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Distances and volumina for graphs

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It has long been realized that connected graphs have some sort of geometric structure, in that there is a natural distance function (or metric), namely, the shortest-path distance function. In fact, there are several other natural yet intrinsic distance functions, including: the resistance distance, correspondent "square-rooted" distance functions, and a so-called "quasi-Euclidean" distance function. Some of these distance functions are introduced here, and some are noted not only to satisfy the usual triangle inequality but also other relations such as the "tetrahedron inequality". Granted some (intrinsic) distance function, there are different consequent graph-invariants. Here attention is directed to a sequence of graph invariants which may be interpreted as: the sum of a power of the distances between pairs of vertices of G, the sum of a power of the "areas" between triples of vertices of G, the sum of a power of the "volumes" between quartets of vertices of G, etc. The Cayley–Menger formula for n-volumes in Euclidean space is taken as the defining relation for so-called "n-volumina" in terms of graph distances, and several theorems are here established for the volumina-sum invariants (when the mentioned power is 2).

1. Introduction

Graphs are well-known [31] to be a natural mathematical correspondent to molecular formulas, so that graphs and functions thereon are of chemical interest. One such function would be a distance function (or metric) on the set of vertices of a graph, especially if the function were intrinsic to the graph rather than dependent on an extrinsic embedding in Euclidean space. The *shortest-path* distance function on a connected graph is intrinsic, the distance between vertices i and j being the minimum number of steps on a path between i and j. Indeed, this distance function has long been studied in the graph theory literature, as indicated by Buckley and Harary's book on graph distances [4]. But, in fact, there are (many) other possible choices for an intrinsic distance function – perhaps most simply by weighting the graph edges (and consequent paths), and this decoration has been considered often. But we have in mind more fundamental alternatives such as the *resistance* distance [18] (for which the distance between vertices i and j may be viewed as just the effective electrical resistance between i and j when unit resistors are placed on every edge of the graph). In contrast to the shortest-path distance, this resistance distance has a notable oft-plausible feature: if vertices i and j are connected by two (or more) paths, then they are closer than if connected by only the shorter of these two paths. And often one may view different parts of a molecule to communicate more readily the more pathways

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which interconnect the two parts, so that a chemical distance might plausibly lessen without any change in the Euclidean or shortest-path distances. Perhaps the shortest-path distance is more appropriate when dealing with localized particulate motion in the network, whereas the resistance distance is more appropriate when dealing with delocalized wave-like motion in the network. This resistance distance and other novel intrinsic distances on graphs are discussed briefly in section 2. There also are noted some sequences of conditions which (when satisfied by a distance function) implicate an ever closer mimicking of the standard Euclidean circumstance. Then, e.g., natural more faithful mimics are obtained as "square-roots" of other distance functions.

But granted some distance function d on a connected graph G there arise questions as to what to do with d, and perhaps most suggestively what they might reveal about a "geometry" of graphs. Such questions include:

- What are relevant consequent graph-geometric invariants to be defined in terms of the distance function d?
- How do such invariants compare to corresponding quantities computed using Euclidean distances for relevant embeddings in Euclidean space?
- Do such comparisons when favorable (at least for suitable d) indicate a special chemical feasibility or stability?
- Could any of these distance functions lead to some sort of intrinsic "geometry of graphs"?

As a first step toward addressing such questions attention is here directed to seemingly natural double sequences of geometrically motivated graph invariants, which consist of sums of powers of distances between pairs of vertices of G, sums of powers of "areas" between triples of vertices of G, sums of powers of "volumes" between quartets of vertices, etc. Of course, to do this we need to make some sort of sense of the n-dimensional "volumina": areas (for $n = 2$), volumes (for $n = 3$), etc.

The recollection of results for a standard n-dimensional Euclidean space is of use. The standard volume function for an n-dimensional polytope specified by the vectors $\mathbf{v}_i$, $1, \ldots, n$, issuing from a given vertex 0 is

$$\mathrm{vol}_n(\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n) = \pm C \det(\mathbf{V}), \tag{1.1}$$

where $\mathbf{V}$ is the $n \times n$ matrix with ith column $\mathbf{v}_i$ (while the sign records the "chirality" of the ordered set of vectors), and the constant C scales the volume measure. The polytope is usually viewed to be the n-parallelepiped with the n edges from vertex 0 being coincident with the $\mathbf{v}_i$, and $C = +1$ is chosen so that the n-dimensional hypercube has such a measure of $+1$ (or -1). But here we are interested in n-simplices, each of which is also is specified by the $\mathbf{v}_i$, and we make the non-standard choice for C whence the regular n-simplex with unit edges has a unit n-volume. But it is well known that an n-simplex has an n-volume $n!$ times smaller than the corresponding n-parallelepiped. Thus, we choose $C = 1/n!$ if we wish to interpret (1.1) as giving the n-volume of an n-parallelepiped, or alternatively we choose $C = 1$ if we wish to interpret (1.1) as giving the n-volume of an n-simplex. Further squaring the above n-volume formula leads one ultimately to the following result [5,20] (which is now standard [3]):

Cayley–Menger theorem. For Euclidean space the square of the n-volume of the n-simplex determined by the $n+1$ points at the vertices is

$$\left\{V_n(\mathbf{D}_1)\right\}^2 = -(-2)^{-n} \det \begin{pmatrix} \mathbf{D}_2 & \mathbf{1}_{n+1} \\ \mathbf{1}^+_{n+1} & 0 \end{pmatrix}, \tag{1.2}$$

where $\mathbf{D}_q$ is here the $n+1$ by $n+1$ matrix with (i,j)th element being the qth power of the distance between the ith and jth vertices of this n-simplex, $\mathbf{1}_{n+1}$ is the $n+1$ by 1 column vector with all elements 1, and $\mathbf{1}^+_{n+1}$ is the transpose of $\mathbf{1}_{n+1}$.

