alpha_S = 0\,, & \text{otherwise} \end{cases}
$$

that is if $S \notin \mathcal{S}$, then S is not a d-split.

We conclude that $\mathcal{S} = \mathcal{S}_d(X)$.

COROLLARY 4. *Let $\mathscr{S}$ be a collection of weakly compatible splits of X. Then the split metrics δ_S $(S \in \mathscr{S})$ are linearly independent. Consequently, $\mathscr{S}$ has at most $\binom{\# X}{2}$ members.*

Proof. Assume that

$$\sum_{S \in \mathscr{S}} \lambda_S \cdot \delta_S = 0$$

for some real numbers λ_S $(S \in \mathscr{S})$. Put

$$\mathscr{S}^+ := \{S \in \mathscr{S} \mid \lambda_S > 0\},$$

$$\mathscr{S}^- := \{S \in \mathscr{S} \mid \lambda_S < 0\}.$$

Then consider the metric d given by either expression

$$\sum_{S \in \mathscr{S}^+} \lambda_S \cdot \delta_S = \sum_{S \in \mathscr{S}^-} (-\lambda_S) \cdot \delta_S.$$

Since $\mathscr{S}^+$ and $\mathscr{S}^-$ are disjoint, weakly compatible collections of splits, we infer from Theorem 3 that both $\mathscr{S}^+$ and $\mathscr{S}^-$ must be empty; that is, $\lambda_S = 0$ for all $S \in \mathscr{S}$. Therefore the split metrics δ_S $(S \in \mathscr{S})$ are linearly independent.

Finally, as the linear space of all symmetric functions $d: X \times X \to \mathbb{R}$ with "zero diagonal," i.e., $d(x, x) = 0$ for all $x \in X$, has dimension $\binom{\# X}{2}$, the collection $\mathscr{S}$ has at most that many members. ∎

Cor. 4 Let $\mathcal{S}$ be a set of weakly compatible splits of X.

Then the split metrics $\{\delta_S\}_{S \in \mathcal{S}}$ are linearly independent.
Also $|\mathcal{S}| \leq \binom{n}{2}$, where $n = |X|$.

Dim. In order to prove the linear independence, suppose

$$\sum_{S \in \mathcal{S}} \lambda_S \cdot \delta_S = 0$$

for some $\lambda_S \in \mathbb{R}$ for each $S \in \mathcal{S}$.

Let

$$\mathcal{S}^+ := \{\, S \in \mathcal{S} \mid \lambda_S > 0 \,\}$$

$$\mathcal{S}^- := \{\, S \in \mathcal{S} \mid \lambda_S < 0 \,\}$$

We can decompose the previous expression in

$$\sum_{S \,\in\, \mathcal{S}^+} \lambda_S \cdot \delta_S + \sum_{S \,\in\, \mathcal{S}^-} \lambda_S \cdot \delta_S = 0$$

Consider the pseudo-metric

$$d := \sum_{S \,\in\, \mathcal{S}^+} \lambda_S \cdot \delta_S = \sum_{S \,\in\, \mathcal{S}^-} (-\lambda_S) \cdot \delta_S$$

Observe that both $\mathcal{S}^+$ and $\mathcal{S}^-$ are weakly compatible.
Applying **Teo**. 3 to the first expression of d we get

$$\mathcal{S}^+ = \mathcal{S}_d(X)$$

and doing the same with the second expression we get

$$\mathcal{S}^- = \mathcal{S}_d(X)$$

So $\mathcal{S}^+ = \mathcal{S}^-$.
But $\mathcal{S}^+$ and $\mathcal{S}^-$ are disjoint due to how they are defined.
So they are both empty: $\mathcal{S}^+ = \mathcal{S}^- = \emptyset$.

We conclude that $\lambda_S = 0,\ \forall\, S \in \mathcal{S}$.
Therefore the split metrics $\{\delta_S\}_{S\in\mathcal{S}}$ are linearly independent.

Since $\delta_S \in M(X),\ \forall\, S \in \mathcal{S}$ and $\dim_{\mathbb{R}}\langle M(X)\rangle = \binom{n}{2}$ then

$$|\mathcal{S}| = \#\{\delta_S\} \leq \binom{n}{2}$$

Since the number of d-splits of an n-set X is bounded by $\binom{n}{2}$, one can compute all d-splits and thus determine the corresponding decomposition in polynomial time. Namely, suppose that the $d|_{Y\times Y}$-splits have already been determined for a proper k-subset Y of X. Then pick any $x \in X - Y$, and check whether $\{x\}$, Y is a partial d-split and whether $A \cup \{x\}$, B or A, $B \cup \{x\}$ is a partial d-split for any $d|_{Y\times Y}$-split A, B. In this way we obtain

all splits of $Y \cup \{x\}$ which are partial d-splits. This step requires no more than

$$\text{const} \cdot \left(k^2 + k^3 \cdot \binom{k}{2}\right)$$

comparisons, so that the whole algorithm is of complexity $O(n^6)$. The isolation indices are updated in each iteration, and hence the decomposition of d is found in $\mathcal{O}(n^6)$ time.

Oss. Since $\mathcal{S}_d(X)$ is weakly compatible, from **Cor.** 4 we have that the number of d-splits is at most $\binom{n}{2}$.

A brute force approach to find all the d-splits of X would be to compute the isolation indices of all the splits of X and discard those that are zero. But, since $|\mathcal{S}(X)| = 2^{n-1} - 1$, this is an exponential algorithm.

We can instead use a more "inductive" approach:
suppose that the $d|_{Y\times Y}$-splits of a proper subset $Y \subset X$ of size k have already been determined. Then pick any $x \in X \setminus Y$ and check

- if $\{Y, \{x\}\}$ is a partial d-split
- if $\{A, B \cup \{x\}\}$ and $\{A, B \cup \{x\}\}$ are partial d-split
  for any $\{A, B\}$ d-split of Y

In this way we obtain all the d-splits of $Y \cup \{x\}$.

Crucially, we just have to check at most $2 \cdot \binom{k}{2} + 1$ splits at each step, thanks to the previous observation. So we can compute the d-splits of X (and their decomposition) in polynomial time.

$|Y| = k$ Contiamo le quaterne che contengono x

$Y \mid \{x\} \rightsquigarrow \frac{k \cdot k - k}{2} + k = \frac{k(k+1)}{2}$

2 scelte* 0 scelte

*possono anche essere uguali

$|A| = i, \; |B| = k - i$

$A \cup \{x\} \mid B \rightsquigarrow i \cdot \frac{(k-i)(k-i+1)}{2}$ (1, 2)

$A \mid B \cup \{x\} \rightsquigarrow \frac{i(i+1)}{2} \cdot (k-i)$ (2, 1)

in tutto $\frac{1}{2} i (k-i) \left[(k - \cancel{i} + 1) + \cancel{i} + 1 \right]$

$= \frac{1}{2} i (k-i)(k+2) =: f_k(i)$

$\frac{\partial}{\partial i} f_k(i) = \frac{1}{2}(k-i)(k+2) - \frac{1}{2} i (k+2) = \frac{1}{2}[(k-i) - i](k+2)$

$= \frac{1}{2}(k - 2i)(k+2) \quad = 0 \iff i = \frac{k}{2}$

$\max_i f_k(i) = \frac{1}{2} \frac{k}{2} \left(k - \frac{k}{2}\right)(k+2) = \frac{k^2}{8}(k+2) = \frac{k^3}{8} + \frac{k^2}{4}$

Ci sono al più $\binom{k}{2}$ d-split $A|B$ su Y

$\leq \frac{k(k+1)}{2} + \left(\frac{k^3}{8} + \frac{k^2}{4}\right)\binom{k}{2}$ #β (non già calcolati prima)

$\leq (\underbrace{6}_{2<,\,3+,\,1-} + \underbrace{1}_{\#<\ \text{per min}\ \beta}) \left[\frac{k(k+1)}{2} + \left(\frac{k^3}{8} + \frac{k^2}{4}\right)\frac{k(k-1)}{2} \right] + \underbrace{\left(1 + \frac{k(k-1)}{2}\right)}_{\#<\ \text{per}\ \alpha > 0}$

#op. / β

(#β-1 nuovi + 1 con l'α precedente)

$= \frac{1}{16}(7k^5 + 7k^4 - 14k^3 + 64k^2 + 48k + 16)$ op. el.

$\sum_{k=2}^{n-1} \cdots = \frac{7}{96}n^6 - \frac{21}{160}n^5 - \frac{49}{192}n^4 + \frac{23}{12}n^3 - \frac{145}{192}n^2 + \frac{73}{480}n - 9$

The reason why the algorithm works is that once we find splits that are not partial d-splits (that is they have zero isolation index), we know that also their extensions won't be d-splits – since the isolation index can only get lower by extending.

A similar improvement in the actual implementation can be made: once we find that a quartet has zero β index, then also the α index is zero; so we can stop checking the other quartets.
Also when computing the β index we can exploit the symmetry of d to skip about $^3/_4$ of quartets.

Another consequence of the above results is the following fact.

COROLLARY 5. *Let a symmetric function $d\colon X \times X \to \mathbb{R}$ on an n-set X be decomposed as $d = d_0 + \sum_S \alpha_S^d \cdot \delta_S$ according to Theorem 2. Then d_0 is linearly independent from $\{\delta_S \mid S$ is a d-split$\}$. In particular, if there are $\binom{n}{2}$ d-splits, then $d_0 = 0$. Similarly, if d is a metric, then d_0 is linearly independent from $\{\delta_S \mid S$ is a d-split or $S = \{x\}, X - \{x\}$ for some $x \in X\}$. Consequently, $d_0 = 0$ in case that there are $\binom{n}{2} - n$ d-splits A, B with* $\min\{\#A, \#B\} \geqslant 2$.

Proof. Suppose that d_0 is a linear combination of the split metrics δ_S for which $\alpha_S^d > 0$,

$$d_0 = \sum_S \lambda_S \cdot \delta_S,$$

where each λ_S is a real number, and the sum extends over all d-splits S. Put

$$\mathscr{S}^+ := \{S \mid S \text{ is a } d\text{-split with } \lambda_S \geqslant 0\},$$
$$\mathscr{S}^- := \{S \mid S \text{ is a } d\text{-split with } \lambda_S < 0\}.$$

Consider the metric

$$d' := \sum_{S \in \mathscr{S}^-} \alpha_S^d \cdot \delta_S + \sum_{S \in \mathscr{S}^+} (\alpha_S^d + \lambda_S) \cdot \delta_S.$$

For any split S of X,

$$\alpha_S^{d'} = \begin{cases} \alpha_S^d + \lambda_S & \text{if} \quad S \in \mathscr{S}^+, \\ \alpha_S^d & \text{if} \quad S \in \mathscr{S}^-, \\ 0 & \text{otherwise,} \end{cases}$$

by Theorem 3. On the other hand, as

$$d' = d - \sum_{S \in \mathscr{S}^-} \lambda_S \cdot \delta_S,$$

we infer from Theorem 2 that

$$\alpha_S^{d'} = \begin{cases} \alpha_S^d & \text{if} \quad S \in \mathcal{S}^+, \\ \alpha_S^d - \lambda_S & \text{if} \quad S \in \mathcal{S}^-. \end{cases}$$

Hence $\lambda_S = 0$ for all $S \in \mathcal{S}$. Consequently, d_0 is the zero metric, thus proving the first assertion of the corollary. The second assertion is then immediate from Corollary 4.

Finally, the first two assertions, applied with respect to

$$d^* := d + \sum_{x \in X} \delta_{\{x\}, X - \{x\}},$$

yield the last assertions in view of Corollary 2. ∎

Cor. 5 Let $d : X \times X \to \mathbb{R}$ be a symmetric function.

Then the residue d_0 is linearly independent from $\{\delta_S\}_{S \in \mathcal{S}_d(X)}$.
In particular, if there are $\binom{n}{2}$ d-splits, then $d_0 = 0$.

If d is a pseudo-metric,
then d_0 is linearly independent from $\{\delta_S\}_{S \in \mathcal{S}_d(X)} \cup \{\delta_x\}_{x \in X}$.
If there are $\binom{n}{2} - n$ non trivial d-splits, then $d_0 = 0$.

Dim. Suppose that

$$d_0 = \sum_{S \in \mathcal{S}_d(X)} \lambda_S \cdot \delta_S$$

so that

$$\begin{aligned} d = d_0 + \sum_{S \in \mathcal{S}(X)} \alpha_S^d \cdot \delta_S \\ = \sum_{S \in \mathcal{S}_d(X)} \lambda_S \cdot \delta_S + \sum_{S \in \mathcal{S}_d(X)} \alpha_S^d \cdot \delta_S \\ = \sum_{S \in \mathcal{S}_d(X)} \left(\alpha_S^d + \lambda_S\right) \cdot \delta_S \end{aligned}$$

Let

$$\mathcal{S}^+ := \{\, S \in \mathcal{S}_d(X) \mid \lambda_S \geq 0 \,\}$$

$$\mathcal{S}^- := \{\, S \in \mathcal{S}_d(X) \mid \lambda_S < 0 \,\}$$

Observe that $\mathcal{S}_d(X) = \mathcal{S}^+ \sqcup \mathcal{S}^-$.

