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Graph Geometry, Graph Metrics, & Wiener

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Abstract

A line of thought suggesting the idea of "graph geometry" and its potential mathematical and chemical relevances is discussed. The development building from intrinsic graph metrics is emphasized, recent independent approaches toward "graph geometry" are inter-related, and a connection is traced back to the work of Wiener a half century ago.

1. Introduction

Wiener's original work [1,2] may be viewed as having three important features:

* first, the utilization of a metric, or distance function, definable on a general (connected) molecular graph G;
* second, the introduction of a "topological index" (or graph invariant) W(G) for use in structure-property correlations, to which end he used it; and
* third, the enunciation of a simple proposition concerning the computation for this now so-called Wiener index W(G).

Of these features perhaps the last two are more often emphasized, e.g., in discussions [3,4,5,6] reviewing more comprehensively

the application and theoretical results for W(G) than is to be done here. But though somewhat less explicit in Wiener's work, the first feature concerning a metric on a graph might be expected to have many more fundamental consequences, even of potential chemical utility. The mathematical utility of such a distance function is attested to by the book *Distance in Graphs* by Buckley and Harary [7], though even here the matter of what metric is referred to seems to be taken for granted, it apparently being assumed that there is be but one fundamental possibility for an intrinsic graph metric. Chemically "molecular geometry" is generally accepted as a relevant part of the full description of molecules, and rather extensively studied. Here too the metric is conventionally taken for granted (being that manifested in Euclidean 3-space), though there has long been a realization that graphical aspects are also very important - e.g., thus the rather cosmopolitan phrases "through-space" and "through-bond" as applied to relevant interactions - and there is some trend to examine (at least partially) topological aspects, e.g., as in [8]. Of course distances (or metrics) are intimately related to geometry. Mathematically a metric is not by itself generally viewed to be sufficient for a "geometry", which at least classically entails a nice continuum, and more modernly a geometry is defined (i.e., axiomatized) in different (even inequivalent) ways - see, e.g., [9]. Rather than finite geometries in the axiomatic mathematical sense, one might imagine a greater chemical relevance arising via correlations between aspects of an intrinsic graph metric and features of conventional molecular embeddings in Euclidean space. Indeed steps [10-14] toward such vague ideas have been made, primarily in developing some of the mathematics believed to be valuable in this matter. The potential relevance of alternative intrinsic metrics for (molecular) graphs has been noted [10,12-14], a number of general theorems obtained [10-13], and some rather empiric computational investigations carried out [14,15]. Comparisons between

different metric aspects (particularly graph-theoretic vs. those of Euclidean embeddings) have been suggested as of fundamental importance [12,14,16]. From the purely mathematical graph-theoretic side some degree of geometric concepts other than via the standard "shortest-path" metric [11,17,18] have been at least implicitly been suggested in the now rather intensive study of the so-called "Laplacian" matrix $\mathbf{L}(G)$ of a graph G, e.g., as reviewed in [17] - the name for $\mathbf{L}(G)$ here referring to a finite-differential geometrical analogy to the standard Laplacian ∇^2 of mathematical analysis involving application to (Euclidean and Riemannian) geometric spaces. Indeed Fiedler in [11] evidently seeks to emphasize and develop more explicitly the geometrical analogy, obtaining correspondences to (Euclidean) geometrical structures, and entitling his work "*A Geometric Approach to the Laplacian Matrix of a Graph*".

In the present manuscript the idea of some sort of an intrinsic "graph geometry" is pursued. In the next section a selective review is made of some relevant aspects of the graph Laplacian, with a qualitative discussion of geometrically suggestive aspects. Section **3** describes a few fundamental alternative intrinsic graph metrics, with some attention to potential relevance and to already known mathematical relations involving correspondences to Euclidean metrics for embeddings in Euclidean space. Section **4** relates Fiedler's work to that described in section **3**.

With the newly recognized alternative graph metrics and such consequent Euclidean correspondences there naturally arises the question of the degree to which such intrinsic "graph geometry" relates to what is traditionally termed "molecular geometry", and which has so often been deemed not to be intrinsic to a molecular graph G. Certainly such "graph-geometric" questions deserve chemical investigation as well as mathematical - e.g., it being imaginable that a close correspondence between intrinsic graph

geometry and molecular geometry (for the embedded molecular structure) might correlate with chemical stability. Here though a consideration of some of the mathematical ideas is the focus of attention. In any event surely such ideas follow a thread of argument leading back to Wiener's pioneering work [1,2], and these ideas seemingly hold promise of yet further interesting mathematical and chemical results.