This Cayley–Menger formula then is suitable for our present purposes in that all that is required is the set of intersite distances. That is, granted a distance function for a graph G, we presume equation (1.2) to be the defining relation for the n-volumen associated to of an $n+1$-element set of vertices of G, though on a general (non-Euclidean) space this "square" of (1.2) need not be non-negative. (To remind that these quantities as defined on such general spaces need not be fully like the ordinary Euclidean-space n-volumes of n-simplices, we use Latinized names.) When (1.2) is non-negative it seems natural to choose $V_n(\mathbf{D}_1)$ as the non-negative square root.

The graph invariants proposed for study here are of the form

$$S_G\{V_n\}^p = \sum \left\{V_n(\mathbf{D}_1)\right\}^p, \tag{1.3}$$

where N is the number of vertices of the graph G, the sum is over all sets of $n+1$ vertices of G, and the $\{V_n(\mathbf{D}_1)\}^2$ are the n-volumina of (1.2) for these n+1-element sets of vertices. For $n = 1$ and for the usual shortest-path distance function some of these invariants are already studied especially for $p = 1$ or 2. In particular, the $p = 1$ case is what is often called the "Wiener number" of G and has been utilized for some time in making correlations with molecular properties – see Wiener's original work [32,33] or recent reviews [14,26,29] of the chemical literature – also there is some mathematical work [7,9,22,23,25]. The $p = 2$ case turns out to be closely related [17] to what has been introduced [19,27] as the "hyper-Wiener" index. Balaban [1] has proposed that the root-mean-square distance should be a chemically useful invariant, and in a similar context other moments [1,28] have been mentioned. The resistance-distance analog of the Wiener index has also been noted [18] and there has been some initial comment [17,36] on the resistance-distance analog of the "hyper-Wiener" index and other related indices. Indeed, that for each formula for the Weiner index (based on the shortest-path distance) there seems [36] to be an equally elegant corresponding one for the resistance-distance analog.

In section 3 we present some results for the $p = 2$ power (which from the defining relation (1.2) might be anticipated to be an exceptional case). Indeed, we introduce a novel polynomial invariant

$$\mathcal{P}_G(x) = \det\left\{\begin{pmatrix} \mathbf{D}_2 & \mathbf{1}_N \\ \mathbf{1}_N^+ & 0 \end{pmatrix} - x\begin{pmatrix} \mathbf{I} & \mathbf{0}_N \\ \mathbf{0}_N^+ & 0 \end{pmatrix}\right\}, \tag{1.4}$$

where $\mathbf{D}_q$ is now the full $N \times N$ matrix of qth powers of distances, $\mathbf{I}$ is the $N \times N$ identity matrix, and $\mathbf{0}_N$ is the $N \times 1$ column vector of all zeroes. In light of theorem 2 proved in section 3 we term $\mathcal{P}_G(x)$ the *volumina* polynomial for G – this is further shown to lead to an efficient method for the computation of the $p = 2$ volumina-sum invariants of (1.3). In section 4 some simplified results for graphs of higher vertex transitivity are noted, applying for so-called "graph-symmetric" distance functions. In section 5 some further theorems for so-called "graph-geodetic" distance functions are established for our invariants.

2. Distance functions and their characterization

The distance functions under consideration are defined with reference to a set V of N distinct points (to be identified to the vertices of a graph). Such functions are a special subclass of the class $\mathcal{C}$ of functions from $V \times V$ onto the real numbers. More particularly, a *distance* function d is such that $d \in \mathcal{C}$ and

$$d(i,i) = 0, \qquad \text{for all } i \in V, \tag{2.1}$$

$$d(i,j) = d(j,i) > 0, \qquad \text{for all distinct pairs } i,j \in V, \tag{2.2}$$

$$d(i,j) + d(j,k) \geqslant d(i,k), \qquad \text{for all distinct triples } i,j,k \in V. \tag{2.3}$$

We emphasize that on graph G there are relevant distance functions besides the standard [4] shortest-path-based ones. One such of particular note is given in terms of the effective resistance function Ω with Ω_{ij} being the resistance between vertices i and j granted fixed (say unit) resistors on each edge of G. Another (non-electrical) interpretation [8] of Ω_{ij} is $1/\delta_i P(i \to j)$, where δ_i is the degree of vertex i and $P(i \to j)$ is the probability of a random walker leaving i to arrive at j before returning to i. A combinatorial interpretation [30] is that Ω_{ij} is a ratio with denominator being the number of spanning trees of G and numerator being the number of spanning "bi-trees", one component of which contains vertex i and the other component of which contains j. An algebraic representation of Ω_{ij} may be [18] given in terms of the *Laplacian* matrix $\Delta - \mathbf{A}$ with Δ the diagonal matrix of vertex degrees and $\mathbf{A}$ the adjacency matrix. Then (as is perhaps "standard" in electrical engineering)

$$\Omega_{ij} = \phi_{i-j}^+ \left\{\frac{Q}{\Delta - \mathbf{A}}\right\} \phi_{i-j}, \tag{2.4}$$

where ϕ_{i-j} is the column vector of all 0s except $+1$ and -1 in the ith and jth positions, Q is the idempotent projection matrix onto the orthogonal complement to the null-space of $\Delta - \mathbf{A}$, and $\{Q/(\Delta - \mathbf{A})\}$ is the generalized inverse, which is 0 on the null-space of $\Delta - \mathbf{A}$ while on the Q-space it is a nonsingular inverse. We term $\boldsymbol{\Omega}$ the *resistance* distance, though a possible alternative nomenclature (noted by Prof. F. Harary) would term this the "electric metric". But to emphasize that $\boldsymbol{\Omega}$ has a formal definition independent of electric circuits the phrase "electric metric" seems slightly less favorable (there being other kinds of resistance than electrical).

Various distance-function subclasses of relevance can be identified through constraining conditions forcing the functions to "mimic" in further ways the standard Euclidean distance (function), denoted d_E. In fact, we identify three natural sequences of conditions, the first two of which have been investigated by Menger [21] and by Blumenthal [2,3].