Consider the pseudo-metric

$$d' := \sum_{S \,\in\, \mathcal{S}^-} \alpha_S^d \cdot \delta_S + \sum_{S \,\in\, \mathcal{S}^+} (\alpha_S^d + \lambda_S) \cdot \delta_S$$

Applying **Teo**. 3 we get

$$\alpha_S^{d'} = \begin{cases} \alpha_S^d + \lambda_S & S \in \mathcal{S}^+ \\ \alpha_S^d & S \in \mathcal{S}^- \end{cases},$$

We can write

$$d' = d - \sum_{S \,\in\, \mathcal{S}^-} \lambda_S \cdot \delta_S$$

and by applying **Teo**. 2 we get

$$\alpha_S^{d'} = \begin{cases} \alpha_S^d, & S \in \mathcal{S}^+ \\ \alpha_S^d - \lambda_S, & S \in \mathcal{S}^- \end{cases}$$

Thus $\lambda_S = 0$ for every split S, proving the linear independence.
The second assertion follows from **Cor**. 4.

Consider

$$d^* := d + \sum_{x \,\in\, X} \delta_x$$

By **Teo**. 2, $d_0^* = d_0$. Also notice that

$$\mathcal{S}_{d^*}(X) = \mathcal{S}_d(X) \cup \bigcup_{x \,\in\, X} \{\{x\}, X \setminus \{x\}\}$$

We get the thesis by applying the first assertion on d^*.

We record another straightforward consequence of Theorem 3 that will be of use in the next section. The *trace* of a collection $\mathscr{S}$ of splits of X on a subset Y of X is the set

$$\mathscr{S}|_Y := \{\{A \cap Y, B \cap Y\} \mid \{A, B\} \in \mathscr{S} \text{ with } Y \not\subseteq A \text{ and } Y \not\subseteq B\}.$$

COROLLARY 6. *Let $\mathscr{S}$ and $\mathscr{T}$ be collections of weakly compatible splits of a set X (with at least five points). Then $\mathscr{S} = \mathscr{T}$ whenever the traces of $\mathscr{S}$ and $\mathscr{T}$ on each 4-subset of X are identical. In addition, for every member S of $\mathscr{S}$ there exists a partial split $\{t, u\}$, $\{v, w\}$ such that S is the unique member of $\mathscr{S}$ extending $\{t, u\}$, $\{v, w\}$.*

Proof. Compare the metrics

$$d_1 := \sum_{S \in \mathscr{S}} \delta_S \qquad \text{and} \qquad d_2 := \sum_{T \in \mathscr{T}} \delta_T$$

on X. The isolation index of a partial split $\{t, u\}$, $\{v, w\}$ is positive with respect to d_1 if and only if it is positive with respect to d_2 since $\mathscr{S}|_{\{t,u,v,w\}}$ equals $\mathscr{T}|_{\{t,u,v,w\}}$. Therefore

$$\alpha^{d_1}_{A,B} > 0 \Leftrightarrow \alpha^{d_2}_{A,B} > 0 \qquad \text{for all splits } A, B \text{ of } X,$$

whence $\mathscr{S} = \mathscr{T}$ by Theorem 3. The second assertion then follows from Corollary 1. ▮

Def. Let $\mathcal{S}$ be a collection of splits of X and $Y \subseteq X$ a subset.
Then the **trace** of $\mathcal{S}$ on Y is the set

$$\mathcal{S}|_Y \coloneqq \{\, \{A \cap Y, B \cap Y\} \mid \{A, B\} \in \mathcal{S},\ Y \not\subseteq A \ \wedge\ Y \not\subseteq B \,\}$$

In practice, it is the restriction of the splits to Y such that they are still splits: in particular the members cannot be empty and, since the set of all splits is a partition of X, it is equivalent to ask that Y is not contained in a single member.

Cor. 6 Let $\mathcal{S}$ and $\mathcal{T}$ be collections of weakly compatible splits of X.

Then $\mathcal{S} = \mathcal{T}$ if and only if
their traces are identical on every 4-subset of X.

Dim. The $(\Rightarrow)$ implication is obvious.

Consider the pseudo-metrics
(since they are conical combinations of split metrics)

$$d_1 := \sum_{S \in \mathcal{S}} \delta_S \ , \qquad d_2 := \sum_{T \in \mathcal{T}} \delta_T$$

Observe that, given $Y = \{t, u, v, w\}$ a 4-subset of X,

$$d_1|_Y = d_2|_Y$$

because they depend only by (the restrictions of) the splits on Y, and $\mathcal{S}, \mathcal{T}$ have the same trace on 4-subsets.

If we consider a split on Y, for example $\{\{t,u\},\{v,w\}\}$,
and the fact that d_1, d_2 are pseudo-metrics, we have

$$\alpha^{d_1}_{\{t,u\},\{v,w\}} = \beta^{d_1}_{\{t,u\},\{v,w\}} = \beta^{d_2}_{\{t,u\},\{v,w\}} = \alpha^{d_2}_{\{t,u\},\{v,w\}}$$

In particular, the isolation index on quartets is positive with respect to d_1 if and only if it is positive with respect to d_2.

This is true also for generic splits because
the isolation index on a generic split is the minimum of
the isolation indices on appropriate quartets.
In particular, the d_1-splits coincide with the d_2-splits.

By **Teo**. 3 we have

$$\mathcal{S} = \mathcal{S}_{d_1}(X) = \mathcal{T}_{d_2}(X) = \mathcal{T}$$

Prop. Let $\mathcal{S}$ be a collection of weakly compatible splits of X.

Then for every $S \in \mathcal{S}$ there exists a partial split $\{\{t, u\}, \{v, w\}\}$ such that S is its unique split extension in $\mathcal{S}$.

Dim. Let $\{\{t, u\}, \{v, w\}\}$ such that

$$\alpha_S = \beta_{\{t,u\},\{v,w\}}$$

with respect to the distance $d \coloneqq \sum_{S \in \mathcal{S}} \delta_S$.

Since by **Teo**. 3 it holds $\mathcal{S} = \mathcal{S}_d(X)$, then S is a d-split. Applying **Cor**. 1 we conclude that S is the unique d-split (that is equivalent to saying element of $\mathcal{S}$) extending $\{\{t, u\}, \{v, w\}\}$.

Solo enunciati.

Next we provide an extension of Theorem 3, allowing one to recover certain collections of split metrics from their sums with a given nonzero symmetric function d from $X \times X$ to $\mathbb{R}$.

Let us call a split $S = \{A, B\}$ of X a *virtual d-split* if

$$aa' + bb' \leqslant \max\{ab + a'b', ab' + a'b\} \qquad \text{for all} \quad a, a' \in A \text{ and } b, b' \in B,$$

or equivalently, if S is a $(d + \lambda \cdot \delta_S)$-split for every $\lambda > 0$. In other words, S is a virtual d-split if and only if there exists a sequence d_i $(i = 1, 2, ...)$ of symmetric functions converging to d such that S is a d_i-split for all $i = 1, 2, ...$. Two virtual d-splits $S_1 = \{A_1, B_1\}$ and $S_2 = \{A_2, B_2\}$ of X are said to be *d-compatible* if

$$xy + uv \geqslant xu + yv, \qquad xy + uv \geqslant xv + yu$$

$$\text{for all} \quad x \in A_1 \cap A_2,\ y \in B_1 \cap B_2,\ u \in A_1 \cap B_2,\ v \in A_2 \cap B_1,$$

or equivalently, if S_1 and S_2 are $(d + \lambda_1 \cdot \delta_{S_1} + \lambda_2 \cdot \delta_{S_2})$-splits for all $\lambda_1, \lambda_2 > 0$; this in turn is equivalent to the condition that for every positive $\lambda \in \mathbb{R}$ the split S_2 is a virtual $(d + \lambda \cdot \delta_{S_1})$-split. By definition, two compatible virtual d-splits are d-compatible. Given any collection $\mathscr{S}$ of weakly compatible splits S with positive weights λ_S, Theorem 3 says that each $S' \in \mathscr{S}$ is a virtual $(\sum_{S \in \mathscr{S} - \{S'\}} \lambda_S \cdot \delta_S)$-split. Moreover, three splits S_1, S_2, S_3 are weakly compatible if and only if S_1 and S_2 are δ_{S_3}-compatible.

THEOREM 4. *Let $d: X \times X \to \mathbb{R}$ be a symmetric function on X, and let $\mathscr{S}$ be a collection of splits of X. Then $\mathscr{S}$ is included in the system of all d'-splits for every function d' of the form*

$$d' := d + \sum_{S \in \mathscr{S}} \lambda_S \cdot \delta_S,$$

where $\lambda_S > 0$ for all $S \in \mathscr{S}$ if and only if all splits in $\mathscr{S}$ are virtual d-splits, any two splits in $\mathscr{S}$ are d-compatible, and any three splits in $\mathscr{S}$ are weakly compatible.

In particular, if d_0 and d_1 are symmetric functions on X such that d_0 is split-prime and the canonical decomposition of d_1 leaves no nonzero residue, then d_0 is the residue of $d_0 + d_1$ exactly when the system of all d_1-splits consists of virtual d_0-splits which are pairwise d_0-compatible.

Finally, as announced above, we characterize the split-prime 5-point metrics.

LEMMA 1. *Up to a scalar every split-prime metric d on X with $\# X=5$ and $d(x, y) \neq 0$ for $x \neq y$ is isometric to the metric induced by $K_{2,3}$; that is, there exists a split $X=Y \cup Z$ with $\# Y=3$ and $\# Z=2$ such that for some $\alpha>0$ one has $d(y, z)=\alpha$ for $y \in Y$ and $z \in Z$, and $d(y, y')=d(z, z')=2\alpha$ for any distinct $y, y' \in Y$ or $z, z' \in Z$.*

In particular, if d is a metric on a five-point set X with nonzero split-prime residue d_0, then one can label the elements of X so that $X=\{y_1, y_2, y_3\} \cup \{z_1, z_2\}$ and $\{z_1, y_i\}$, $\{z_2, y_j\}$ is a partial d-split for all $i, j \in \{1, 2, 3\}$ with $i \neq j$.

Lemma 1 and Theorem 4 pave the way to a painless verification of the useful fact (first stated in (1.16) of [11]) that there are exactly three "generic" types of 5-point metrics. Let X be a set of cardinality 5. Note that a family $\mathscr{S}$ of splits of X is weakly compatible if and only if

$$\mathscr{S}^{(2)} := \{\{A, B\} \in \mathscr{S} \mid \min\{\# A, \# B\}=2\}$$

is weakly compatible. The members of $\mathscr{S}^{(2)}$ are then conveniently coded as the edges of an undirected graph with vertex-set X, briefly referred to as the graph of $\mathscr{S}^{(2)}$ (or $\mathscr{S}$). Weak compatibility simply rephrases in graph-theoretic terms as follows: there are no triangles and no vertices of degree larger than 2. Hence $\mathscr{S}$ is weakly compatible if and only if its graph is isomorphic to a subgraph of the 5-cycle or the 4-cycle plus an isolated vertex. There are thus exactly two types of weakly compatible split systems that are maximal with respect to inclusion. In view of Theorem 3 and this observation one can easily describe the metrics on X which totally decompose into split metrics (thus yielding only zero residues); see Fig. 8 and Fig. 9 (with $\alpha=0$) below.

[...]

So we arrive at three generic types of 5-point metrics d: (I) the residue d_0 of d is zero and the graph of $\mathscr{S}_d^{(2)}$ is a 5-cycle; (II) $d_0 \neq 0$ and the graph of $\mathscr{S}_d^{(2)}$ is a 4-cycle plus an isolated vertex; (III) $d_0 \neq 0$ and the graph of $\mathscr{S}_d^{(2)}$ is a path (of length 4). More explicitly, these metrics are generated as follows.

Type I. For $X=\{x_0, x_1, x_2, x_3, x_4\}$ and positive real numbers ξ_i, β_i ($i=0, 1, 2, 3, 4$) put

$$d := \sum_{i=0}^{4} \xi_i \cdot \delta_{\{x_i\}, X-\{x_i\}} + \sum_{i=0}^{4} \beta_i \cdot \delta_{\{x_i, x_{i+1}\}, X-\{x_i, x_{i+1}\}}$$

(indices modulo 5), cf. Fig. 8.