2. The Laplacian Matrix and Geometry

The graph-theoretic nomenclature followed in this and later sections is fairly standard, both in mathematics [19] and in mathematical chemistry [20]. A *graph* G is specified first by a *vertex* set $V(G)$ and second by an *edge* set $E(G)$ comprised from (unordered) pairs of vertices from $V(G)$. Often we denote the order of $V(G)$ by N. The *adjacency* matrix $\mathbf{A}(G)$ has N rows and N columns in correspondence to the vertices of $V(G)$ with all elements A_{ij} being 0 except those corresponding to pairs $\{i,j\} \epsilon E(G)$ for which $A_{ij}=1$. The *degree* matrix $\mathbf{\Delta}(G)$ has similarly labelled rows and columns and is diagonal with the ith diagonal element being the number of edges $e \epsilon E(G)$ such that $i \epsilon e$. That is, $\mathbf{\Delta}(G)$ is diagonal with Δ_{ii} the *degree* of $i \epsilon V(G)$.

The graph Laplacian of a graph G is mathematically very fundamental, with several recent reviews [17,18]. Indeed the graph Laplacian can be traced back over a century to Kirchoff's seminal electrical-network article [21] (appearing in a chemistry journal), though this application now typically is a focus in electrical engineering. More recent but meagre chemical applications are identified by Kunz [22]. The *Laplacian* matrix of G is defined

$$\mathbf{L}(G) \equiv \mathbf{\Delta}(G) - \mathbf{A}(G) \tag{2.1}$$

though sometimes this matrix has been termed the Kirchhoff matrix, or (in electrical engineering) the admittance matrix. The rationale for the Laplacian name is that: were G to be a regular (perhaps suitably dense) lattice graph in a Euclidean manifold and if the values of a function f on this manifold as evaluated at these lattice points were formed into a vector $\mathbf{f}$, then $\mathbf{L}(G)\mathbf{f}$ would give the finite-difference approximant for the classical Laplacian ∇^2 applied to f. Indeed $\mathbf{L}(G)$ and ∇^2 share some important properties: both are positive semi-definite with lower eigenvalues corresponding to eigenvectors with fewer nodal regions, i.e., to eigenvectors for which the components vary more slowly between adjacent vertices. More rigorously these results for $\mathbf{L}(G)$ can be readily seen if one notes that for an arbitrary column N-vector $\mathbf{v}$ it can be shown that

$$\mathbf{v}^\dagger \mathbf{L}(G)\mathbf{v} = \sum_{i-j} (v_i - v_j)^2 \qquad (\mathbf{2}.2)$$

where the summation is over the edges $\{i,j\} \epsilon E$, v_k is the kth component of $\mathbf{v}$, and $\mathbf{v}^\dagger$ is the (complex-conjugate) transpose of $\mathbf{v}$. Thence evidently one obtains 0 if all the v_k are equal, and if G is connected, then the result is >0 for any other vector. Thus for such connected G, there is a unique (up to phase and normalization) 0-eigenvalue vector, while all other eigenvalues are positive. Later we denote this unique eigenvector with all components 1 by ϕ. If G were to have two components, one sees from (**2**.2) that there would be exactly two 0 eigenvalues, while all other eigenvalues are positive. So , again for a connected graph G one might anticipate the lowest positive eigenvalue (which would collapse towards 0 as one disconnects the graph) would be a measure of the graph's connectivity - and indeed Fiedler [23] has proposed that this eigenvalue $\lambda_2(G)$ be called the *algebraic connectivity* of G. Generally from (**2**.2) one can see that the lower-eigenvalue eigenvectors are expected to vary

slowly from a site of V to its neighbors. These lower-eigenvalue eigenvectors may be spoken of as *long wave-length*, much as is done in connection with ∇^2, whose eigenvalues for a region of space represent standing waves in that region. Naturally too these lower eigenvalues are the ones for which the greatest correspondence to the standard Laplacian ∇^2 eigensolutions might be anticipated (when the wavelength is large compared to the neighbor-site spacing). Because of the evident singular character of especially the lowest-eigenvalue eigenvector ϕ some attendant notation might be introduced - we let the idempotent projection operator onto this (null-eigenvalue) space be denoted $\mathbf{\Phi}$ and its complement be $\mathbf{\Lambda}$, whence the two add to the identity $\mathbf{I}$. Then