The first sequence of conditions on a function $d \in C$ consists of the n*-Euclidean conditions*, for $n = 0, 1, 2, \ldots, N-1$. For a given n the condition is that for every $(n+1)$-element subset $\mathcal{S} \subseteq V$ there exists a corresponding $(n+1)$-point subset $\mathcal{S}'$ of n-dimensional Euclidean space $\mathcal{E} = \mathcal{E}_n$ such that if $i' \in \mathcal{S}'$ corresponds to $i \in \mathcal{S}$, then

$$d(i,j) = d_E(i',j'), \quad \text{for all } i,j \in \mathcal{S}. \tag{2.5}$$

That is, every set $\mathcal{S}$ of $(n+1)$ points in V can be isometrically (or faithfully) embedded into Euclidean space so that d gives values corresponding to the Euclidean distances on this subset $\mathcal{S}$. The 0-Euclidean condition is equivalent to the "identity" condition (2.1). The 1-Euclidean condition is equivalent to the "symmetry/positivity" condition (2.2). The 2-Euclidean condition is equivalent to the "triangle" condition (2.3). That is, the usual definition of a distance function d is seen to be equivalent to demanding that d satisfy the Euclidean $n =$ 0-, 1- and 2-Euclidean conditions. The 3-Euclidean condition demands an even greater degree of mimicry, which not all distance functions satisfy. For example, the shortest-path distance function for the 4-cycle graph does not satisfy the 3-Euclidean condition. However, there are transformed distance functions guaranteed to satisfy the 3-Euclidean condition. Given d, one can define

$$d_\alpha(i,j) \equiv \bigl\{d(i,j)\bigr\}^\alpha, \quad \text{for all } i,j \in V, \tag{2.6}$$

whence there can be proved [2] the following:

Blumenthal's "Square-Root" theorem. For $0 \leqslant \alpha \leqslant 1/2$, the function d_α is a distance function satisfying the 3-Euclidean condition.

Of all these d_α evidently $d_{1/2}$ bears the greatest "similarity" to d, and so may be viewed to play a special role. This $d_{1/2}$ corresponding to the standard shortest-path distance function d on graphs has seemingly not been previously explored, and the same statement applies as regards the square-rooted resistance distance. Of related interest are functions $d^{(m)}$ (for real m) from $V \times V$ taking values

$$d^{(m)}(i,j) \equiv \left(\phi_{i-j}^{+}\left\{\frac{Q}{\Delta - \mathbf{A}}\right\}^m \phi_{i-j}\right)^{1/2}, \tag{2.7}$$

where the notation follows that of equation (2.4). Evidently, $d^{(1)}$ is the $d_{1/2}$ corresponding to the resistance distance. Generally, $d^{(m)}$ satisfies the condition of (2.1), and the interchange symmetry of its arguments is evident. A well-known (and readily verified) fact is that the column-vector $\mathbf{1}_N$ of all ones is an eigenvector to $\Delta - \mathbf{A}$ with eigenvalue 0. Evidently, too ϕ_{i-j} is orthogonal to $\mathbf{1}_N$, so that the matrix elements of ϕ_{i-j} over the matrix $\{Q/(\Delta - \mathbf{A})\}^m$ must be the same as over the mth power of $\mathbf{M}_x \equiv \{Q/(\Delta - \mathbf{A})\} + xQ$. But too since (for a connected graph) all other eigenvalues of $\{Q/(\Delta - \mathbf{A})\}$ exceed 0, it is evident that $\mathbf{M}_x$ is positive definite so long as $x > 0$. But then the function $d^{(m)}$ is a standard Euclidean-type vector-space distance function using this positive definite matrix $\mathbf{M}_x$ to define the metric. Thus there follows:

Theorem 1. The graph functions $d^{(m)}$ are distance functions satisfying all the n-Euclidean conditions.

Of all these distance functions $d^{(2)}$ shares a particular feature with $\boldsymbol{\Omega}$: both scale linearly with inverses of the (non-zero) elements of $\mathbf{A}$. Such an inversive scaling also applies for the shortest-path distance if we imagine an increase in a non-zero element of $\mathbf{A}$ to indicate an enhanced "contact", corresponding to shorter distances. This distance function $d^{(2)}$ we term *quasi-Euclidean*.

A second natural sequence of conditions on a function satisfying equations (2.1) and (2.2) consists of the n*-volumina positivity conditions*, for $n = 2, 3, \ldots, N-1$. For a given n the condition is that every $(n+1)$-element subset $\mathcal{S}$ of V is such that formula (1.2) for $\{V_n(\mathbf{D}_1)\}^2$ gives a non-negative result. Here the $(n = 2)$-volumina positivity condition is equivalent to the triangle condition, as may be seen on expanding the $(n = 2)$-determinant of (1.2) to give

$$\left\{V_2(\mathbf{D}_1)\right\}^2 = \frac{1}{4} s\Delta_i(j,k)\Delta_j(k,i)\Delta_k(i,j), \tag{2.8}$$

where $\Delta_i(j,k) \equiv d(i,j) + d(k,i) - d(j,k)$ and s is the sum of the three different distances – then (granted (2.1) and (2.2)) one sees that $s > 0$ and no more than one of the Δ may be negative, so that non-negativity of (2.8) implies nonnegativity of every Δ-term there and consequently the triangle inequality is implied. The n-volumina positivity conditions and n-Euclidean conditions turn out to be [21] in general equivalent. See also section 40 of Blumenthal [3]. Further, 4-Euclideanicity implies [34] n-Euclideanicity.