Type II. For $X=\{z_1, z_2, y_1, y_2, y_3\}$ and positive real numbers ζ_1, ζ_2, η_1, η_2, η_3, β_1, β_2. β_3, β_4, α put

$$\begin{aligned} d := {} & \sum_{i=1}^{2} \zeta_i \cdot \delta_{\{z_i\}, X-\{z_i\}} + \sum_{i=1}^{3} \eta_i \cdot \delta_{\{y_i\}, X-\{y_i\}} \\ & + \beta_1 \cdot \delta_{\{y_1, z_1\}, X-\{y_1, z_1\}} + \beta_2 \cdot \delta_{\{z_1, y_2\}, X-\{z_1, y_2\}} \\ & + \beta_3 \cdot \delta_{\{y_2, z_2\}, X-\{y_2, z_2\}} + \beta_4 \cdot \delta_{\{z_2, y_1\}, X-\{z_2, y_1\}} \\ & + \alpha \cdot d', \end{aligned}$$

where d' is the $K_{2,3}$ metric defined by

$$d'(z_1, z_2) = d'(y_i, y_j) = 2 \qquad (1 \leqslant i < j \leqslant 3),$$

$$d'(z_i, y_j) = 1 \qquad (i=1, 2;\ j=1, 2, 3) \text{ (see Fig. 9).}$$

Type III. The labels and parameters are as in type II, but now put

$$\begin{aligned} d := {} & \sum_{i=1}^{2} \zeta_i \cdot \delta_{\{z_i\}, X-\{z_i\}} + \sum_{i=1}^{3} \eta_i \cdot \delta_{\{y_i\}, X-\{y_i\}} \\ & + \beta_1 \cdot \delta_{\{y_1, z_1\}, X-\{y_1, z_1\}} + \beta_2 \cdot \delta_{\{z_1, y_2\}, X-\{z_1, y_2\}} \\ & + \beta_3 \cdot \delta_{\{y_2, z_2\}, X-\{y_2, z_2\}} + \beta_4 \cdot \delta_{\{z_2, y_3\}, X-\{z_2, y_3\}} \\ & + \alpha \cdot d'. \end{aligned}$$

All other ("degenerate") 5-point metrics are obtained by setting some of the parameters equal to zero. For instance, the 5-point tree metric with 7 splits is obtained from each type by letting either $\beta_1 = \beta_3 = \beta_4 = 0$ (type I), or $\beta_2 = \beta_4 = \alpha = 0$ (types II and III), say.

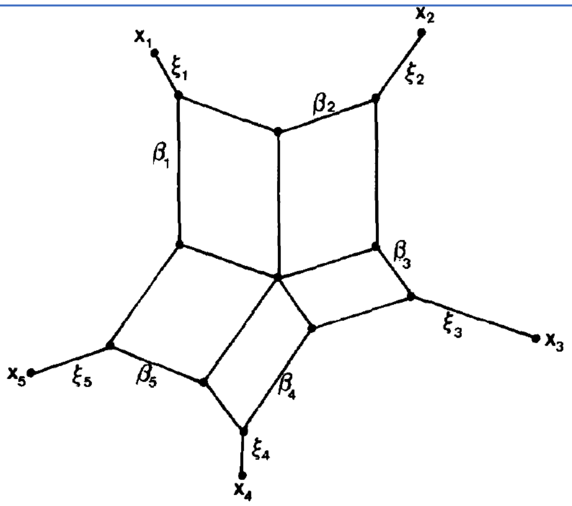


FIG. 8. A generic 5-point metric: type I.

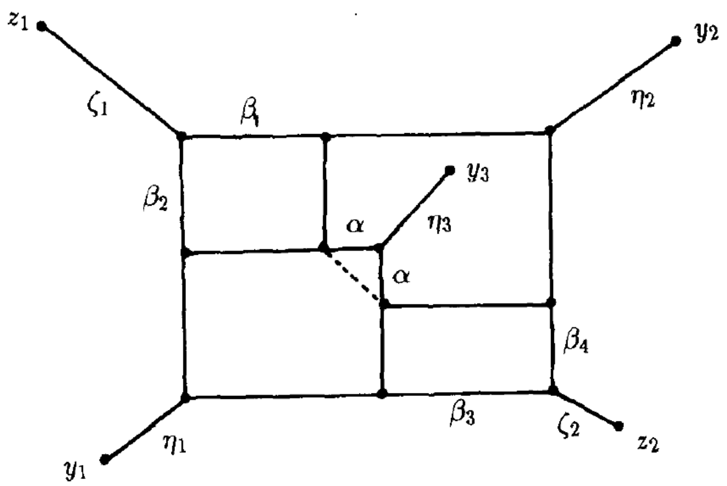


FIG. 9. A generic 5-point metric: type II.

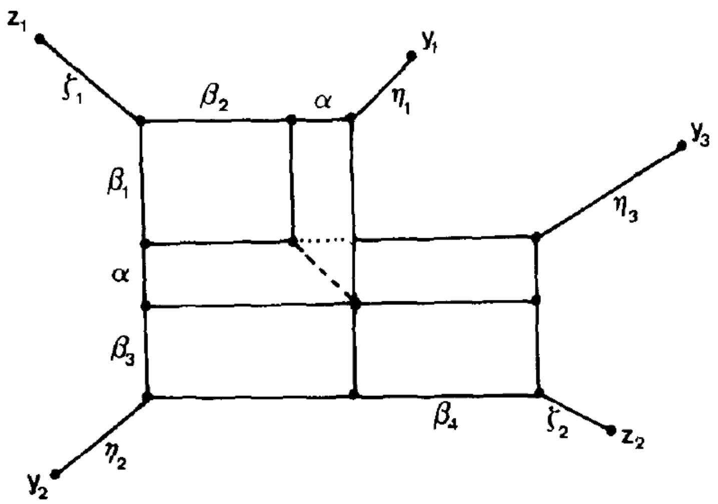


FIG. 10. A generic 5-point metric: type III.

3. Maximum Collections of Weakly Compatible Splits

The upper bound $\binom{n}{2}$ in Corollary 4 for the total number of d-splits is actually attained for a circular configuration. Namely, let $x_0, ..., x_n = x_0$ (in this order) be the vertices of a convex n-gon. Any pair of distinct edges (x_i, x_{i+1}), (x_j, x_{j+1}), where $i < j$, gives rise to a split $\{x_{i+1}, x_{i+2}, ..., x_j\}$, $\{x_{j+1}, ..., x_{i-1}, x_i\}$, that is, the split induced by any line crossing the edges (x_i, x_{i+1}) and (x_j, x_{j+1}). It is clear that the forbidden configuration of partial splits on four points cannot occur here. Hence the collection of all these $\binom{n}{2}$ splits is weakly compatible. We call any subset of such a collection of splits *circular*.

Next we want to show that every "maximum collection" of $\binom{n}{2}$ weakly compatible splits is circular. To this end we first give a convenient description of cycles in terms of the *crossing relation* $|$: four distinct points are related as $tv|uw$ in a cycle when the line segment from t to v crosses the line segment from u to w (see Fig. 11). Notice that a cycle is uniquely determined by its crossing relation.

The following result should actually belong to folklore.

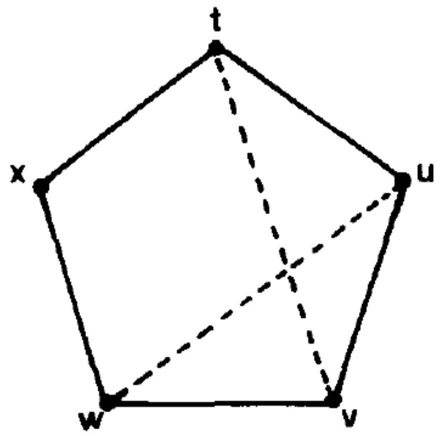


FIG. 11. The instance $tv|uw$ on a pentagon.

I circular splits sono weakly compatible perché 4 punti disposti in cerchio non sono linearmente separabili.

PROPOSITION 1. *A quaternary relation* $|$ *on a set* X *is the crossing relation of a cycle if and only if the following three conditions hold for distinct* $t, u, v, w, x \in X$:

(1) $tu|vw$ *implies* $ut|vw$ *and* $vw|tu$;

(2) *either* $tu|vw$, *or* $tv|uw$, *or* $tw|uv$ (*exclusively*);

(3) $tv|uw$ *and* $tw|vx$ *imply* $tv|ux$.

THEOREM 5. *The following conditions are equivalent for a weakly compatible collection* $\mathscr{S}$ *of splits of an n-set* X:

(i) $\mathscr{S}$ *is the circular collection of all splits of a convex n-gon with vertices from* X;

(ii) $\#\mathscr{S} = \binom{n}{2}$;

(iii) *the split metrics* δ_S $(S \in \mathscr{S})$ *form a basis of the linear space* $\langle M(X) \rangle$ *of all symmetric functions* $d: X \times X \to \mathbb{R}$ *satisfying* $d(x, x) = 0$ *for all* $x \in X$;

(iv) *for every* $S \in \mathscr{S}$ *there is exactly one partial split* $\{t, u\}$, $\{v, w\}$ *which extends to S but to no other member of* $\mathscr{S}$.

Proof. We already know that (ii) and (iii) are equivalent (cf. Corollary 4). Evidently, (i) implies (ii).

To prove that (ii) or (iii) implies (i), first note that for every subset Y of X, the restrictions $\delta_S|_{Y \times Y}$ $(S \in \mathscr{S})$ generate the space of all symmetric functions on Y with zero diagonal. This is because every such function extends to a symmetric function on X with zero diagonal, which then can be expressed as a linear combination of the split metrics δ_S $(S \in \mathscr{S})$. The splits corresponding to the nonzero metrics of the form $\delta_S|_{Y \times Y}$ $(S \in \mathscr{S})$ constitute the trace of $\mathscr{S}$ on Y. Therefore $\#\mathscr{S}|_Y = \binom{\# Y}{2}$. In particular, for any subset Y with $\# Y = 4$, exactly two of the three splits A, B of Y with $\# A = \# B = 2$ extend to splits in $\mathscr{S}$. So, the relation $|$, defined for distinct

Circular collections of splits (which are not necessarily maximum) are further studied in a forthcoming paper by Bandelt, Dress, and Möller.

Finally note that if $\mathscr{S}$ is a circular collection of splits S with positive weights α_S then the "circular" metric $d = \sum_{S \in \mathscr{S}} \alpha_S \cdot \delta_S$ admits an optimal travelling salesperson tour of length $2 \cdot \sum_{S \in \mathscr{S}} \alpha_S$. If d is an arbitrary metric and $\mathscr{S}$ is its system of d-splits S with isolation indices α_S, then this length is still a lower bound for the lengths of tours through all points (because each d-split must be "traversed" at least twice).

4. Total Decomposability

In Theorem 1 we have seen that the isolation index of a partial d-split T is greater than or equal to the sum of the isolation indices of the d-splits extending T. When does equality always hold? To state the answer, let us define a symmetric function $d: X \times X \to \mathbb{R}$ to be *totally decomposable* if d equals the sum of $\alpha_S^d \cdot \delta_S$ where S runs through all d-splits. That is, in the decomposition of d according to Theorem 2 there is no split-prime remainder: $d_0 = 0$. Then d is necessarily a metric. As we have seen in the introduction, metric spaces having at most four points are always totally decomposable. In contrast, on a 5-set there is a nonzero split-prime metric, namely the one associated with the graph $K_{2,3}$ (see Fig. 4). In general, the following holds.

Def. A symmetric function $d : X \times X \to \mathbb{R}$ is **totally decomposable** if its split-prime residue is zero $d_0 = 0$;
or equivalently, if it can be written as

$$d = \sum_{S \in \mathcal{S}_d(X)} \alpha_S^d \cdot \delta_S$$

Oss. A totally decomposable function is a pseudo-metric.

In fact, it is a conical combination of split metrics (that are pseudo-metrics).

Fact If $|X| \leq 4$, then every pseudo-metric is totally decomposable.

If $|X| = 5$, then there is a non-zero split-prime pseudo-metric, namely the one associated with the graph $K_{2,3}$.