$$(2.3) \qquad \mathbf{\Phi} \equiv (1/N)\phi\phi^{\dagger} , \qquad \mathbf{\Phi\Lambda} = \mathbf{\Lambda\Phi} = \mathbf{0} , \text{ and } \qquad \mathbf{\Phi}+\mathbf{\Lambda} \equiv \mathbf{I}$$

and resolutions of a general vector $\mathbf{v}$ or matrix $\mathbf{T}$ with regard to these two subspaces are introduced

$$\mathbf{v} = \mathbf{v}_{\Phi}+\mathbf{v}_{\Lambda} \qquad \text{with} \qquad \mathbf{v}_{\Phi} \equiv \mathbf{\Phi v} \quad \& \quad \mathbf{v}_{\Lambda} \equiv \mathbf{\Lambda v}$$

$$(2.4)$$

$$\mathbf{T} = \mathbf{T}_{\Phi\Phi}+\mathbf{T}_{\Phi\Lambda}+\mathbf{T}_{\Lambda\Phi}+\mathbf{T}_{\Lambda\Lambda}$$

$$\text{with} \quad \mathbf{T}_{\Phi\Phi} \equiv \mathbf{\Phi T\Phi} , \quad \mathbf{T}_{\Phi\Lambda} \equiv \mathbf{\Phi T\Lambda} , \quad \mathbf{T}_{\Lambda\Phi} \equiv \mathbf{\Lambda T\Phi} , \ \& \ \mathbf{T}_{\Lambda\Lambda} \equiv \mathbf{\Lambda T\Lambda}$$

Use of these notations is made later in the following sections.

As a hopefully potent general conclusion one might reasonably suspect that the Laplacian $\mathbf{L}(G)$ naturally encodes information in some finite-differential fashion about a subregion of a Euclidean space as reasonably "spanned" by a set of points corresponding to those of G - that is, $\mathbf{L}(G)$ might encode geometric information about such a subregion. Evidently this information is intrinsic to G though it is in some sense "geometric".

3. Graph Metrics

Though the general concept of a metric is a standard (and important) mathematical concept, it is perhaps appropriate to first recall the definition. See, e.g., Blumenthal [24]. A *metric* ρ on a set V is a function from $V\times V$ onto the reals satisfying three conditions:

(**3.**1) (0) $i\in V \Rightarrow \rho(i,i)=0$

(1) $i,j\in V \;\&\; i\neq j \Rightarrow \rho(i,j)=\rho(j,i)>0$

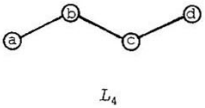
(2) $i,j,k\in V \Rightarrow \rho(i,j)+\rho(j,k)\geq\rho(i,k)$

The last condition is often called the *triangle inequality*, while often the first two conditions are "usually remixed". As stated here these conditions accumulated up through the nth guarantee that any set of n+1 points of V be faithfully (or *isometrically*) embeddable in n-dimensional Euclidean space $\mathscr{E}_n$. And with this last interpretation one readily imagines further refining conditions which might be satisfied by some metrics. That is, a metric ρ is *n-Euclidean* if all sets of n+1 points of V are isometrically embeddable in $\mathscr{E}_n$. Thence the conditions (0), (1), and (2) in the definition of a metric ρ are identified with 0-, 1-, and 2-Euclidean-ness.

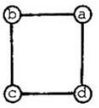
It is emphasized that several metrics, being both "natural" and "intrinsic", are possible [12-14] on graphs, which are here typically assumed to be *connected*. Then presumably there too will emerge chemical relevance. A listing of some such metrics indicating some arguments for their fundamental "meaningfulness' is of value.

The shortest-path metric d

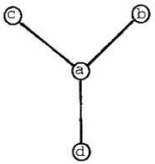
This is the common metric of Buckley and Harary [7], of the extensive mathematical literature reviewed there, of the preponderance of the chemical graph-theoretic literature (reviewed in [20]), and seemingly too of the early work of Wiener [1,2]. This *shortest-path* distance between two points $i,j \in V(G)$ is taken to be the number d(i,j) of steps in a shortest path in G between i and j. Occasionally a "decoration" of this metric is made for weighted graphs, wherein each edge {i,j} is given a (positive) weight w_{ij}, path lengths are given as the sum of the component edge weights, and the (so weighted) distance between two points is the minimum path length between these two vertices. This metric is 2-Euclidean (by definition) but frequently is not 3-Euclidean. Failure at being 3-Euclidean is possible only with N=4 or more points, so that one might consider the (connected) 4-point graphs:



L_4



C_4



Y

Here L_4 is faithfully (or isometrically) embeddable in $\mathscr{E}_1$ (and thence too in $\mathscr{E}_3$) as a straight line segment of length 3, with the distinguished vertices located at 0,1,2,3 along this segment. But neither C_4 or Y is isometrically embeddable, one being led to contradictions if an isometric embedding is assumed. E.g., for Y the vertices b,a,c (for which d(b,a)=d(a,c)=1 and d(b,c)=2) must all lie along a straight line, as likewise must c,a,d lie along a second straight line, with the segment between c and a shared with the first line - whence one concludes (for a Euclidean

space) that the two lines coincide with a and d lying atop one another, though the distance d(a,d) is to be 2, which of course is a contradiction. It is to be noted that the weighting decorations earlier mentioned do not affect these failures at isometric embeddings into Euclidean space.

The resistance-distance metric Ω

This metric may be given in several different ways [10,12-14], one involving the generalized inverse $\mathbf{\Gamma}(G)$ of $\mathbf{L}(G)$, this $\mathbf{\Gamma}(G)$ having the same null space (with projector $\mathbf{\Phi}$) as $\mathbf{L}(G)$ and being otherwise the inverse to $\mathbf{L}(G)$ on the orthogonal complement to this null space. Then for $i,j \in V(G)$ the resistance distance between i and j is

$$\Omega(i,j) = \boldsymbol{\phi}_{ij}{}^{T}\mathbf{\Gamma}\boldsymbol{\phi}_{ij} = \Gamma_{ii}-\Gamma_{ij}-\Gamma_{ji}+\Gamma_{jj} \qquad (3.2)$$

where $\mathbf{\Gamma} \equiv \mathbf{\Gamma}(G)$ and $\boldsymbol{\phi}_{ij}$ is an N-vector all of whose elements are 0 excepting the ith and jth which are +1 and -1. This may be argued to be a "reasonable" distance function if one makes a full eigen-resolution of $\mathbf{\Gamma}$ to obtain

$$\Omega(i,j) = \sum_{\lambda} (c_{\lambda i}-c_{\lambda j})^{*} \lambda^{-1} (c_{\lambda i}-c_{\lambda j}) \qquad (3.3)$$

where the λ are the non-zero eigenvalues of $\mathbf{L}$ (and in turn are the inverses of the non-zero eigenvalues of $\mathbf{\Gamma}$) and $c_{\lambda k}$ is the kth component of the orthonormalized eigenvector $\mathbf{c}_{\lambda}$ corresponding to λ. Evidently (because of the factor λ^{-1}) there is a preference for the so-called "long-wavelength" eigensolutions (with smaller values of λ), and for these values of λ the factors $(c_{\lambda i}-c_{\lambda j})$ tend to be smaller the closer together the sites i and j are, since for such "long-wavelength" λ the components (whose values represent wave amplitudes) vary slowly with separation from one another. That is, $\Omega(i,j)$ tends to measure dissimilarity of long-

wavelength wave amplitudes at i and j, so that with this interpretation Ω seems intuitively somewhat like a "metric". Another suggestive presentation of this metric is in terms of random walks on G, such as discussed at some length in the charming book [25] by Doyle & Snell. It turns out that $\Omega(i,j)$ is inversely proportional to the probability that a random walker leaving from site i will arrive at site j before returning to i. Again $\Omega(i,j)$ so interpreted intuitively should be larger the "harder" it is to travel from i to j - i.e., Ω should intuitively act like a metric. But originally the definition was presented in another suggestive form familiar from the theory of electrical networks: first, one imagines a network with a unit resistor between each pair of nodes interconnected by an edge of G; and second, one identifies $\Omega(i,j)$ as the effective resistance between nodes i and j (were a battery to be connected between i and j). From this definition many people seem to have an intuitive feeling that Ω satisfies the conditions of a metric. Now it seems that this metric need not be 3-Euclidean, e.g., this metric being identical to the shortest-path metric for all trees. But for many (cycle-containing) graphs Ω is 3-Euclidean while d is not. Anyway via any of the triumvirate of possible interpretations noted here it seems that Ω might be surmised to be a "reasonable" or "meaningful" metric - even if one were to introduce weights corresponding to the inverse values of the resistors placed on each edge (or into the inverse values for walking along different edges, or into the inverse values identified to the edges in $\mathbf{A}$ as appear in $\mathbf{L}$). It might seem rather remarkable that comparatively so little attention has been directed to Ω as a metric despite the (here only partially developed) intuitive appeal of each of the three indicated interpretations.