A third natural sequence of conditions on a function satisfying equations (2.1) and (2.2) consists of the n*-simplex conditions*, for $n = 2, 3, \ldots, N-1$. For a given n the condition is that every $(n+1)$-element subset $\mathcal{S}$ of V is such that the $(n-1)$-volumen of any n-element subset of $\mathcal{S}$ is no larger than the sum of the $(n-1)$-volumina of the n other n-element subsets of $\mathcal{S}$. Evidently, the $n = 2$ condition here is the familiar "triangle" condition of equation (2.3). The present $n = 3$ condition says that the area of any face of a tetrahedron does not exceed the sum of the areas of the other three faces – thence it is naturally called the "tetrahedron" inequality. Clearly, the

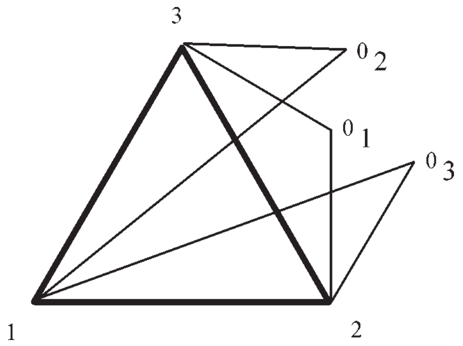

Figure 1. Construction to illustrate failure of 3-Euclideanicity even though the tetrahedron inequality is satisfied.

n-Euclidean condition implies the n-simplex condition. But, contrary to a statement made elsewhere [24], the converse is not generally true. As an example to this effect for $n = 3$, consider four points 0,1,2,3 with $d(1,0) = 3/2$, $d(2,0) = d(3,0) = 2/3$, $d(1,2) = d(2,3) = d(3,1) = 1$ – here the veracity of this as an example is seen from figure 1, where we have faithfully embedded the vertices 1,2,3 in the Euclidean plane of the paper, and then added the point 0 in three possible ways forming three new faithful triangles, each having one of its sides in common with the 1,2,3-triangle. Evidently, if the 1,3- and 1,2-edges of the 0,1,3- and 0,1,2-triangles are to be fixed on the 1,2,3-triangle there is no way for their 0,1-edges to be brought into contact (while keeping the Euclidean distances fixed). That is, there is no faithful embedding for this tetrahedron (in 3-dimensional Euclidean space), though the tetrahedron-inequality is clearly satisfied.

3. General theorematic results for volumina sums

There are some volumina-polynomial-related theorems which may be established for general distance functions on $V = V(G)$, though these results are concerned with the special power $p = 2$ (appearing in (1.3) and (1.4)). A distance function is viewed to be specified by the matrix $\mathbf{D}_1$ of its values. It turns out that the volumina polynomial of (1.4) is intimately related to the power $p = 2$ volumina sums.

Theorem 2. For the definitions of section 1, with N the order of V,

$$\mathcal{P}_G(x) = -\sum_{n=1}^{N-1} (-2)^n S_G\{V_n\}^2 (-x)^{N-n-1}. \tag{3.1}$$

Proof. From the determinantal definition of $\mathcal{P}_G(x)$ in (1.4) one sees that factors of x arise whenever a permutation in the expansion of this determinant leaves some indices fixed (since the only elements on the diagonal of the net matrix being operated on are x, and no others involve x). That is,

$$\mathcal{P}_G(x) = \sum_{n=0}^{N-1} (-x)^{N-n-1} \sum_{i(n+1)} \det \begin{pmatrix} \mathbf{D}_{2,i(n+1)} & \mathbf{1}_{n+1} \\ \mathbf{1}_{n+1}^{+} & 0 \end{pmatrix}, \tag{3.2}$$

where $i(n+1) \equiv (i_1, i_2, \ldots, i_{n+1})$ is an ordered $(n+1)$-tuple of row (and column) indices $1 \leqslant i_1 < i_2 < \cdots < i_{n+1} \leqslant N$, $\mathbf{D}_{2,i(n+1)}$ is the submatrix of $\mathbf{D}_2$ associated to the indicated rows and columns, and $\mathbf{1}_{n+1}$ is the column vector of $(n+1)$ elements of 1. Here we have not included in the sum a term for the power x^N since it is recognized that no permutation fixing the last index $(N+1)$ can survive (because this diagonal element is 0), and so the only surviving permutations must also move some other index as well. Now from equation (1.2) one identifies the present determinantal quantities as n-volumina for the implicit n-simplices specified by the points of $i(n+1)$. That is,

$$\mathcal{P}_G(x) = \sum_{n=0}^{N-1} -(-x)^{N-n-1} (-2)^n \sum_{i(n+1)} \left\{ V_n(\mathbf{D}_{2,i(n+1)}) \right\}^2, \tag{3.3}$$

and comparison of this with equation (1.3) yields the theorem. □

This result (of theorem 2) leads to an efficient means of computation of the $S_G\{V_n\}^2$ even for larger n:

Theorem 3. For the definitions of section 1,

$$S_G\{V_n\}^2 = (-2)^{-n} \sum_j u_j^2 S_n(j), \tag{3.4}$$

where u_j is the sum of the components of jth orthonormal eigenvector to $\mathbf{D}_2$, and $S_n(j)$ is the sum over all n-fold products of eigenvalues to $\mathbf{D}_2$ excluding the jth eigenvalue.

Proof. The determinant appearing in the definition of $\mathcal{P}_G(x)$ remains invariant under the application of a unitary transformation, say

$$\begin{pmatrix} \mathbf{U} & \mathbf{0}_N \\ \mathbf{0}_N^{+} & 1 \end{pmatrix}, \tag{3.5}$$

with $\mathbf{U}$ diagonalizing $\mathbf{D}_2$, thusly

$$\left(\mathbf{U}^{+}\mathbf{D}_2\mathbf{U}\right)_{ij} = \delta_{ij}\Lambda_i, \tag{3.6}$$

where Λ_i is the ith eigenvalue to $\mathbf{D}_2$. Then, letting Λ be the diagonal matrix of these Λ_i, one has

$$\mathcal{P}_G(x) = \det \begin{pmatrix} \Lambda - x\mathbf{I} & \mathbf{U}^{+}\mathbf{1}_N \\ \mathbf{1}^{+}\mathbf{U}_N & 0 \end{pmatrix}, \tag{3.7}$$

a result involving an $(N+1)\times(N+1)$ matrix which is diagonal except for the last row and column. Since the last index must be moved by the permutations in the expansion of this determinant (the last diagonal element being 0), one has

$$\mathcal{P}_G(x) = \sum_{j=1}^{N}(-1)\big(\mathbf{U}^{+}\mathbf{1}_N\big)_j\big(\mathbf{1}_N^{+}\mathbf{U}\big)_j\prod_{i\neq j}(\Lambda_i - x). \tag{3.8}$$