THEOREM 6. *The following conditions are equivalent for a symmetric function* $d: X \times X \to \mathbb{R}$ *with zero diagonal*:

(i) d *is a totally decomposable metric*;

(ii) *every partial d-split T extends to d-splits so that*

$$\alpha_T = \sum \{\alpha_S \mid S \text{ is a } d\text{-split extending } T\};$$

(iii) *for all* $t, u, v, w, x \in X$,

$$\alpha_{\{t,u\},\{v,w\}} = \alpha_{\{t,u,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,w,x\}};$$

(iv) *for all* $t, u, v, w, x \in X$,

$$\alpha_{\{t,u\},\{v,w\}} \leqslant \alpha_{\{t,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,x\}}.$$

Proof. (i) implies (ii). By definition we have

$$d = \sum_S \alpha_S \cdot \delta_S.$$

For any proper subset Y of X,

$$d|_{Y \times Y} = \sum_S \alpha_S \cdot \delta_S|_{Y \times Y} = \sum \{\lambda_T \cdot \delta_T \mid T \text{ is a split of } Y\},$$

where λ_T is the sum of $\alpha_{A,B}$ for all d-splits A, B extending T. Since the collection of splits T of Y for which $\lambda_T > 0$ is weakly compatible, it follows from Theorem 3 that each λ_T is the isolation index of T.

(ii) implies (iii). This is clear, for

$$\begin{aligned}
\alpha_{\{t,u\},\{v,w\}} &= \sum \{\alpha_S \mid S \text{ extends } \{t,u\}, \{v,w\}\} \\
&= \sum \{\alpha_S \mid S \text{ extends } \{t,u,x\}, \{v,w\}\} \\
&\quad + \sum \{\alpha_S \mid S \text{ extends } \{t,u\}, \{v,w,x\}\} \\
&= \alpha_{\{t,u,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,w,x\}}.
\end{aligned}$$

(iii) implies (iv). This is also clear, for

$$\begin{aligned}\alpha_{\{t,u\},\{v,w\}} &= \alpha_{\{t,u,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,w,x\}} \\ &\leqslant \alpha_{\{t,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,x\}}.\end{aligned}$$

(iv) implies (iii). By Theorem 1, we always have

$$\alpha_{\{t,u\},\{v,w\}} \geqslant \alpha_{\{t,u,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,w,x\}}.$$

On the other hand,

$$\alpha_{\{t,u,x\},\{v,w\}} = \min\{\alpha_{\{t,u\},\{v,w\}}, \alpha_{\{t,x\},\{v,w\}}, \alpha_{\{u,x\},\{v,w\}}\}$$

and

$$\alpha_{\{t,u\},\{v,w,x\}} = \min\{\alpha_{\{t,u\},\{v,w\}}, \alpha_{\{t,u\},\{v,x\}}, \alpha_{\{t,u\},\{w,x\}}\}$$

implies that $\alpha_{\{t,u,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,w,x\}}$ is not smaller than the minimum of $\alpha_{\{t,u\},\{v,w\}}$, $\alpha_{\{t,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,x\}}$, $\alpha_{\{t,x\},\{v,w\}} + \alpha_{\{t,u\},\{w,x\}}$, $\alpha_{\{u,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,x\}}$, and $\alpha_{\{u,x\},\{v,w\}} + \alpha_{\{t,u\},\{w,x\}}$. Hence, (iv) applied with respect to x and either t, u; v, w, or t, u; w, v, or u, t; v, w, or u, t; w, v, implies

$$\alpha_{\{t,u,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,w,x\}} \geqslant \alpha_{\{t,u\},\{v,w\}}$$

and therefore

$$\alpha_{\{t,u\},\{v,w\}} = \alpha_{\{t,u,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,w,x\}}.$$

(iii) implies (i). Clearly d is a metric: from (iii) and the equality $aa=0$ for all $a \in X$ we infer

$$\begin{aligned}uv = \alpha_{\{u\},\{v\}} &= \alpha_{\{u,x\},\{v\}} + \alpha_{\{u\},\{v,x\}} \\ &\leqslant \alpha_{\{x\},\{v\}} + \alpha_{\{u\},\{x\}} \\ &= xv + ux\end{aligned}$$

for all $u, v, x \in X$.

Now, suppose that the metric space (X, d) is not totally decomposable, where $\# X$ is as small as possible. In addition, assume that the number of d-splits is minimal under this condition. We claim that in this case d must be split-prime. To verify this it suffices to show that

$$\tilde{d} := d - \alpha_{A,B} \cdot \delta_{A,B}$$

for any d-split A, B would also satisfy condition (iii), contrary to the minimality assumption. So we assert that for all $t, u, v, w, x \in X$ the isolation indices with respect to $\tilde{d}$ satisfy the inequality

$$\tilde{\alpha}_{\{t,u\},\{v,w\}} = \tilde{\alpha}_{\{t,u,x\},\{v,w\}} + \tilde{\alpha}_{\{t,u\},\{v,w,x\}}. \tag{+}$$

First observe that

$$\tilde{\alpha}_{A_0,B_0} = \begin{cases} \alpha_{A_0,B_0} - \alpha_{A,B} & \text{if } A, B \text{ extends } A_0, B_0, \\ \alpha_{A_0,B_0} & \text{otherwise} \end{cases} \tag{++}$$

for all $A_0, B_0 \subseteq X$. This follows immediately from Theorem 2 applied to the restriction of d to $A_0 \cup B_0$. Now, either A, B extends $\{t, u\}$, $\{v, w\}$, in which case it extends $\{t, u, x\}$, $\{v, w\}$ or $\{t, u\}$, $\{v, w, x\}$ but not both, or A, B does not extend $\{t, u\}$, $\{v, w\}$, in which case it extends neither $\{t, u, x\}$, $\{v, w\}$ nor $\{t, u\}$, $\{v, w, x\}$. In either case $(+)$ follows from $(++)$ and (iii). We conclude that indeed d is split-prime.

Next assume that $\# X = 5$. If $\alpha_{\{t,u\},\{v,w\}} = 0$ for all distinct $t, u, v, w \in X$, then

$$tu + vw = tv + uw = tw + uv$$

would hold throughout, and thus letting $X = \{a_1, a_2, a_3, a_4, a_5\}$ and $\alpha_i := \frac{1}{2} \cdot (a_i a_j + a_i a_k - a_j a_k)$ for $i = 1, 2, 3, 4, 5$ (which would be independent of $j, k \in \{1, 2, 3, 4, 5\}$ as long as $\# \{i, j, k\} = 3$) d would be totally decomposable in the form

$$d = \sum_{i=1}^{n} \alpha_i \cdot \delta_{\{a_i\}, X - \{a_i\}},$$

a contradiction. On the other hand, if the partial split $\{t, u\}$, $\{v, w\}$ has a positive isolation index, where $X = \{t, u, v, w, x\}$, then by (iii) either $\alpha_{\{t,u,x\},\{v,w\}}$ or $\alpha_{\{t,u\},\{v,w,x\}}$ is positive as well, contrary to our assumption that d is split-prime. This settles the case $\# X = 5$. Conditions (i), (ii), (iii), and (iv) are therefore equivalent whenever $\# X = 5$.

Finally assume that $\# X > 5$. By the initial hypothesis (viz., minimality of $\# X$), $d|_{Y \times Y}$ is totally decomposable for every proper subset Y of X. Let $\mathscr{T}$ be the set of all partial d-splits A, B of X such that $\#(A \cup B) = \# X - 1$.

We claim that $\max\{\# A, \# B\} = 3$ for each member A, B of $\mathscr{T}$. Say, $A \cup B = X - \{x\}$. If a_1, a_2, a_3 are distinct points in A, then for at least one index i we have

$$(A - \{a_i\}, B \cup \{x\}) \notin \mathscr{T},$$

for otherwise, A, $B \cup \{x\}$ is a d-split of X. Suppose that A contains at least four distinct points a_1, a_2, a_3, a_4. Then, by the preceding argument, there are two distinct indices $i \neq j$ such that neither $A - \{a_i\}$, $B \cup \{x\}$ nor $A - \{a_j\}$, $B \cup \{x\}$ belongs to $\mathscr{T}$. Hence, as $A - \{a_i\}$, B and $A - \{a_j\}$, B are partial d-splits of the totally decomposable subspaces $X - \{a_i\}$ and $X - \{a_j\}$, respectively, they must extend to the respective members $(A - \{a_i\}) \cup \{x\}$, B and $(A - \{a_j\}) \cup \{x\}$, B of $\mathscr{T}$. But then $A \cup \{x\}$, B is a d-split which is impossible. This proves our claim.

So, given A, B as before, we may assume that $\# A \geqslant 2$ and $\# B = 3$. Then, as above, there exists $a \in A$ such that $(A - \{a\}) \cup \{x\}$, B is not in $\mathscr{T}$, whence $A - \{a\}$, $B \cup \{x\}$ belongs to $\mathscr{T}$. This contradicts the just proven claim since $\#(B \cup \{x\}) = 4$. This final contradiction concludes the proof of the theorem. ∎

Teo. 6 Let $d : X \times X \to \mathbb{R}$ be a symmetric function with zero diagonal. Then the following conditions are equivalent:

(i) d is totally decomposable

(ii) for every partial split T

$$\alpha_T = \sum \{\, \alpha_S \mid S \in \mathcal{S}_d(X),\ S \succcurlyeq T \,\}$$

(iii) for all $t, u, v, w, x \in X$

$$\alpha_{\{t,u\},\{v,w\}} = \alpha_{\{t,u,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,w,x\}}$$

(iv) for all $t, u, v, w, x \in X$

$$\alpha_{\{t,u\},\{v,w\}} \leq \alpha_{\{t,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,x\}}$$

Dim. (i ⇒ ii) By definition of total decomposability, we have

$$d = \sum_{S \in \mathcal{S}_d(X)} \alpha_S \cdot \delta_S$$

For any proper subset $Y \subset X$

$$d|_{Y\times Y} = \sum_{S \in \mathcal{S}_d(X)} \alpha_S \cdot \delta_S|_{Y\times Y} = \sum \{ \lambda_T \cdot \delta_T \mid T \in \mathcal{S}(Y) \}$$

where $\lambda_T = \sum\{ \alpha_S \mid S \in \mathcal{S}_d(X),\ S \succcurlyeq T \}$.

From **Teo**. 1, we have $\lambda_T \leq \alpha_T$ for every T split of Y. Thus

$$\{ T \in \mathcal{S}(Y) \mid \lambda_T > 0 \} \subseteq \mathcal{S}_d(Y)$$

so it is weakly compatible. Applying **Teo**. 3 to this set we get

$$\alpha_T = \lambda_T$$

(ii ⇒ iii) Let $t, u, v, w, x \in X$. Then

$$\begin{aligned} \alpha_{\{t,u\},\{v,w\}} &= \sum \left\{ \alpha_S \,\middle|\, S \in \mathcal{S}_d(X),\ S \succcurlyeq \{\{t,u\},\{v,w\}\} \right\} \\ &= \sum \left\{ \alpha_S \,\middle|\, S \in \mathcal{S}_d(X),\ S \succcurlyeq \{\{t,u,x\},\{v,w\}\} \right\} \\ &\quad + \sum \left\{ \alpha_S \,\middle|\, S \in \mathcal{S}_d(X),\ S \succcurlyeq \{\{t,u\},\{v,w,x\}\} \right\} \\ &= \alpha_{\{t,u,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,w,x\}} \end{aligned}$$

(iii ⇒ iv) Let $t, u, v, w, x \in X$. Then

$$\begin{aligned} \alpha_{\{t,u\},\{v,w\}} &= \alpha_{\{t,u,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,w,x\}} \\ &\leq \alpha_{\{t,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,x\}} \end{aligned}$$

(iv ⇒ iii) Let $t, u, v, w, x \in X$. By **Teo**. 1 we have

$$\alpha_{\{t,u,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,w,x\}} \leq \alpha_{\{t,u\},\{v,w\}}$$

On the other hand

$$\alpha_{\{t,u,x\},\{v,w\}} = \min\{\alpha_{\{t,u\},\{v,w\}}, \alpha_{\{t,x\},\{v,w\}}, \alpha_{\{u,x\},\{v,w\}}\}$$

$$\alpha_{\{t,u\},\{v,w,x\}} = \min\{\alpha_{\{t,u\},\{v,w\}}, \alpha_{\{t,u\},\{v,x\}}, \alpha_{\{t,u\},\{w,x\}}\}$$

Applying condition (iv) with respect to x and either

$$t,u;v,w\,, \qquad t,u;w,u\,, \qquad u,t;v,w\,, \qquad u,t;w,v$$

we get

$$\begin{aligned}
\alpha_{\{t,u\},\{v,w\}} &\leq \alpha_{\{t,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,x\}} \\
\alpha_{\{t,u\},\{w,v\}} &\leq \alpha_{\{t,x\},\{w,v\}} + \alpha_{\{t,u\},\{w,x\}} \\
\alpha_{\{u,t\},\{v,w\}} &\leq \alpha_{\{u,x\},\{v,w\}} + \alpha_{\{u,t\},\{v,x\}} \\
\alpha_{\{u,t\},\{w,v\}} &\leq \alpha_{\{u,x\},\{w,v\}} + \alpha_{\{u,t\},\{w,x\}}
\end{aligned}$$