Square-rooted metrics

As it turns out there is a general theorem of Blumenthal [26] that given a metric ρ there are corresponding metrics ρ_α with $\rho_\alpha(i,j) \equiv \{\rho(i,j)\}^\alpha$ such that ρ_α is n-Euclidean for all $n \geq 0$ so long as $0 \leq \alpha \leq 1/2$. Evidently $\alpha = 1/2$ plays a special role in maintaining some sort of maximal similarity between ρ and one of these ρ_α achieving n-Euclidean-ness. Thence we have two more natural metrics of interest - namely $d_{1/2}$ and $\Omega_{1/2}$. Their "meaningfulness" derives from that of d or Ω.

Quasi-Euclidean metric

There is a further rather general class of n-Euclidean metrics for which one takes $\rho(i,j) \equiv \{\phi_{ij}^\dagger \Pi \phi_{ij}\}^{1/2}$ where ϕ_{ij} is the column vector all of whose elements are 0 excepting the ith and jth which are +1 and -1 while Π is a positive definite matrix. Indeed this is a standard vector-space-theoretic result [26] where one would identify ϕ_{ij} as the difference of position vectors for points i and j - the space evidently being identified as N-dimensional with the N graph vertices being located at unit (positive) positions along each of the different axes. The choice $\Pi = \Gamma(G)$ evidently gives $\Omega_{1/2}$, though $\mathbf{L}(G)$ and hence also $\Gamma(G)$ are well-known to be [11,17,18] only positive semi-definite - basically the possibility of a 0 value for $\rho(i,j)$ can not occur if one constrains attention to the "graph-theoretic" points at unit positive distances along each axis, the null-eigenvalue eigenvector ϕ to $\Gamma(G)$ being unrealizable as a difference ϕ_{ij} of two such positions. The choice $\Pi = \{\Gamma(G)\}^2$ obviously gives a related metric but also scales linearly with inverse edge weights, just as is the case with d and Ω. This metric has been termed the *quasi-Euclidean* metric $\rho_{q\text{-}E}$.

Neumaier's metric

Neumaier [28] has established a metric ρ_N with

(3.4) $$\rho_N(i,j) = \{\mu\cdot(1-I_{ij})-A_{ij}\}^{1/2}$$

where $-\mu$ is the lowest eigenvalue of the adjacency matrix $\mathbf{A}\equiv\mathbf{A}(G)$. But though this is a metric it can be argued to not be so chemically "meaningful". E.g., for an even-length cycle, $\mu=2$ and every pair of (distinct) non-neighbor vertices are a distance 2 apart while all neighbor pairs are a distance 1 apart - and any correspondence to a Euclidean embedding seems "far-fetched".

The feature of making a metric n-Euclidean is just one conceivable criterion to seek for a "meaningful" graph geometry. Of some interest is that both $\Omega_{1/2}$ and $\rho_{q\text{-}\varepsilon}$ associate not only to norms but also naturally associate to an inner-product

(3.5) $$\langle \mathbf{u}|\mathbf{v}\rangle \equiv \mathbf{u}^{\dagger}\,\mathbb{L}^{n}\,\mathbf{v}$$

where n=1 for $\Omega_{1/2}$ or n=2 for $\rho_{q\text{-}\varepsilon}$. But there are other ways to look for the "meaningfulness" of a metric, one such being to compare the inter-site distances for G to those for an embedding of interest in a Euclidean space. Of course, different embeddings are of interest for different circumstances so that one should not expect (or even perhaps seek) a perfect correspondence. Such an initial study [14] looking at other "geometric" features has indeed been undertaken (along with the introduction of novel intrinsic graph-geometric invariants - net linear curvature, net torsion, and net Gaussian curvature), and especial promise suggested for $\rho_{q\text{-}\varepsilon}$ and Ω. Another (theorematic) approach is considered in the next section.