Here

$$\big(\mathbf{1}_N^{+}\mathbf{U}\big)_j = \sum_i U_{ij} \equiv u_j \tag{3.9}$$

is the sum of the elements of the jth eigenvector (when it is normalized). Then expanding our last formula for $\mathcal{P}_G(x)$ it is seen that the coefficient of $(-x)^{N-n-1}$ is

$$\sum_{j=1}^{N}\big(-u_j^2\big)\sum_{i(n)\not\ni j}\prod_{i_k\in i(n)}\Lambda_{i_k}, \tag{3.10}$$

where also we have presumed that u_j is real (as may be done for eigenvectors of a real symmetric matrix, as $\mathbf{D}_2$). Recognition of the inner summation here as giving $S_n(j)$ followed by a comparison to the coefficients in theorem 2 yields the present theorem. □

The volumina polynomial may be related to another polynomial of a type already introduced (for the shortest-path distance) elsewhere [6,12,13,15]. We define the qth *distance* polynomial as

$$\mathcal{D}_G^{(q)}(x) \equiv \det\{\mathbf{D}_q - x\mathbf{I}\}. \tag{3.11}$$

The $q = 1$ case is that previously defined [6,12,13,15] (for the shortest-path distance), but the $q = 2$ case may be more directly related to our present volumina polynomial. To see this define coefficients $S_n(0)$ in the expansion of the $q = 2$ distance polynomial thus

$$\mathcal{D}_G^{(2)}(x) = \sum_{n=0}^{N} S_n(0)(-x)^{N-n}. \tag{3.12}$$

The basic inter-relation between coefficients of the two types of polynomials now is given by:

Theorem 4. Let Λ_j be the jth eigenvalue to $\mathbf{D}_2$. Then

$$S_{n+1}(0) = \Lambda_j S_n(j) + S_{n+1}(j) = \frac{1}{N-n}\sum_{j=1}^{N} S_{n+1}(j), \quad n = 0,\ldots,N-1, \tag{3.13}$$

where $S_0(j) \equiv S_0(0) \equiv 1$, and conversely,

$$S_n(j) = \sum_{k=0}^{n} (-\Lambda_j)^k S_{n-k}(0). \tag{3.14}$$

Proof. Following much the same idea as in theorem 3 one obtains the coefficient $S_{n+1}(0)$ of $(-x)^{N-n+1}$ to be the sum over all products of $n+1$ eigenvalues of $\mathbf{D}_2$. But such a sum is clearly given in terms of the sums $S_n(j)$ as indicated by the first equality of the present theorem. The expression giving $S_n(j)$ in terms of the $S_{n-k}(0)$ is obtained by inversion. □

Of course the polynomial $\mathcal{D}_G^{(2)}(x)$ for $d_{1/2}$ is identical with $\mathcal{D}_G^{(1)}(x)$ for d, so that these results can relate back to the already discussed [6,12,13,15] $\mathcal{D}_G^{(1)}(x)$ case.

But too an effective means to compute the $S_G\{V_n\}^2$ is obtained. The coefficients $S_n(0)$ are computable in polynomial time in N as the coefficients of the secular equation (3.11) for $q = 2$, and so to are the eigenvalues Λ_i and eigenvector sums u_j of (3.9). Then the $S_n(j)$ are computed by (3.14), and finally, the desired volumina-sum invariants $S_G\{V_n\}^2$ are obtained via (3.4).

4. Transitivity and volumina sums

Whenever a (connected) graph has suitable "transitivity" features, somewhat more explicit results apply for our volumina-sum invariants for several of the considered distance functions on graphs. Let $\mathcal{A}(G)$ denote the *automorphism group* of the graph, this group consisting of permutations on the $V(G)$ such that when any $P \in \mathcal{A}(G)$ is applied (in the natural fashion) to the edges of $E(G)$ the consequent graph is just G again. For $P \in \mathcal{A}(G)$ and $i \in V(G)$ denote the vertex to which P sends i by Pi. Now define a distance function on G to be *graph-symmetric* iff

$$d(Pi, Pj) = d(i, j), \quad \forall i, j \in V(G),\ \forall P \in \mathcal{A}(G). \tag{4.1}$$

Evidently, the shortest-path and resistance distance as well as their square-rooted derivative distances are all so symmetric, though often Euclidean distances associated to embeddings in Euclidean 3-space are not. Throughout the remainder of the paper we presume that all distances are graph-symmetric.

The consequent simplifications of the results in the preceding section relate to the orbit structure of G, the *orbits* being equivalence classes of $V(G)$ under the action of elements of $\mathcal{A}(G)$. Let $\alpha = 1, 2, \ldots, r$ label the distinct orbits O_α of $V(G)$, and let $\mathbf{u}_\alpha$ denote the $N \times 1$ column vector with elements labelled by $i \in V(G)$ being 1 or 0 as $i \in O_\alpha$ or $i \notin O_\alpha$. Then since $\mathbf{D}_q$ commutes with the natural matrix representation $\mathbf{P}$ for $P \in \mathcal{A}(G)$ (for a graph-symmetric distance function), one sees that the r-dimensional space spanned by the different $\mathbf{u}_\alpha$ is invariant under action by $\mathbf{D}_q$ – that is, $\mathbf{P}\mathbf{u}_\alpha = \mathbf{u}_\alpha$ and $\mathbf{P}\mathbf{D}_q\mathbf{u}_\alpha = \mathbf{D}_q\mathbf{u}_\alpha$. Thus there are r independent eigenvectors to $\mathbf{D}_q$ entirely within this r-dimensional "symmetric" subspace. Moreover, the eigenproblem on this subspace is soluble in terms of an $r \times r$ *contracted* distance power matrix $\mathbf{D}_q^{\text{con}}$, with elements

$$\left(\mathbf{D}_q^{\text{con}}\right)_{\alpha\beta} \equiv (\#_\alpha \#_\beta)^{-1/2} \sum_{i\in O_\alpha} \sum_{j\in O_\beta} d(i,j)^q, \tag{4.2}$$

where $\#_\alpha$ is the order of the αth orbit O_α. This (real symmetric) matrix has r independent eigensolutions

$$\mathbf{D}_q^{\text{con}} \mathbf{w}_\xi^{\text{con}} = \Lambda_\xi \mathbf{w}_\xi^{\text{con}}. \tag{4.3}$$