Therefore

$$\begin{aligned}
\alpha_{\{t,u,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,w,x\}} &= \min\left\{\begin{matrix}
\alpha_{\{t,u\},\{v,w\}} + \alpha_{\{t,u\},\{v,w\}}, \\
\alpha_{\{t,u\},\{v,w\}} + \alpha_{\{t,u\},\{v,x\}}, \\
\alpha_{\{t,u\},\{v,w\}} + \alpha_{\{t,u\},\{w,x\}}, \\
\alpha_{\{t,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,w\}}, \\
\alpha_{\{t,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,x\}}, \\
\alpha_{\{t,x\},\{v,w\}} + \alpha_{\{t,u\},\{w,x\}}, \\
\alpha_{\{u,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,w\}}, \\
\alpha_{\{u,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,x\}}, \\
\alpha_{\{u,x\},\{v,w\}} + \alpha_{\{t,u\},\{w,x\}}
\end{matrix}\right\} \\
&\geq \min\left\{\begin{matrix}
\alpha_{\{t,u\},\{v,w\}} \\
\alpha_{\{t,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,x\}}, \\
\alpha_{\{t,x\},\{v,w\}} + \alpha_{\{t,u\},\{w,x\}}, \\
\alpha_{\{u,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,x\}}, \\
\alpha_{\{u,x\},\{v,w\}} + \alpha_{\{t,u\},\{w,x\}}
\end{matrix}\right\} \\
&\geq \alpha_{\{t,u\},\{v,w\}}
\end{aligned}$$

(iii $\Rightarrow$ i) [DA FARE]

As an immediate consequence of the above equivalence (i) $\Leftrightarrow$ (ii) we note the following fact (compare Corollary 1). For a totally decomposable metric d and a d-split A, B with $a_1, a_2 \in A$ and $b_1, b_2 \in B$, the partial d-split $\{a_1, a_2\}$, $\{b_1, b_2\}$ extends to no d-split other than A, B if and only if $\alpha_{\{a_1,a_2\},\{b_1,b_2\}} = \alpha_{A,B}$.

Cor. Let d a totally decomposable pseudo-metric, $\{A, B\}$ a d-split and $a_1, a_2 \in A$, $b_1, b_2 \in B$.

Then $\{A, B\}$ is the only d-split extension of $\big\{\{a_1, a_2\}, \{b_1, b_2\}\big\}$ if and only if $\alpha_{\{a_1,a_2\},\{b_1,b_2\}} = \alpha_{A,B}$.

Dim. $(\Rightarrow)$ By **Teo**. 6

$$\alpha_{\{a_1,a_2\},\{b_1,b_2\}} = \sum \big\{ \alpha_S \,\big|\, S \in \mathcal{S}_d(X),\ S \succcurlyeq \big\{\{a_1, a_2\}, \{b_1, b_2\}\big\} \big\}$$
$$= \alpha_{A,B}$$

$(\Leftarrow)$ By **Teo**. 6

$$\alpha_{A,B} = \alpha_{\{a_1,a_2\},\{b_1,b_2\}}$$
$$= \sum \big\{ \alpha_S \,\big|\, S \in \mathcal{S}_d(X),\ S \succcurlyeq \big\{\{a_1, a_2\}, \{b_1, b_2\}\big\} \big\}$$

and since $\alpha_{A,B}$ is a term of the sum, it must be the only one.

The preceding theorem confirms that total decomposability is a "five-point" condition. Therefore deciding whether a symmetric function d on an n-set X is totally decomposable is of complexity at most $O(n^5)$. In this case one can also determine all d-splits S and their isolation indices in at most $O(n^5)$ simple computational steps. Indeed, for each quadruple $(a_1, a_2, a_3, a_4) \in X^4$ with $\alpha_{\{a_1,a_2\},\{a_3,a_4\}} > 0$ one determines in $\#(X - \{a_1, a_2, a_3, a_4\})$ steps whether for all $x \in X - \{a_1, a_2, a_3, a_4\}$ the identity $\alpha_{\{a_1,a_2\},\{a_3,a_4\}} = \alpha_{\{a_1,a_2,x\},\{a_3,a_4\}} + \alpha_{\{a_1,a_2\},\{a_3,a_4,x\}}$ holds. If this is true, consider

$$A := \{x \in X \mid \alpha_{\{a_1,a_2\},\{a_3,a_4,x\}} = 0\},$$
$$B := \{x \in X \mid \alpha_{\{a_1,a_2,x\},\{a_3,a_4\}} = 0\},$$

and check whether $A \cup B = X$, in which case A, B is a d-split whose isolation index equals $\alpha_{\{a_1,a_2\},\{a_3,a_4\}}$. According to Corollary 1 every d-split is found in this manner. This algorithm for finding all d-splits improves the $O(n^6)$-algorithm described after Corollary 4 in case that d is totally decomposable. It would be interesting to find out whether there exists an $O(n^5)$-algorithm for computing all d-splits along with their isolation indices in the case of a general metric d.

Consider $a_1, a_2, a_3, a_4 \in X$ such that $\alpha_{\{a_1,a_2\},\{a_3,a_4\}} > 0$ and the sets

$$A := \left\{\, x \in X \;\middle|\; \alpha_{\{a_1,a_2\},\{a_3,a_4,x\}} = 0 \,\right\}$$
$$B := \left\{\, x \in X \;\middle|\; \alpha_{\{a_1,a_2,x\},\{a_3,a_4\}} = 0 \,\right\}$$

Suppose that the following identity holds for all $x \in X,\; x \neq a_1, a_2, a_3, a_4$

$$\alpha_{\{a_1,a_2\},\{a_3,a_4\}} = \alpha_{\{a_1,a_2,x\},\{a_3,a_4\}} + \alpha_{\{a_1,a_2\},\{a_3,a_4,x\}}$$

Then we have $a_1, a_2 \in A$ and $a_3, a_4 \in B$.

Since $\alpha_{\{a_1,a_2\},\{a_3,a_4,x\}} = 0$ and, by extending the (partial) splits, the isolation index cannot increase, then all extensions of $\{\{a_1,a_2\},\{a_3,a_4\}\}$ with at least one element of A in the second part have isolation index equal to 0.

Idem for extensions of $\{\{a_1,a_2\},\{a_3,a_4\}\}$ with at least one element of B in the first part.

So between the extensions of $\{\{a_1, a_2\}, \{a_3, a_4\}\}$, the only possibly non zero isolation index is that of the split $\{A, B\}$ (that is all elements of A in the first part and all elements of B in the second one).

If d is totally decomposable, then the sum of the isolation indexes of the extensions equals the isolation index of the base partial split, and so

$$\alpha_{A,B} = \alpha_{\{a_1,a_2\},\{a_3,a_4\}}$$

This gives an $O(n^5)$ algorithm to check whether a symmetric function d is totally decomposable and to compute d-splits and their isolation indexes:

- check the identity for all quartets a_1, a_2, a_3, a_4
  (only those whose partial split have positive isolation index)
- if the identity holds, then check if $A \cup B = X$
- if this is true, then $\{A, B\}$ is a d-split and its isolation index is
  $$\alpha_{\{a_1,a_2\},\{a_3,a_4\}}$$

Question: Does it exist an $O(n^5)$ algorithm for the general case?

Note that the set of all totally decomposable metrics on a finite set X is a closed subset of $\mathbb{R}^{X\times X}$ and that it contains an open subset of

$$\langle M(X)\rangle = \{d \in \mathbb{R}^{X\times X} \mid d \text{ is symmetric and vanishes on the diagonal}\}.$$

Indeed, if a metric d is the (pointwise) limit of metrics d_i $(i \to \infty)$, then $\alpha^{d_i}_{A,B} \to \alpha^{d}_{A,B}$ for all A, $B \subseteq X$ when $i \to \infty$. Therefore if the metrics d_i satisfy condition (iii) of Theorem 6, then so does d. On the other hand, if $\mathscr{S}$ is a maximal collection of weakly compatible splits as discussed in the preceding section, and if $d := \sum_{S\in\mathscr{S}} \delta_S$, then $\alpha^{d'}_S > 0$ for all $S \in \mathscr{S}$ and all $d' \in \langle M(X)\rangle$ sufficiently close to d. Hence d' must be totally decomposable in view of Corollary 5.

As an illustrative example, consider any finite subspace X of the boundary of a convex polygon (or any compact convex set) in the Euclidean plane. We assert that X is totally decomposable. First assume that X is the set Y of all vertices of this polygon. Obviously, every 4-subset

[...]

Arbitrary finite subspaces of the Euclidean plane, of course, are not totally decomposable in general. For instance, let t, u, v, w be the vertices of any convex quadrangle in the plane such that $tv|uw$. Let x be any interior point of the line segment from w to the crossing point of the two diagonals (see Fig. 13). Then

$$\begin{aligned}
&\alpha_{\{t,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,x\}} - \alpha_{\{t,u\},\{v,w\}} \\
&\quad = \tfrac{1}{2} \cdot \max\{tv + wx - tx - vw,\ tw + vx - tx - vw,\ 0\} \\
&\qquad + \tfrac{1}{2} \cdot (tv + ux - tu - vx) - \tfrac{1}{2} \cdot (tv + uw - tu - vw) \\
&\quad = \tfrac{1}{2} \cdot \max\{tv - tx - vx,\ tw - tx - wx,\ vw - vx - wx\} < 0,
\end{aligned}$$

thus violating condition (iv) of Theorem 6.

Examples of totally decomposable metrics are, of course, the tree metrics, as was already mentioned in the introduction. Indeed, the well-known results concerning tree metrics (cf. [9]) can be deduced quite easily from Theorem 6 in the following form:

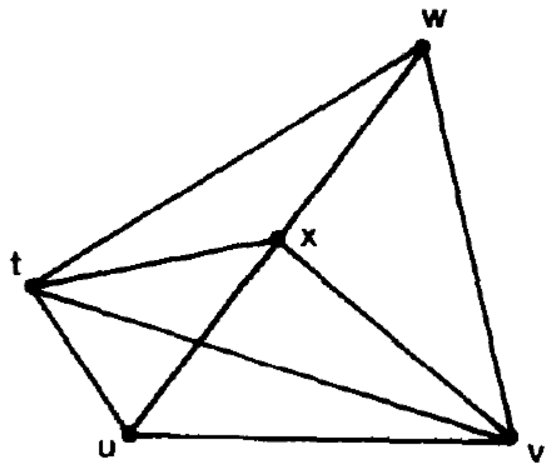


FIG. 13. A 5-subspace of the Euclidean plane which is not totally decomposable.

COROLLARY 7. *For a metric d defined on X, the following two conditions are equivalent*:

(i) *d is totally decomposable and any two d-splits A, B and A', B' are compatible (that is, one of the four intersections $A \cap A'$, $A \cap B'$, $B \cap A'$, and $B \cap B'$ is empty)*;

(ii) *for any four points $t, u, v, w \in X$ the four-point condition*

$$tu + vw \leqslant \max\{tv + uw, tw + uv\}$$

is fulfilled.

Proof. (i) implies (ii). This follows trivially from the fact that condition (i) holds for $d|_{Y \times Y}$ for all $Y \subseteq X$, once it is true for X, so it holds in particular for $\{t, u, v, w\}$. Hence (ii) follows from the standard analysis of 4-point metrics.

(ii) implies (i). At first we show that d is totally decomposable. Indeed, if $t, u, v, w, x \in X$ and if $\alpha_{\{t,u\},\{v,w\}} > 0$ then $tu + vw < tw + vu = tv + wu$ and therefore

$$\begin{aligned}\alpha_{\{t,u\},\{v,w\}} &= \tfrac{1}{2} \cdot (tw + uv - tu - vw) \\ &= \tfrac{1}{2} \cdot (tw + xv - tx - vw) + \tfrac{1}{2} \cdot (tx + uv - tu - vx) \\ &\leqslant \alpha_{\{t,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,x\}}.\end{aligned}$$

In addition, if there would be two incompatible d-splits A, B and A', B', so that for, say, $t, u, v, w \in X$ one has $t, u \in A$, $v, w \in B$, $t, v \in A'$, and $u, w \in B'$, then one verifies easily by restricting d to $\{t, u, v, w\}$ that $tw + uv$ exceeds $tu + vw$ as well as $tv + uw$, contradicting condition (ii). ∎

Def. (compatible splits)

Given two splits $\{A, B\}$ and $\{A', B'\}$ we say that they are **compatible** if one of the following four intersections is empty

$$A \cap A', \qquad A \cap B', \qquad B \cap A', \qquad B \cap B'$$

We say that a set of splits is **compatible** if its splits are (pairwise) compatible.

Oss. Subsets of compatible sets are compatible.

Oss. A compatible set is weakly compatible.