4. Fiedler's Geometric Approach

Fiedler's results [11] give support to the general idea of intrinsic geometric aspects to a graph, and proceed by way of some particular geometric ideas and notation. The Euclidean metric is denoted by ρ_E with $\rho_E(i,j)$ being the distance between points i and j of a Euclidean space. For a discrete set S of N such points the N×N matrix $\mathbf{M}$ with elements $M_{ij} \equiv \{\rho_E(i,j)\}^2$ is termed the *Menger* matrix for the set S of points. Also let $\mathbf{0}$ denote the column N-vectors whose elements are all 0, let $\mathbf{I}$ denote the N×N identity matrix, and recall the notation of section 2 as regards Φ- and Λ-projections related to the null-eigenvalue eigenvector of $\mathbf{L}$. Then Fiedler [11] makes a development leading to his theorem 5.2, which here is stated in an altered corrected form:

Fiedlerian Theorem — For a graph G of N vertices with Laplacian $\mathbf{L}$ and a column N-vector $\mathbf{q}$ with a given value of r and a given Λ-component $\mathbf{q}_\Lambda$, there exists a unique Φ-component $\mathbf{q}_\Phi$ and a unique matrix $\mathbf{M}$ such that

$$(4.1) \qquad \begin{pmatrix} 0 & \phi^\dagger \\ \phi & \mathbf{M} \end{pmatrix} \begin{pmatrix} r & \mathbf{q}^\dagger \\ \mathbf{q} & \mathbf{L} \end{pmatrix} = -2 \begin{pmatrix} 1 & \mathbf{0}^\dagger \\ \mathbf{0} & \mathbf{I} \end{pmatrix}$$

For suitable r and $\mathbf{q}_\Lambda$ the matrix $\mathbf{M}$ is a Menger matrix for a set of points in a Euclidean space.

Evidently to each connected N-vertex graph G this theorem manages to establish a correspondent geometric structure - namely N-1-simplices (in turn corresponding to the N points associated to $\mathbf{M}$) in an N-1-dimensional Euclidean space $\mathcal{E}_{N-1}$. There are additional results leading up to this and further results

elaborating the character of this simplex analogue implied in this theorem. But one can still wonder how this revealed correspondent geometric structure (an explicitly geometric graph invariant) might relate in other perhaps more "understandable" ways with the graph G. That is, the real problem is not to make just an embedding in $\mathscr{E}_{N-1}$ but to make a "meaningful" embedding. E.g., if one imagines each of the N graph points placed at one (positive) unit along each of N orthogonal axes of $\mathscr{E}_N$, then such an embedding is achieved but it knows little about the graph G and thence is generally not "meaningful". Fiedler's embedding clearly "knows" about the graph G but the question of "meaningfulness" remains. E.g., a graph embedding for the complement of G (wherein bonded and non-bonded pairs of sites are interchanged) also "knows" about G, but both this embedding and that for G itself are not both likely to be "meaningful" in the sense of giving faithful reasonable embeddings with bonded vertices a corresponding unit distance apart while non-bonded vertices are somewhat farther apart. Presumably the choice for the suitable $\Lambda\mathbf{q}=\mathbf{q}_\Lambda$ may reveal something about the possible meaningfulness of any derived "geometry", and to better understand such choices it is useful to proceed toward a proof, a first step of which is:

Lemma A — Under the hypotheses of the theorem the various consequent quantities are uniquely determined by

$$\mathbf{q}_\Phi = -(2/N)\,\phi$$

$$\mathbf{M}_{\Lambda\Lambda} = -2\Gamma$$

(4.2)

$$\mathbf{M}_{\Phi\Lambda}{}^\dagger = \mathbf{M}_{\Lambda\Phi} = -\Gamma\mathbf{q}_\Lambda\phi^\dagger$$

$$\mathbf{M}_{\Phi\Phi} = (N/2)\{r-(\mathbf{q}_\Lambda{}^\dagger\Gamma\mathbf{q}_\Lambda)\}\Phi$$

Proof: One can begin by performing the indicated matrix multiplication in the matrix equation of the prospective theorem

$$(4.3) \qquad \begin{pmatrix} \phi^{\dagger}q & \phi^{\dagger}L \\ r\phi+Mq & \phi q^{\dagger}+ML \end{pmatrix} = \begin{pmatrix} -2 & 0^{\dagger} \\ 0 & -2I \end{pmatrix}$$