Then defining $\mathbf{w}_\xi \equiv \sum_\alpha w_{\xi\alpha}^{\text{con}} \#_\alpha^{-1/2} \mathbf{u}_\alpha$, one sees (for $i \in O_\alpha$)

$$\begin{aligned}(\mathbf{D}_q \mathbf{w}_\xi)_i &= \sum_\beta \sum_{j\in O_\beta} d(i,j)^q w_{\xi\beta}^{\text{con}} \#_\beta^{-1/2} = \sum_\beta \#_\alpha^{-1/2} \left(\mathbf{D}_q^{\text{con}}\right)_{\alpha\beta} w_{\xi\beta} \\ &= \Lambda_\xi \#_\alpha^{-1/2} w_{\xi\alpha}^{\text{con}} = \Lambda_\xi w_{\xi i},\end{aligned} \tag{4.4}$$

so that r eigensolutions to $\mathbf{D}_q$ are obtained. But now the vector $\mathbf{1}_N$ appearing in the u_j of theorem 3 is clearly contained within the present r-dimensional symmetric subspace, whence $\mathbf{1}_N$ is orthogonal to the other $n - r$ "non-symmetric" eigenvectors to $\mathbf{D}_q$. That is, only r terms survive in the j-sum of theorem 3, and there results:

Theorem 5. For a graph-symmetric distance function for a graph G with r orbits under $\mathcal{A}(G)$,

$$S_G\{V_n\}^2 = (-2)^{-n} \sum_\xi w_\xi^2 S_n(\xi), \tag{4.5}$$

where $w_\xi \equiv \sum_\alpha w_{\xi\alpha}^{\text{con}} \#_\alpha^{-1/2}$ with $w_{\xi\alpha}^{\text{con}}$ the αth component of the ξth orthonormal eigenvector to $\mathbf{D}_2^{\text{con}}$.

We may specialize this to the *transitive* (or, more precisely, *vertex-transitive*) case, this being defined to be the case where there is a single orbit ($r = 1$).

Corollary 1. For the $r = 1$ case with a graph-symmetric distance function,

$$S_G\{V_n\}^2 = \frac{(-2)^{-n}}{N} S_n(1), \tag{4.6}$$

where $\xi = 1$ labels the maximum eigenvalue.

Of course, there are many types of transitive graphs including the cyclic graphs and the complete graphs K_N. For K_N, the final n-volumina mean can easily be seen directly from the definition to be δ^n, if δ is the common distance between every pair of vertices.

The next simplest case involves $r = 2$ orbits. One class of such graphs are the *complete bipartite* graphs $K_{A,B}$ comprised of A-element and B-element sets of vertices, every member of either set being joined by edges to exactly all of those of the other set. (For $A = B$, there is just $r = 1$ orbit.) Let a, b and c be the intersite distances, respectively, between: two elements of the first set O_α, two elements of the second set O_β, and two elements one from each set. Here A and B are the numbers of elements in O_α and O_β. Now

$$\mathbf{D}_2^{\text{con}} = \begin{pmatrix} a^2/A & c^2/\sqrt{AB} \\ c^2/\sqrt{AB} & b^2/B \end{pmatrix}, \tag{4.7}$$

so that the ξth eigenproblem is readily solved, and the w_ξ of theorem 5 determined. But further, the additional eigenvalues going into the $S_n(\xi)$ are also readily found. As a first step toward obtaining these note that $\mathbf{D}_2$ can be written in the form

$$\mathbf{D}_2 = \begin{pmatrix} a^2(\mathbf{J}_{\alpha\alpha} - \mathbf{I}_\alpha) & c^2\mathbf{J}_{\alpha\beta} \\ c^2\mathbf{J}_{\beta\alpha} & b^2(\mathbf{J}_{\beta\beta} - \mathbf{J}_\beta) \end{pmatrix}, \tag{4.8}$$

where $\mathbf{I}_\alpha$ and $\mathbf{I}_\beta$ are the identity matrices on the α- and β-subspaces while $\mathbf{J}_{\alpha\alpha}, \mathbf{J}_{\alpha\beta}, \mathbf{J}_{\beta\alpha}$ and $\mathbf{J}_{\beta\beta}$ are the $A \times A$, $A \times B$, $B \times A$ and $B \times B$ matrices of all ones. Next, let $\mathbf{v}_\alpha$ be any vector of the α-subspace such that it is orthogonal to $\mathbf{u}_\alpha$ (the vectors of all ones within the α-subspace), so that

$$\sum_{i \in O_\alpha} \nu_{\alpha i} = \mathbf{v}_\alpha^+ \mathbf{u}_\alpha = 0. \tag{4.9}$$

Then

$$(\mathbf{D}_2\mathbf{v}_\alpha)_i = \begin{cases} a^2 \sum_{j \in O_\alpha} (1 - \delta_{ij}) v_{\alpha j} = -a^2 v_{\alpha i}, & i \in O_\alpha, \\ c^2 \sum_{j \in O_\alpha} v_{\alpha j} = 0, & i \in O_\beta, \end{cases} \tag{4.10}$$

whence every vector of this $(A-1)$-dimensional α-subspace is seen to be an eigenvector with eigenvalue $-a^2$. Likewise, one may define β-subspace vectors $\mathbf{v}_\beta$ such that $\mathbf{v}_\beta^+ \mathbf{u}_\beta = 0$ and find they span the $(B-1)$-dimensional β-subspace with eigenvalue $-b^2$. Thus we have (after a little straight-forward manipulation):