In fact, if we call $\mathcal{S}_0, \mathcal{S}_1, \mathcal{S}_2$ the sets of splits extending the three respective quartets,
then weak compatibility is equivalent to saying that
at most two of them are non-empty,
while compatibility is equivalent to saying that
at most one of them is non-empty
(the splits from two different sets are not compatible).

Def. (four-point condition)

We say that (X, d) (or just d) satisfies the **four-point condition** if for any four points $t, u, v, w \in X$ it holds

$$tu + vw \leq \max\{tv + uw, tw + uv\}$$

or equivalently

$$tu + vw \leq tv + uw = tw + uv$$

Dim. $(\Leftarrow)$ It is clear.

$(\Rightarrow)$ Applying the first formula

$$tv + uw \leq \max\{tu + vw, tw + uv\} = tw + uv$$

$$tw + uv \leq \max\{tv + uw, tu + vw\} = tv + uw$$

Oss. If X satisfies the four-point condition and $t, u, v, w \in X$ are such that $\alpha_{\{t,u\},\{v,w\}} > 0$, then

$$tu + vw < tv + uw = tw + uv$$

In fact, $tu + vw$ cannot be the maximum among the three (otherwise the isolation index would be zero).

Prop. If d is a totally decomposable pseudo-metric, then

$$\mathcal{S}_d(Y) = \mathcal{S}_d(X)|_Y , \qquad \forall\, Y \subseteq X$$

Dim. Let $Y \subseteq X$. Clearly a d-split of X is also a d-split of Y, because by extending the isolation index does not increase (and so by restricting it does not decrease). So $\mathcal{S}_d(Y) \supseteq \mathcal{S}_d(X)|_Y$.

From **Teo**. 6, the isolation index of a d-split of Y coincides with the sum of the indices of its extensions.
In particular, there must be an extension that is also a d-split of X. Thus $\mathcal{S}_d(Y) \subseteq \mathcal{S}_d(X)|_Y$.

Cor. 7 Let d be a pseudo-metric on X.

Then d is totally decomposable and any two d-splits are compatible if and only if d satisfies the four-point condition.

Dim. $(\Rightarrow)$ Let $t, u, v, w \in X$. Since compatibility is preserved by restriction, from the previous **Prop**. we get that $\mathcal{S}_d(Y)$ is compatible for all subsets Y of X.
In particular $\mathcal{S}_d(\{t, u, v, w\})$ is compatible.

By compatibility, at least two quartets cannot be d-splits – suppose WLOG $\big\{\{t, v\}, \{u, w\}\big\}$ and $\big\{\{t, w\}, \{u, v\}\big\}$.

If $\alpha_{\{t,u\},\{v,w\}} = 0$, then

$$tu + vw = tv + uw = tw + uv$$

If $\alpha_{\{t,u\},\{v,w\}} > 0$, then

$$tu + vw < tv + uw = tw + uv$$

In both cases the four-point condition is satisfied.

(⇐) Let $t, u, v, w \in X$. If $\alpha_{\{t,u\},\{v,w\}} > 0$, then for every $x \in X$

$$
\begin{aligned}
\alpha_{\{t,u\},\{v,w\}} &= \frac{1}{2}(tw + uv - tu - vw) \\
&= \frac{1}{2}(tw + xv - tx - vw) + \frac{1}{2}(tx + uv - tu - vx) \\
&\leq \alpha_{\{t,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,x\}}
\end{aligned}
$$

where we used the previous **Oss**. in the first line.

By **Teo**. 6 this proves that d is totally decomposable.

Suppose to have two incompatible d-splits $\{A, B\}$ and $\{A', B'\}$. Then we can suppose that exist $t, u, v, w \in X$ such that

$$
t, u \in A\,, \qquad v, w \in B\,, \qquad t, v \in A', \qquad u, w \in B'
$$

Since d is totally decomposable, its restriction to $\{t, u, v, w\}$ is a linear combination of split metrics that splits 2-2 (that is they extend one of the quartets) and 3-1.
But the latter contribute equally to the three distances.
Since the set of d-splits is weakly compatible and

$$
\{A, B\} \succcurlyeq \big\{\{t, u\}, \{v, w\}\big\}\,, \qquad \{A', B'\} \succcurlyeq \big\{\{t, v\}, \{u, w\}\big\}
$$

then $\big\{\{t, w\}, \{u, v\}\big\}$ does not have any d-split extension.

So the only different contributions come from split metrics that splits like $\delta_{A,B}$ and $\delta_{A',B'}$. As a consequence we have

$$
tw + uv > \begin{matrix} tv + uw \\ tu + vw \end{matrix}
$$

violating the four-point condition. ↯

Oss. Tree metrics are totally decomposable pseudo-metrics (since they satisfy the four-point condition).

Further examples of totally decomposable metrics that are not simply tree metrics are provided by the sums of two tree metrics. In this case the system of d-splits is obtained as the union of the respective systems of splits of the summands. So, as a corollary to Theorem 3 we record here the following

COROLLARY 8. *The sum $d = d_1 + d_2$ of two tree metrics on a set X is totally decomposable. A split of X is a d-split if and only if it is a d_1- or d_2-split.*

It follows that we can decide whether or not a metric d on an n-set X is a sum of two tree metrics in at most $O(n^5)$ simple computational steps: in that many steps we can decide whether or not d is totally decomposable, as well as produce its decomposition in case d is such. Since two systems of pairwise compatible splits encompass together at most $3n-6$ different splits, d cannot be a sum of two tree metrics when the number of d-splits exceeds this bound. Then it remains to check whether the *incompatibility graph* of the d-splits is bipartite; in this graph the vertices are the d-splits, and two vertices are adjacent if and only if the respective d-splits are incompatible. The feasible decompositions correspond to the 2-colourings of this graph, however modified in the following way: each isolated vertex may simultaneously receive both colours.

We conclude this section with a brief look at operations which preserve total decomposability. The first operation that comes to mind is the Cartesian product, for which the distance between two points is the sum of the coordinate distances. This operation, however, preserves total decomposability only in a fairly special case. Namely we have the following result, which is an easy consequence of Corollary 8 and Theorem 6.

COROLLARY 9. *Let d_i be a nonzero metric on a set X_i (having therefore at least two points), for $i = 1, 2$. Then the metric $d = d_1 \times d_2$ of the Cartesian product of the two spaces is totally decomposable if and only if both d_1 and d_2 are tree metrics.*

A (weighted) tree is built up by successively glueing together subtrees along single points. There is a more general operation available which preserves total decomposability. First some necessary terminology: a subspace Y of a metric space X is *gated* if for every point $x \in X$ there exists a (up to distance zero unique) point $x' \in X$ (the *gate* for x in Y) such that $xy = xx' + x'y$ for all $y \in Y$; if $x \in Y$, then trivially $x' = x$. See [13] for further information on gated subspaces. A gated subspace Y is *convex* in the following sense: for all $w, y \in Y$ and $x \in X$ such that x is between w and y, that is, $d(w, x) + d(x, y) = d(w, y)$, it follows that x belongs to Y. The same holds, for example, for the two sides A and B of any d-split A, B because otherwise, if $x \in B$ were between $t, u \in A$, then $\{t, u\}$, $\{x\}$ could not be a partial d-split.

PROPOSITION 2. *Let Y, Z be gated, totally decomposable subspaces of a metric space X such that $X = Y \cup Z$ and $Y \cap Z \neq \emptyset$. Then X is totally decomposable.*

LEMMA 2. *If $\mathcal{S}$ is a system of weakly compatible splits of X and if $f\colon X' \to X$ is a map, then the system $\mathcal{S}'$ of splits $f^{-1}(A), f^{-1}(B)$, where A, B runs through all splits in $\mathcal{S}$, is weakly compatible, too.*

Still another simple consequence of Theorem 6, phrased in the terminology of abstract convexity, is worth mentioning. Recall that a subset A of a metric space X is called d-convex if every point x of X satisfying $ax + a'x = aa'$ for some $a, a' \in A$ belongs to A (cf. [24]). The *d-convexity* of the space is the collection of all d-convex sets. The *d-convex hull* of a subset Y of X is the smallest d-convex set containing Y. A *d-convex split* A, B consists of complementary d-convex sets A and B. We have already observed that every d-split is a d-convex split. As one would expect the converse is not true in general (see Fig. 14 below). The d-convexity is said to be *regular* if for every d-convex set C and $x \notin C$ there exists a d-convex split A, B with $C \subseteq A$ and $x \in B$. The *Carathéodory number* is the least number k such that the d-convex hull of every subset Y of X with $\# Y > k$ is the union of the d-convex hulls of the k-subsets of Y (cf. [19]).

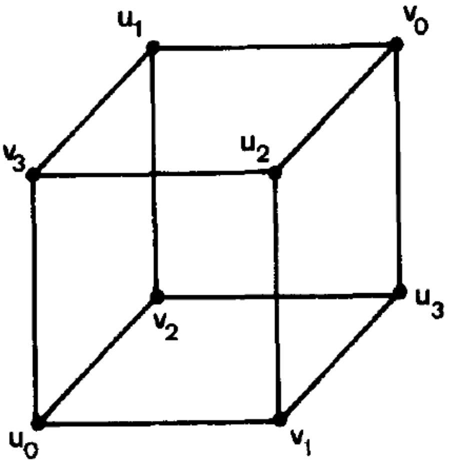


FIG. 14. A split-prime Hamming metric.

PROPOSITION 3. *The d-convexity of a totally decomposable metric space has Carathéodory number at most 2 and is regular.*

In some instances the preceding fact can be used to verify that a given metric space is not totally decomposable. For example, the d-convexity of the graph $K_{2,3}$ (see Fig. 4) has Carathéodory number 2 but is not regular. On the other hand, the cube graph (see Fig. 14) has a regular d-convexity, but its Carathéodory number equals 3. Actually, the metric d of this graph is split-prime since there are evidently no more than three d-convex splits (corresponding to the pairs of opposite "faces"), each of which fails to be a d-split because each d-convex set with d-convex complement contains exactly two of the four vertices u_0, u_1, u_2, u_3 (mutually at distance 2) in Fig. 14.

The latter example indicates that the class of (graph) metrics belonging to the Hamming cone (cf. [2, 4, 5]) is considerably larger than the class of (graph) metrics that are totally decomposable. It also shows that the condition $Y \cap Z \neq \emptyset$ cannot be dropped from the above Proposition 2. Indeed, the split-prime cube is the (disjoint) union of its two gated subspaces $Y = \{u_0, u_1, v_2, v_3\}$ and $Z = \{v_0, v_1, u_2, u_3\}$, both of which are totally decomposable.

CHAPTER 5: COHERENT DECOMPOSITION

5. Coherent Decomposition

The decomposition of metrics via splits can be identified as a particular instance of a more general additive decomposition scheme that respects the combinatorial structure of the metrics in question. Isbell [18] already observed that the injective hull $T(X, d)$ of a finite metric space (X, d) (in the category of metric spaces and nonexpansive mappings) has a certain polytopal structure. If d is a tree metric, then the space $T(X, d)$ is nothing but the tree representing d. More generally, optimal graphical representations of metric spaces (as considered by Imrich and Stotskii [17] and others) are closely related to the corresponding injective hull (see [11]). The case of trees suggests that certain additive decompositions of d correspond to decompositions of the polytopal structure of the given metric.

To be more specific, let us recall that the injective hull of a metric space (X, d) can be regarded as the set

$$T(X, d) := \{f \in \mathbb{R}^X \mid f(x) = \sup_{y \in X}(d(x, y) - f(y)) \text{ for all } x \in X\}$$

endowed with the L_∞-metric

$$\|f, g\| := \sup_{x \in X} |f(x) - g(x)| \qquad (f, g \in T(X, d)).$$

The canonical embedding $x \mapsto f_x$ $(x \in X)$ of (X, d) into $T(X, d)$ is defined by

$$f_x(y) := d(x, y) \qquad \text{for} \quad y \in X.$$

In what follows the set X is fixed, and so we briefly write $T(d)$ instead of $T(X, d)$. The set $T(d)$ is included in the closed convex subset

$$P(d) := \{f \in \mathbb{R}^X \mid f(x) + f(y) \geqslant d(x, y) \text{ for all } x, y \in X\}$$

of the linear space $\mathbb{R}^X$. Namely, $T(d)$ consists of the minimal members of $P(d)$ with respect to the pointwise (partial) ordering (where $f \leqslant g$ if and only if $f(x) \leqslant g(x)$ for all $x \in X$). To give an example, let $S = \{A, B\}$ be a split of X; then $P(\delta_S)$ is the collection of all mappings $f: X \to \mathbb{R}_0^+$ satisfying $f(a) + f(b) \geqslant 1$ for all $a \in A$ and $b \in B$, while $T(\delta_S)$ is an isomorphic copy of the closed interval $[0, 1]$.