Then upon resolution of the lower-right element into the (Φ,Φ)-, (Φ,Λ)-, (Λ,Φ)-, and (Λ,Λ)-projected components, one obtains

$$\begin{aligned} \phi q_{\Phi}^{\dagger} &= -2\Phi \\ \phi q_{\Lambda}^{\dagger}+M_{\phi\Lambda}L &= 0 \\ 0 &= 0 \\ M_{\Lambda\Lambda}L &= -2\Lambda \end{aligned} \qquad (4.4)$$

As a direct consequence of the first and fourth of these four equations, the first two expressions of the lemma follow. The first result here also leads to the satisfaction of the condition for the upper-left element of (4.3), and the condition for the upper-right element of (4.3) is a result already known to be satisfied by L. Next substitution of the now established first two expressions of (4.2) into the lower-left element of the matrix equation of (4.3) leads for the Φ- and Λ-components to

$$\begin{aligned} \{r-(2/N)M_{\phi\Phi}\}\phi+M_{\phi\Lambda}q_{\Lambda} &= r\phi+M_{\phi\Phi}q_{\Phi}+M_{\phi\Lambda}q_{\Lambda} = 0 \\ -(2/N)M_{\Lambda\Phi}\phi-2\Gamma q_{\Lambda} &= M_{\Lambda\Phi}q_{\Phi}+M_{\Phi\Lambda}q_{\Lambda} = 0 \end{aligned} \qquad (4.5)$$

The second of these two equations leads to the third of the

expressions (4.2) of the lemma, and utilization of this in the remaining (second) condition of (4.4) an identity is reached (checking the consistency of the results obtained so far). Now substitution of the third expression of (4.2) in the first expression of the first equation of (4.5) leads to the fourth expression of (4.2). Thus the lemma is proved.

With the characterization of the algebraic solution of the Fiedlerian equation (4.1) the next point to address concerns the identification of at least one "suitable" choice for $\mathbf{q}_\Lambda$ realizing $\mathbf{M}$ as a Menger matrix. This is done by:

Lemma B -- For the Fiedlerian theorem the choices

$$r=4(Tr\Gamma)+(\gamma^T\mathbf{L}\gamma)\ , \quad \mathbf{q}_\Lambda=-\mathbf{L}\gamma\ , \text{ and } \quad \gamma_i=\Gamma_{ii} \tag{4.6}$$

yield a Menger matrix $\mathbf{M}$ associated to the square-rooted resistance-distance metric $\Omega_{1/2}$.

Proof: Given $\mathbf{q}_\Lambda$ one determines first the components of $\mathbf{M}$ via the expressions (4.2) of lemma A, thusly

$$\mathbf{M}_{\Lambda\Phi} = -\Gamma(-\mathbf{L}\gamma)\phi^\dagger = \Lambda\gamma\phi^\dagger = \{\mathbf{I}-(1/N)\phi\phi^\dagger\}\gamma\phi^\dagger = \{\gamma-(Tr\Gamma)\phi\}\phi^\dagger \tag{4.7}$$

and also

$$\mathbf{M}_{\Phi\Phi} = (N/2)\{4(Tr\Gamma)+(\gamma^T\mathbf{L}\gamma)-(\gamma^T\mathbf{L}\Gamma\mathbf{L}\gamma)\}\Phi = 2N(Tr\Gamma)\Phi \tag{4.8}$$

As a consequence the different components of $\mathbf{M}$ may be now summed over to give the full $\mathbf{M}$ matrix as

$$\mathbf{M} = 2N(Tr\Gamma)\Phi+\{\gamma-(Tr\Gamma)\phi\}\phi^\dagger+\phi\{\gamma^\dagger-(Tr\Gamma)\phi^\dagger\}-2\Gamma \tag{4.9}$$

whence the individual matrix elements are

(**4**.10) $M_{ij} = 2N(Tr\Gamma)(1/N)+\{\gamma_i-(Tr\Gamma)\}+\{\gamma_j-(Tr\Gamma)\}-2\Gamma_{ij} = \Gamma_{ii}+\Gamma_{jj}-2\Gamma_{ij}$

But the final result here is recognized as $\Omega(i,j)$, so that $M_{ij}=\{\Omega_{1/2}(i,j)\}^2$, and lemma B is established.

Indeed, for the case that G is a tree, this is the solution to (**4**.1) which Fiedler [11] illustrates - trees being just the case for which $\Omega_{1/2}$ and $d_{1/2}$ coincide and thence give the Menger matrix as the standard shortest-path distance matrix. More comprehensively it is seen here that without the restriction to trees the relation is better identified to the resistance-distance metric, and the metric which it actually implicates is the square-rooted resistance-distance metric $\Omega_{1/2}$. Thus the Fiedlerian theorem is proved.