Theorem 6. Let a, b, c be the $\alpha\alpha$, $\beta\beta$, $\alpha\beta$ distances between vertices of the α and β sets of $G = K_{A,B}$. Then

$$S_G\{V_n\}^2 = (-2)^{-n}\bigl\{w_+^2 S_n(+) + w_-^2 S_n(-)\bigr\}, \tag{4.11}$$

where for $\sigma = +$ or $-$,

$$\begin{aligned} w_\sigma^2 &= 1 + \sigma c^2/\bigl(R\sqrt{AB}\bigr), \\ R &= \left\{ \left(\frac{a^2B - b^2A}{2AB}\right)^2 + \frac{c^4}{AB} \right\}^{1/2}, \\ S_n(\sigma) &= \lambda_\sigma S_{n-1}(\pm) + S_n(\pm), \end{aligned} \tag{4.12}$$

$$\lambda_\sigma = \frac{a^2B + b^2A}{2AB} + \sigma R,$$
$$S_n(\pm) = \sum_{x,y}^{x+y=n} \binom{A-1}{x}\binom{B-1}{y}\left(-a^2\right)^x\left(-b^2\right)^y.$$

Here the λ_σ are the eigenvalues to $\mathbf{D}_2^{\mathrm{con}}$ and $S_n(\pm)$ is the sum over n-fold products of the $A-1$ and $B-1$ eigenvalues of $-a^2$ and $-b^2$ of $\mathbf{D}_2$.

5. Volumina-sum recursions for “square-rooted” distances

For particular “square-rooted” distance functions, systematic recursion formulas for the mean n-volumina may be developed. A distance function d on a graph G is said to be *graph-geodetic* iff: whenever all paths between two vertices $i, k \in V(G)$ pass through a third point $j \in V(G)$, it follows that $d(i,j) + d(j,k) = d(i,k)$. The shortest-path distance function clearly is so graph-geodetic, and as it turns out [18] the resistance distance is too. Some proofs for theorems concerning the shortest-path distance function apply directly to any graph-geodetic distance function. For example, the theorem of [18, section 7] for the resistance distance is an analogue of the earlier result [12] for the shortest-path distance – but it applies for any graph-geodetic distance. Here for a graph-geodetic distance d we consider the mean n-volumina for the associated “square-rooted” distance $d_{1/2}$ (this thereby satisfying the $(n = 3)$-Euclidean conditions of section 2).

The recursions to be developed involve related graphs differing in but one or two vertices. Of particular relevance will be graphs related as in figure 2. That is, the two graphs are the same except that a cut-edge (between vertices x and y) in L – R is eliminated in L · R with the previous other connections in L – R to y replaced by connections to x. Notably the distances between vertices i of L and j of R will be $d(x,y)$ less in L · R than in L – R. A useful (working) lemma is:

Lemma 7. Let L – R and L · R be related as in the preceding figure, let d be a graph-geodetic distance function (on L – R and L · R), and let $\mathbf{D}_1$ be the $(n+1)\times(n+1)$ matrix of $d_{1/2}$ distances associated with a set $\mathcal{S}$ of $n+1$ vertices of L – R. Then:

(a) for no vertices of R in $\mathcal{S}$,

$$\left\{V_n(\mathbf{D}_1)\right\}^2 = \left\{V_n\left(\mathbf{D}_1'\right)\right\}^2; \tag{5.1}$$

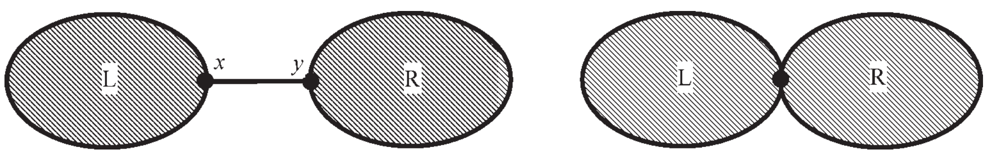

Figure 2. Graphs L – R and L · R.

(b) for one vertex j of R in $\mathcal{S}$,

$$\{V_n(\mathbf{D}_1)\}^2 = \{V_n(\mathbf{D}'_1)\}^2 = d(x,y)\{V_{n-1}(\mathbf{D}'_{1(j)})\}^2; \tag{5.2}$$

(c) for x, y both in $\mathcal{S}$,

$$\{V_n(\mathbf{D}_1)\}^2 = d(x,y)\{V_{n-1}(\mathbf{D}'_{1(y)})\}^2, \tag{5.3}$$

where $\mathbf{D}'_1$ denotes the corresponding $d_{1/2}$ distance matrix for L · R and the parenthetic subscript on $\mathbf{D}'_{1(j)}$ indicates that vertex j is deleted.

Proof. The result of (a) is trivial. For the case (b), the matrix appearing in the definition of $\{V_n(\mathbf{D}_1)\}^2$ is of the form

$$\begin{vmatrix} d(i,i') & d(i,x)+\delta+d(y,j) & 1 \\ d(j,y)+\delta+d(x,i') & 0 & 1 \\ 1 & 1 & 0 \end{vmatrix}, \tag{5.4}$$

where $\delta \equiv d(x,y)$ and we have indicated just one representative row i and one representative column i' for the n rows and columns associated to vertices of L. Now the determinant of this matrix remains unchanged upon subtraction of δ times the last column from the next to last – and likewise upon subtraction of δ times the last row from the next to the last. This leaves

$$\det \begin{vmatrix} d(i,i') & d(i,x)+d(y,j) & 1 \\ d(j,y)+d(x,i') & -2\delta & 1 \\ 1 & 1 & 0 \end{vmatrix}. \tag{5.5}$$