Next we study how $P(d_1 + d_2)$ compares with $P(d_1) + P(d_2)$ for metrics d_1, d_2 on X. Here a linear combination $\lambda \cdot Q + \mu \cdot R$ of two sets Q, R of real-valued mappings reads as $\{\lambda \cdot f + \mu \cdot g \mid f \in Q,\ g \in R\}$. It is clear that

$$P(d_1) + P(d_2) \subseteq P(d_1 + d_2)$$

is always true. Further, equality holds if and only if the minimal members of $P(d_1 + d_2)$ decompose, that is, $T(d_1 + d_2) \subseteq T(d_1) + T(d_2)$, in which case we call d_1 and d_2 *coherent* metrics (on X). More generally, we define k metrics $d_1, \ldots, d_k$ to be *coherent* if $P(d_1 + \cdots + d_k) = P(d_1) + \cdots + P(d_k)$, and we also say that in this case the metrics $d_1, \ldots, d_k$ constitute a *coherent decomposition* of $d := d_1 + \cdots + d_k$. Our next result relates this concept with d-splits.

THEOREM 7. *Let $d = d_1 + \lambda \cdot \delta_S$ be a decomposition of a metric d on X such that $\lambda > 0$ and S is a split of X. Then*

$$P(d) = P(d_1) + \lambda \cdot P(\delta_S)$$

if and only if S is a d-split and one has $\lambda \leqslant \alpha_S$.

THEOREM 8. *Let d be a metric on X. Assume that*

$$d = d_0 + \sum_{S \in \mathcal{S}} \lambda_S \cdot \delta_S$$

is a decomposition of d such that d_0 is a split-prime metric, $\mathcal{S}$ is a collection of splits, and $\lambda_S > 0$ for all members S of $\mathcal{S}$. Then this constitutes a coherent decomposition of d, that is,

$$P(d) = P(d_0) + \sum_{S \in \mathcal{S}} \lambda_S \cdot P(\delta_S)$$

holds, if and only if $\mathcal{S}$ is the system of all d-splits and each λ_S equals the isolation index α_S.

From Theorems 3 and 8 we obtain yet another description of weak compatibility:

COROLLARY 10. *Let $\mathcal{S}$ be a collection of splits of X. Then $\mathcal{S}$ is weakly compatible if and only if $d = \sum_{S \in \mathcal{S}} \delta_S$ constitutes a coherent decomposition of d.*

Does the concept of coherent decomposition actually go beyond the decomposition scheme via d-splits? A simple example affirming this is the following. Consider the metric subspace (X, d) consisting of the vertices a_i and b_i ($i = 0, 1, 2, 3$) of the left-hand graph in Fig. 15.

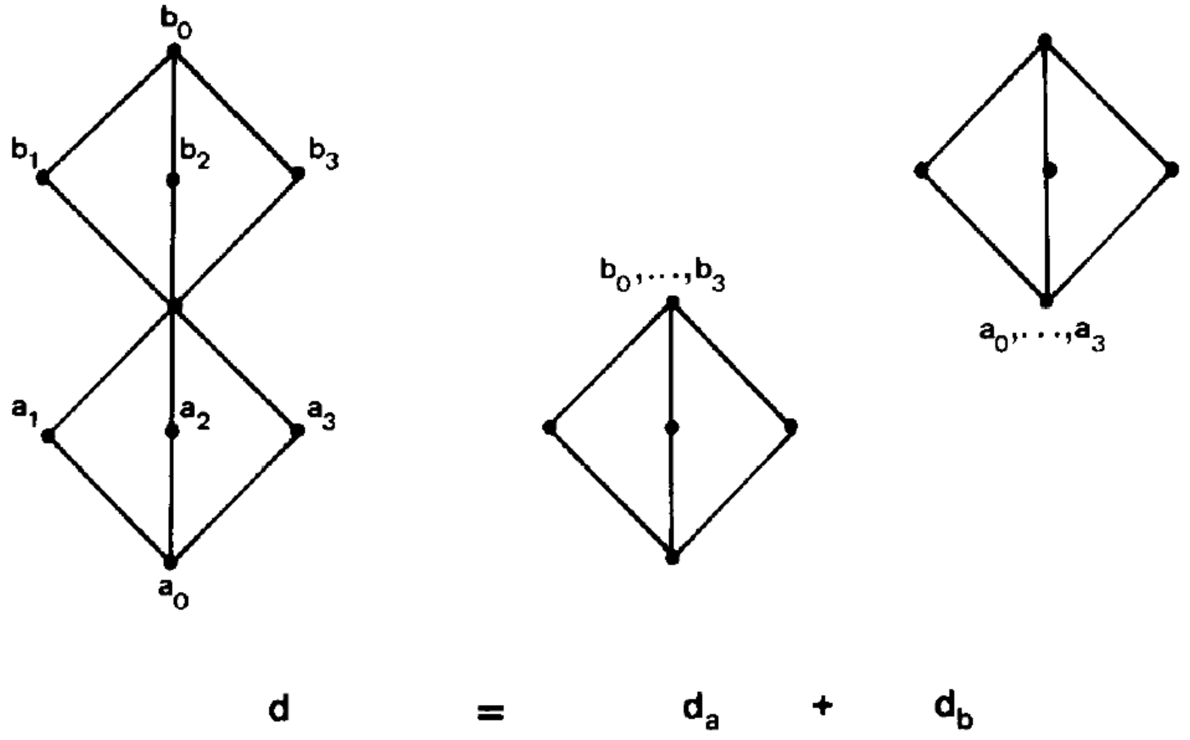


FIG. 15. A coherent decomposition of a split-prime metric.

It is readily seen that d is split-prime, yet a coherent decomposition of d into two metrics d_a and d_b is suggested in Fig. 15. To check this, first note that for $i = 0, 1, 2, 3$, one has

$$d_a(a_i, b_0) = a_i b_0 - 2,$$

$$d_a(a_i, b_j) = a_i b_j - 1 \qquad \text{for} \quad j = 1, 2, 3,$$

$$d_b(a_0, b_i) = a_0 b_i - 2,$$

$$d_b(a_j, b_i) = a_j b_i - 1 \qquad \text{for} \quad j = 1, 2, 3.$$

Now let $f \in P(d)$. Then either

$$f(a_0) \geqslant 2 \text{ and } f(a_j) \geqslant 1 \qquad \text{for} \quad j = 1, 2, 3$$

or

$$f(b_0) \geqslant 2 \text{ and } f(b_j) \geqslant 1 \qquad \text{for} \quad j = 1, 2\ 3.$$

Assume the latter, say. Define mappings f_a and f_b by

$$\begin{aligned}
f_a(a_i) &:= f(a_i) && \text{for} \quad i = 0, 1, 2, 3, \\
f_a(b_0) &:= f(b_0) - 2, && \\
f_a(b_j) &:= f(b_j) - 1 && \text{for} \quad j = 1, 2, 3, \\
f_b(a_i) &:= 0 && \text{for} \quad i = 0, 1, 2, 3, \\
f_b(b_0) &:= 2, && \\
f_b(b_j) &:= 1 && \text{for} \quad j = 1, 2, 3.
\end{aligned}$$

Then $f = f_a + f_b$ with $f_a \in P(d_a)$ and $f_b \in P(d_b)$. We conclude that $d = d_a + d_b$ is in fact a coherent decomposition.

In the preceding example, the metric induced by the graph $K_{2,3}$ (see Fig. 4) constitutes a component of the metric displayed in Fig. 15. More generally, we say that a nonzero metric d_1 on X is a *coherent component* of a metric d on X if there exists a coherent decomposition of the form $d = \lambda \cdot d_1 + d_2$ for some $\lambda > 0$ and a metric d_2. Trivially, every multiple of d

is a coherent component of d. If there are no other coherent components, then d is said to be *coherently prime* or briefly *prime*. Note that every prime metric is split-prime (but not conversely). The smallest example of a prime metric is provided by the $K_{2,3}$-metric. In fact, this metric generates an extremal cone of $M(X)$ (see [3] or [21]): the argument rests on the following lemma, involving the following two notions. Let us say that two pairs $\{x, u\}$ and $\{v, y\}$ are *perspective* in the metric space (X, d) if x, u, v, y form a rectangle, that is if $\{x, u\}$, $\{v, y\}$ is a d'-split of the metric space $(X' := \{x, u, v, y\},\ d' := d|_{X' \times X'})$ and no trivial d'-splits of the form $\{z\}$, $X' - \{z\}$ $(z \in X')$ exist, or equivalently, if either the d'-convex hulls of $\{x, y\}$ and of $\{u, v\}$ both coincide with X' or the same holds for $\{x, v\}$ and $\{u, y\}$. The transitive closure of the perspectivity relation on the set of all pairs with nonzero distance is dubbed *projectivity*. A pair $\{x, u\}$ with $d(x, u) > 0$ is called an *edge* in the space (X, d) if there is no point properly between x and u, that is, $d(x, z) + d(z, u) = d(x, u)$ implies $z \in \{x, u\}$. Then Theorem 2.4 and Lemma 2.2 of [3] can be restated (in a more general form) as follows.

LEMMA 3. *Let $d = d_1 + d_2$ be any decomposition of a metric d on X. Then every d_1- (or d_2-) convex set is d-convex and, hence, the d_1- (or d_2-) convex hull of a subset of X contains its d-convex hull. In particular, if $\{x, u\}$ and $\{v, y\}$ are projective with respect to d, then $d_i(x, u) = d_i(v, y)$ for $i = 1, 2$. Further, if*

$$d_1(x, u)/d(x, u) = d_1(u, y)/d(u, y)$$

for all incident edges $\{x, u\}$, $\{u, y\}$ of the space (X, d), then d_1 and d_2 are multiples of d.

We have already seen at the end of Section 4 that the metric of the cube graph is split-prime although it is not extremal. As one would now expect this metric is even prime. This is caused by the "cubic" product structure: the cube graph is the Cartesian product of three copies of the graph K_2. The argument immediately carries over to arbitrary Cartesian graph products with at least three factors:

PROPOSITION 4. *The Cartesian product G of any three nontrivial, connected graphs (or, more generally, any graph G which for every pair of incident edges $\{t, u\}$, $\{u, v\}$ contains either an isometric subgraph isomorphic to the cube and including t, u, and v, or one additional edge $\{u, w\}$ and two isometric subgraphs isomorphic to the cube, one containing t, u, w, and the other one containing v, u, w) yields a prime metric.*

A slight modification of the above argument shows that the graph obtained from the cube by deleting one vertex also yields a prime metric.

The relaxed condition in Proposition 4 applies to graphs which are not necessarily factorizable but still have a local cube structure. Such graphs do exist: consider, for instance, the extended odd graphs E_k ($k \geqslant 3$) constructed in [22].

The above observations confirm that prime metrics exist in abundance. It is more interesting, however, to find all prime coherent components of a given metric d and thus to determine the set $M(d)$ of all coherent components of d. Which split metrics belong to $M(d)$ is clear by what has been shown: Theorem 7 says that these split metrics are precisely the ones associated with the d-splits. Consequently, a totally decomposable metric d' is a coherent component of d if and only if every d'-split is a d-split. In this case $M(d')$ consists of totally decomposable metrics, viz., the non-negative linear combinations of the split metrics δ_S associated with the d'-splits S. Hence, as these split metrics are linearly independent (by Corollary 4), $M(d')$ is a simplicial closed convex subcone of $M(X)$. It is therefore not really surprising that, in general, $M(d)$ turns out to be a closed convex subcone of $M(X)$, which consists of those metrics d' satisfying the following requirement: for each $f \in P(d)$ there exists some $f' \in P(d')$ such that $K(f) \subseteq K(f')$. Then, if $d' \in M(d)$, the convex cone $M(d')$ is the smallest subcone of $M(d)$ in the lattice of "boundary cones" of $M(d)$ that contains d'. Thus, the family $(M(d) \mid d \in M(X))$ constitutes an interesting stratification of $M(X)$ by closed convex cones. We conjecture that all these subcones $M(d)$ ($d \in M(X)$) are simplicial, that is, their extremals are linearly independent:

Conjecture. There exists a unique coherent decomposition $d = d_1 + \cdots + d_k$ of d into linearly independent metrics $d_1, ..., d_k \in M(d)$ such that

$$M(d) = \left\{ \sum_{i=1}^{k} \lambda_i \cdot d_i \mid \lambda_i \geqslant 0 \text{ for } i = 1, ..., k \right\}.$$

Actually, it was this conjecture, originally suggested by the analysis of 5-point metrics as performed in [11], which prompted us to investigate the relationship between a metric d and the split metrics δ_S in $M(d)$. We view the results presented here as substantial evidence for our conjecture.