Of course, one may still wonder about other metrics in terms of Fiedler's geometric approach. This is in part answered by:

Lemma C -- Suppose in equation (**4**.1) $\mathbf{L}$ is replaced by $\mathbf{L}^2$. Then the Fiedlerian theorem continues to hold. Also lemma A holds with Γ replaced by Γ^2 in (**4**.2). Further if these same replacements are made in (**4**.6) of lemma B, then the new $\mathbf{N}$ is the Menger matrix for the quasi-Euclidean metric $\rho_{q\text{-}E}$.

The proof is not detailed here but closely parallels that already detailed for lemmas A and B in leading to the overall Fiedlerian theorem. Actually even further extensions are formally possible, involving other metrics corresponding to different Π of our discussion leading to $\rho_{q\text{-}E}$ in section **3** - but questions of "meaningfulness" would seem to arise.

5. Further Points and Prospects

That there are several fundamental graph metrics seems for too long to have been overlooked, though there are several

instances where different such metrics have been "almost discovered". Fiedler's work in [11] essentially suggests the metric $\Omega_{1/2}$, but a number of more tangential related results may be found, e.g., where bounds on a graph's size (via the shortest-path metric) are expressed [29] in terms of Fiedler's (Laplacian-based) algebraic connectivity index $\lambda_2(G)$. Because of the electrical-network interpretation of the resistance-distance metric, it seems possible that there may be papers in the electrical-engineering literature suggestive of such ideas (but I am not so familiar with this area).

Merris [30] in some sense came near to finding an alternative metric, in his development of a formula for the Wiener index W(G) for the special case that G is a tree T, this formula being

$$W(T) = \sum_{\lambda} \lambda^{-1} \tag{5.1}$$

where the summation is over non-zero eigenvalues of the Laplacian matrix $\mathbf{L}(T)$. But the summands λ^{-1} being just the nonzero eigenvalues of the generalized inverse $\mathbf{\Gamma}(T)$ of $\mathbf{L}(T)$, one sees that $W(T)=Tr\mathbf{\Gamma}(T)$ as can be readily verified to be the sum of the $\Omega(i,j)$ over distinct pairs $\{i,j\}$, while the resistance-distance and shortest-path distances are the same for trees, so that also W(T) is given as the same sum over the d(i,j), this being the usual defining formula for the Wiener index. But Merris [30] goes on to surmise that the right-hand-side summation of (**5.1**) over non-zero eigenvalues of the Laplacian for a general (connected) graph G may be of interest (and possibly of use in chemistry for making structure-property correlations) - so that what in effect he has done is to suggest that the resistance-distance analog of the Wiener index may be of interest. Indeed (as noted previously [10,13]) Wiener's discussion was really restricted to trees, so that in some sense the resistance-

distance analog is just as valid an extension of Wiener's original work as is the conventional extension using the shortest-path metric. This resistance-distance alternative has now been called W'(G) in [10], the "Kirchoff number" in [16], and the 'quasi-Wiener index" in [31]. In fact in [13] it has been emphasized that many formulas valid for W(T) for the case of trees turn out when extended (in a natural way) to general graphs yield instead W'(G).

Another place where alternative metrics appear in disguised form involves the so-called [32] "distance polynomial"

$$\rho(x) = \det\{\mathbb{D}(G)-x\mathbb{I}\} \tag{5.2}$$

where $\mathbb{D}(G)$ is the N×N matrix of intersite distances d(i,j). Here the nth coefficient of the polynomial turns out [12] to be related to a sum over squares of n+1-point n-volumina for the square-rooted metric $d_{1/2}$. That is, these coefficients evidently are related to an extension of the Wiener number to a whole sequence of sums of squares of n-volumina - the ordinary Wiener number being the first member for distances, the second member being for 3-point (triangular) areas, the third member being for 4-point (tetrahedral) volumes, etc. Indeed the indicated interpretation is intimately related to the identification of $\mathbb{D}$ as a Menger matrix for the metric $d_{1/2}$, somewhat reminiscent of the manner in which Fiedler's work is related to $\Omega_{1/2}$.

Overall it is contended that there seems to be promise for some sort of *graph geometry*, especially using alternative intrinsic graph metrics. Studies to this end seem however to be just at an initial stage - mathematically, physically, and chemically. Further work seems of much potential value.

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