Here the (i,j) and (j,i') entries entail just the d-distances for L · R. Thus on expansion of the determinant one obtains

$$\det \begin{vmatrix} d(i,i') & d'(i,j) & 1 \\ d'(j,i') & 0 & 1 \\ 1 & 1 & 0 \end{vmatrix} - 2\delta \cdot \det \begin{vmatrix} d(i,i') & 1 \\ 1 & 0 \end{vmatrix}, \tag{5.6}$$

which leads directly (via the definition of (1.2)) to part (b) of the lemma. Next, for part (c), the matrix appearing in the definition of $\{V_n(\mathbf{D}_1)\}^2$ takes the form

$$\begin{vmatrix} d(i,i') & d(i,x) & d(i,x)+\delta & d(i,x)+\delta+d(y,j') & 1 \\ d(x,i') & 0 & \delta & \delta+d(y,j') & 1 \\ \delta+d(x,i') & \delta & 0 & d(y,j') & 1 \\ d(j,x)+\delta+d(x,i') & d(j,y)+\delta & d(j,y) & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{vmatrix}, \tag{5.7}$$

where again, we have shown just representative rows and columns for vertices other than x and y – here $i, i' \in V(L)$ while $j, j' \in V(R)$, though it is not required that there necessarily be vertices from one or the other of these two parts of L – R. Again, the determinant of this matrix remains unchanged upon subtraction of row x from rows i, and of column x from columns i'. Further, one can subtract row y from rows j, and column y from columns j'. Yet further, after subtraction of row (and column) x from row (and column) y, one is left with

$$\det\begin{vmatrix} d(i,i') - d(x,i') - d(i,x) & d(i,x) & 0 & 0 & 0 \\ d(x,i') & 0 & \delta & d(y,j') & 1 \\ 0 & \delta & -2\delta & 0 & 0 \\ 0 & d(j,y) & 0 & d(j,j') - d(j,y) - d(y,j') & 0 \\ 0 & 1 & 0 & 0 & 0 \end{vmatrix}. \quad (5.8)$$

Here subtraction of δ times the last column from column y leaves just one non-zero element in column y. Then making a Laplace expansion down this column gives the determinant of our n-volumina square as

$$-2\delta\cdot\det\begin{vmatrix} d(i,i') - d(x,i') - d(i,x) & d(i,x) & 0 & 0 \\ d(x,i') & 0 & d(x,j') & 1 \\ 0 & d(j,y) & d(j,j') - d(j,y) - d(y,j') & 0 \\ 0 & 1 & 0 & 0 \end{vmatrix}. \quad (5.9)$$

Finally, addition of the remnant row x to rows i and j, as well as addition of column x to columns i' and j' leads to the result of part (c). □

With part (c) of lemma 7 in hand, a corollary readily follows (for the case, where the volumina mean consists of a single term):

Corollary 2. Let graphs L − R and L · R be as in lemma 7, let d be graph-geodetic, and let N be the number of vertices in L · R. Then for $d_{1/2}$,

$$S_{L-R}\{V_N\}^2 = d(x,y)S_{L\cdot R}\{V_{N-1}\}^2. \quad (5.10)$$

Of course, n-volumina where $n+1$ is the total number of vertices in the graph form a rather special case. Another special case is for $n = 2$, when there are triples of points with all or 1 vertex in either L or R, so that the recursions of parts (a) and (b) of lemma 7 may be applied. When all 3 points are in the same part (L or R), the recursion (a) does not yield the second term that arises with that of (b), so that not all the terms of $S_{\mathrm{L\cdot R}}\{V_1\}^2$ arise "directly" – but these missing terms are precisely those of $S_{\mathrm{L}}\{V_1\}^2$ and $S_{\mathrm{R}}\{V_1\}^2$. Thus:

Theorem 8. Assume the hypothesis of lemma 7. Then for $d_{1/2}$,

$$S_{L-R}\{V_2\}^2 = S_{L\cdot R}\{V_2\}^2 + d(x,y)\big(S_{L\cdot R}\{V_1\}^2 - S_L\{V_1\}^2 - S_R\{V_1\}^2\big). \quad (5.11)$$

Next, the conditions on n for these n-volumina sums may be related if there is made a further restriction on the graphs involved. In particular, one of the two parts (say R) of L − R may be limited to have just one vertex. That is, the graphs L − R and L · R are presumed limited to the forms shown in figure 3. Now there is never more than one vertex in R for an n-simplex in the n-volumina sum for L − R, and an argument much like that for theorem 8 applies, to give:

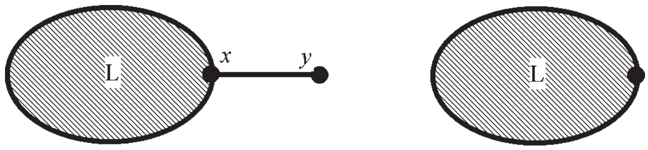

Figure 3. Graphs L $-$ y and L.

Theorem 9. Let L $-$ y and L be as in figure 3, and let d be graph-geodetic. Then for $d_{1/2}$,

$$S_{L-y}\{V_n\}^2 = S_L\{V_n\}^2 + d(x,y)S_L\{V_{n-1}\}^2. \tag{5.12}$$

For trees these recursion relations may be iterated down to the 1- and 2-site graphs.

6. Conclusion

It has here been suggested that for graphs, there are several intrinsic distance functions of natural interest. The present work indicates some possible directions of mathematical inquiry as regards such more general distance functions, particularly as regards the consequent volumina-sum invariants. Section 2 has identified some novel intrinsic metrics on graphs. The results of section 3 encompass an efficient general method for computing these new invariants, and sections 4 and 5 identify some more results for special sorts of graphs or distance functions. But also, there is some other related work. For instance, subsequent to the results reported here, further relations to other mathematical work (particularly, by Fiedler [10,11] and Merris [22]) has been elaborated in [16]. And further "graph-geometric" invariants have been proposed in [35], with an initial indication that for plausible molecular geometries, extrinsic Euclidean distances and consequent graph invariants correspond relatively favorably when the resistance distance or quasi-Euclidean distance is used. Could there be a "geometry of graphs"? Could it have deep relevance for chemistry?

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