CHAPTER 6: SPLITS VERSUS CLUSTERS

6. SPLITS VERSUS CLUSTERS

In a previous paper (see [8]) we developed a decomposition theory for similarity functions, which parallels the split-decomposition of metrics in a way. While the latter makes use of splits and split metrics, the key ingredients of the former are systems of clusters (i.e., subsets) and elementary similarity functions (i.e., binary characteristic functions of clusters). Alluding to the scenario of [25], one can interpret splits as *distinctive features* and clusters as *common features*.

A brief description of the additive decomposition theory for similarity functions will be given next. In what follows X is a finite set. Given a system $\mathscr{H}$ of nonempty subsets of X, the *proper-intersection graph* of $\mathscr{H}$ has the members of $\mathscr{H}$ as its vertices, where two vertices are adjacent if and only if the respective members of $\mathscr{H}$ intersect properly (that is, their intersection is nonempty and neither set is contained in the other). $\mathscr{H}$ is a *hierarchy* over X if its proper-intersection graph is without edges, that is, for all C_1, $C_2 \in \mathscr{H}$, either $C_1 \cap C_2 = \varnothing$, or $C_1 \subseteq C_2$ or $C_2 \subseteq C_1$. More generally, a *weak hierarchy* is a system $\mathscr{H}$ such that there are no three elements $x_1, x_2, x_3 \in X$ and three sets C_1, C_2, $C_3 \in \mathscr{H}$ satisfying $x_i \in C_j$ if and only if $i \neq j$. In the hypergraph terminology weak hierarchies are precisely the "hypergraphs without triangles" (cf. [1]). We assume here that the empty set is not a member of (weak) hierarchies. For every nonempty subset C of X define a similarity function σ_C by

$$\sigma_C(u, v) := \begin{cases} 1 & \text{if} \quad u, v \in C, \\ 0 & \text{otherwise} \end{cases} \qquad (u, v \in X).$$

A similarity function s is said to be *additive* if it is of the form

$$s = \sum_{C \in \mathscr{H}} \alpha_C \cdot \sigma_C$$

for some weak hierarchy $\mathscr{H}$ and positive weights α_C $(C \in \mathscr{H})$, and it is said to be *strictly additive* if $\mathscr{H}$ can be chosen to be a proper hierarchy. The members of $\mathscr{H}$ (along with their weights α_C) can be reconstructed from the function s (in a recursive manner): the intersections of members of $\mathscr{H}$ are recovered as the *s-clusters*, that is, subsets C with

$$m_s(u, v \mid x) := s(u, v) - \min\{s(u, x), s(v, x), s(u, v)\} > 0$$

for all $u, v \in C$ and $x \notin C$. The *isolation index* of a cluster C is defined as

$$\imath(C) := \min_{\substack{a, b \in C \\ x \in X - C}} \{m_s(a, b \mid x)\}.$$

Note that this terminology slightly deviates from the one in [8].

One way to code a system $\mathscr{S}$ of splits of X is to select a point $w \in X$ and record the system $\mathscr{H}^{(w)}$ of the parts C for which $\{C, X - C\} \in \mathscr{S}$ and $w \notin C$. It is this transformation which sets up the analogy between systems of splits and systems of clusters.

LEMMA 4. *Let $\mathscr{S}$ be a system of splits of X, and let $\mathscr{H}^{(w)} = \mathscr{H}^{(w, \mathscr{S})} := \{C \mid \{C, X - C\} \in \mathscr{S}$ and $w \notin C\}$ denote the associated system of clusters with respect to a point $w \in X$. Then the incompatibility graph of $\mathscr{S}$ coincides with the proper-intersection graph of $\mathscr{H}^{(w)}$. In particular, $\mathscr{S}$ is the union of k systems of pairwise compatible splits if and only if $\mathscr{H}^{(w)}$ is the union of k hierarchies.*

LEMMA 5. *The following statements are equivalent for a system $\mathscr{S}$ of splits of X and its family of cluster systems $\mathscr{H}^{(w)}$ $(w \in X)$:*

(i) *$\mathscr{S}$ consists of triplewise weakly compatible splits;*

(ii) *$\mathscr{H}^{(w)}$ is a weak hierarchy with respect to all $w \in X$;*

(iii) *for at least one $w \in X$, the system $\mathscr{H}^{(w)}$ is a weak hierarchy such that there are no points $u_1, u_2, u_3 \in X$ and clusters $C_1, C_2, C_3 \in \mathscr{H}^{(w)}$ with nonempty intersection which satisfy $u_i \in C_j$ if and only if $i = j$.*

Proposition 5. *Let $\mathscr{S}$ be a collection of splits of X. Then the incompatibility graph of $\mathscr{S}$ is bipartite if and only if $\mathscr{S}$ is weakly compatible and satisfies the following two conditions:*

(1) there is no subset $Y = \{y_0, y_1, \ldots, y_5\}$ of X such that each $\{y_i, y_{i+1}, y_{i+2}\}$, $\{y_{i+3}, y_{i+4}, y_{i+5}\}$ (indices modulo 6) belongs to the trace of $\mathscr{S}$ on Y,

(2) there is no subset $Z = \{z_0, z_1, \ldots, z_{k-1}\}$ of X such that $k \geqslant 5$ is odd and each $\{z_i, z_{i+1}\}$, $Z - \{z_i, z_{i+1}\}$ (indices modulo k) belongs to the trace of $\mathscr{S}$ on Z.

Combining this proposition with Corollary 8 we arrive at another characterization of the sum of two tree metrics:

Corollary 11. *A metric d on X is the sum of two tree metrics on X if and only if d is totally decomposable and satisfies the following two conditions:*

(1) there is no subset $Y = \{y_0, y_1, \ldots, y_5\}$ of X such that each $\{y_i, y_{i+1}, y_{i+2}\}$, $\{y_{i+3}, y_{i+4}, y_{i+5}\}$ (indices modulo 6) is a partial d-split,

(2) there is no subset $Z = \{z_0, z_1, \ldots, z_{k-1}\}$ of X such that $k \geqslant 5$ is odd and each $\{z_i, z_{i+1}\}$, $X - \{z_i, z_{i+1}\}$ (indices modulo k) is a partial d-split.

So far, we have associated a family of cluster systems $\mathscr{H}^{(w)}$ ($w \in X$) to a system of splits of X. In an analogous fashion, every metric d on X is accompanied by a family of similarity functions $s^{(w)}$ ($w \in X$). To begin with, assume $C \subseteq X$ and $w \in X - C$. Then the companion of the split metric $\delta_{C,X-C}$ with respect to w is the elementary similarity function $\sigma_C^{(w)} = \sigma_C|_{(X-\{w\})^2}$, namely:

$$\sigma_C^{(w)}(u, v) = \tfrac{1}{2} \cdot (\delta_{C,X-C}(u, w) + \delta_{C,X-C}(v, w) - \delta_{C,X-C}(u, v)) \quad \text{for} \quad u, v \in X - \{w\}.$$

More generally, given a metric d on X, the *Farris transform* of d (to a similarity function) with respect to a given point $w \in X$ is defined by

$$s^{(w)}(u, v) = s^{(w,d)}(u, v) := \tfrac{1}{2} \cdot (d(u, w) + d(v, w) - d(u, v)) \quad \text{for} \quad u, v \in X - \{w\}.$$

Tree metrics are linked with strictly additive similarity functions and hence with ultramerics via this transformation, viz.: d is a tree metric if and only if $s^{(w)}$ is strictly additive, or equivalently, if and only if the dissimilarity function

$$d^{(w)}(u, v) = \begin{cases} 0 & \text{if} \quad u = v, \\ c - s^{(w)}(u, v) & \text{otherwise,} \end{cases}$$

where $c \geqslant s^{(w)}(u, v)$ for all $u, v \in X - \{w\}$, is an ultrametric on $X - \{w\}$ for some (and hence for all) $w \in X$ (see [6]). Further relationships between a metric d and its Farris transforms $s^{(w)}$ are established next. We briefly write $m^{(w)}$ instead of $m_{s^{(w,d)}}$.

LEMMA 6. *Given a symmetric function $d: X \times X \to \mathbb{R}$,*

$$\beta_{\{a,a'\},\{b,w\}} = m^{(w)}(a, a' \mid b)$$

for every $w \in X$ and all $a, a', b \in X - \{w\}$. Hence, if d is a metric on X and A, B is a split of X with $w \in B \neq \{w\}$, then A is an $s^{(w)}$-cluster if and only if

$A, \{w, b\}$ is a partial d-split for all $b \in B - \{w\}$, and A, B is a d-split if and only if A is an $s^{(w)}$-cluster for all $w \in B$. In the latter case the isolation index $\alpha^d_{A,B}$ of the split A, B relative to d coincides with the smallest isolation index of the cluster A with respect to the functions $s^{(w)}$ $(w \in B)$.

In order to establish the link between totally decomposable metrics and additive similarity functions, recall from [8] that a similarity function s is said to be *almost additive* if

$$m_s(t, u \mid u) = 0 \qquad \text{and} \qquad m_s(t, u \mid x) \leqslant m_s(t, u \mid y) + m_s(t, u \mid z) + m_s(y, z \mid x)$$

for all $t, u, x, y, z \in X$.

PROPOSITION 6. *The following conditions are equivalent for a metric d on X and its family of Farris transforms $s^{(w)}$ $(w \in X)$:*

(i) *d is totally decomposable;*

(ii) *$s^{(w)}$ is additive for all $w \in X$;*

(iii) *$s^{(w)}$ is almost additive for all $w \in X$;*

(iv) *for all $t, u, v, w, x \in X$,*

$$m^{(w)}(t,u \mid v) \leqslant m^{(w)}(t, u \mid x) + m^{(w)}(t, x \mid v).$$

COROLLARY 12. *A metric d on X is the sum of two tree metrics if and only if each Farris transform $s^{(w)}$ $(w \in X)$ is a sum of two strictly additive similarity functions. More generally, d is a sum of k coherent tree metrics $d_1, ..., d_k$ if and only if $s^{(w)}$ $(w \in X)$ is a sum of k "coherent" strictly additive similarity functions $s_1, ..., s_k$ (that is, strictly additive similarity functions such that every cluster of $s := s_1 + \cdots + s_k$ is a cluster of some of the s_i $(i = 1, ..., k)$).*

Observe that a metric d need not be totally decomposable when there exists just one point $w \in X$ such that $s^{(w)}$ is additive. For instance, the $K_{2,3}$ metric d has two additive Farris transforms and three nonadditive Farris transforms.

The preceding observations emphasize that much of the information on a metric d is preserved when shifting to the family $s^{(w)}$ $(w \in X)$ of Farris transforms and analyzing them within the additive clustering model. Quite another approach is, of course, taken when one computes the clusters of the similarity function $s = \text{const} - d$ directly corresponding to d. Whether the decomposition based on d-splits or the one based on s-clusters is more appropriate to study the structure inherent in a given data set depends on the nature of the data and the potential interpretation. Note that the d-splits remain unchanged when d undergoes a linear transformation $d \mapsto \lambda \cdot d + \mu$ with $\lambda > 0$, while s-clusters are invariant under all strictly monotone transformations of the reals. So, if the measurement of (dis) similarities is subject to systematic error which considerably deviates from linear transforms of the ideal or "true" distances, then the s-cluster model might be preferable. In any case one should routinely compute both, the d-splits as well as the s-clusters (for $s = \text{const} - d$).

In many case studies the d-splits tend to be small in number (and thus more informative) compared with the s-clusters. Computer simulations (performed by Rainer Wetzel) confirm that perturbing a tree metric d or an ultrametric const $-s$ decreases the number of d-splits quite drastically, but typically increases the number of s-clusters of size at most 2.

How "successful" a decomposition of a given metric d on X into d-splits is can be measured by the following quantity

$$\sum_{x,\,y \in X} \; \sum_{d\text{-splits } S} \alpha_S^d \cdot \delta_S(x, y) \Big/ \sum_{x,\,y \in X} d(x, y),$$

which we call the *splitting index* of d. That is, if $d = d_0 + d_1$ is the coherent decomposition of d into a split-prime metric d_0 and a totally decomposable metric d_1, then the splitting index equals

$$1 - \left(\sum_{x,\,y \in X} d_0(x, y) \Big/ \sum_{x,\,y \in X} d(x, y) \right).$$

A splitting index close to 1 indicates that the split-prime residue possibly is a negligible error term.

For some data sets taken from biology or psychology the observed splitting indices are fairly large, so that much of the structure inherent to the data is then reflected by the corresponding system of d-splits. Detailed analyses of some instructive cases will be performed in subsequent papers.

split	**cluster**
incompatibility graph	proper-intersection graph
compatible splits	hierarchy
weakly compatible splits	weak hierarchy
metric	similarity function
tree metric	strictly additive similarity function
totally decomposable	additive / almost additive
linear transformations	strictly monotone transformations