Inverting Laplace−Kirchhoff Matrices from Their Roots

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Laplace−Kirchhoff matrices, perturbed by rooting a vertex by the unit element e_{ij}, have true inverses, which are combinations of unit matrices and partial inverses. The inverses are quadratic forms of matrices in the lower triangular form. At trees, they determine path coordinates of vertices. The resistance distances are obtained by a graph algorithm.

INTRODUCTION

The Laplace−Kirchhoff matrices are quadratic forms $\mathbf{S^TS}$ of incidence matrices of oriented graphs **S**, where $s_{ij} = -1$ if the arc i goes from the vertex j, $s_{ij} = 1$ if the arc i goes to the vertex j, $s_{ij} = 0$ otherwise. They have one zero eigenvalue, and therefore they are singular. They have generalized inverses,[1] in fact infinitely many generalized inverses.[2] One of these,[3] the Eichinger matrix **E**, can be found summing up partial inverses obtained by deleting jth row and column

$$\mathbf{E} = \sum_j (\vartheta_j \mathbf{S^T S})^{-1}$$

In trees, the diagonal elements of Eichinger matrices are the sums of the distances from the vertex i to all other vertices, where e_{ij} are distances from the vertex i unpassed on the path to the vertex j. The Eichinger matrices are nonsingular. The elements of their inverses are close to elements of the Laplace−Kirchhoff matrices, and I proposed a possibility of perturbation of the vector corresponding to the vector described by a Laplace−Kirchhoff matrix.[3]

If the Laplace−Kirchhoff matrix is n-dimensional, then the other quadratic form in trees is $(n-1)$-dimensional and is not singular. The inverse[4] was formulated as the quadratic form of the path matrix **W**, which elements are $+1$ if the arc j has the same orientation as the path i, -1 if the arc j has the opposite orientation, and 0 if the arc j is not on the path.

Graph theory deals with a problem of coding of rooted trees.[5] These impractical results contain implicitly a simple solution of the given problem.

CODED ROOTED TREES

Only one unit element corresponds to each arc in path and walk matrixes **W**, the arc (or edge) itself. The columns match with the arcs (edges). In the descendant code, a tree is characterized by $(n-1)$ paths from the root. There can be n roots and therefore the whole set of codes to each tree has $n(n-1)$ rows, which is twice that of the path matrix **W**. The root code is thus a submatrix of the matrix **W**. The code is defined in the subspace of vertices, and each path is coded by all its vertices (as columns), including both its ends. Moreover, the root itself is induced as the unit element e_{11} in the first row. The convention is that arcs are always proceeding from the root. The resulting code has the lower triangular form, and the unit matrix **I** is on the diagonal. In trees, the first column is the unit matrix **J**, but the code can be used for forests, too.

The inverses of code matrices **W** are in the lower triangular form, and the unit matrix **I** is on the diagonal. The off-diagonal elements are -1 if the vertex j is the child of the vertex i and 0 otherwise. Since each child has only one parent, only two nonzero elements are in each row, except for the first one, and this part of the matrix **W** is the incidence matrix **S** of the given tree.

The unit element e_{11} is the vector going from the origin of the coordinate system to the vertex 1, or using graph convention, the arc going from the vertex 0 to the vertex 1. The zero column containing one -1 element is deleted.

For our purposes, it is necessary to allow any vertex to become the root without changing the indexes. For this, we define the path matrix as vertices on the path between the vertex i and the root j. It is only a permutation of the lower triangular form. For example

$$\mathbf{W} = \begin{Vmatrix} 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \end{Vmatrix} \qquad \mathbf{W}^{-1} = \begin{Vmatrix} 1 & -1 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 0 & 1 \end{Vmatrix}$$

The row with the unit element is inserted into the incidence matrix, and all arcs are oriented from the vertex 3.

Since both matrices are mutually inverse, their transpose and quadratic forms must have this property taken in proper order. This leads to the relation

$$(\vartheta_j \mathbf{S^T S})^{-1} + \mathbf{J J^T} = (\mathbf{S^T S} + e_{jj})^{-1}$$

which is true not only for trees but also for all connected graphs. Their incidence matrices **S** with the unit element e_{ij} are not square matrices but rectangular m,n matrices, $m > n$. Therefore, they do not have inverses, but their quadratic forms have inverses, since they are overdetermined. This will be shown for the case of simple cycles $C(n)$.

The unit column **J** is the zero eigenvector from the right of all incidence matrices **S**. The matrix $\mathbf{JJ^T}$ leaves on the place of perturbation 1 in the given row and zeroes in in other rows of any Laplace−Kirchhoff matrix multiplied by it from the right. The root row must be balanced by the submatrix, which is inverse to $\vartheta_j \mathbf{S^T S}$. The incidence matrix of a cycle with a column deleted is identical with the

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transposed matrix of the linear chain $L(n)$: $\vartheta_j S(C_n) = \mathbf{S^T}(L_n)$. Its inverse is the quadratic form $\mathbf{W^TW}$ of the path matrix. The chain forms the spanning tree of the cycle. Its square matrix is decomposed into a triangular form and added to the matrix **J**. Since $\mathbf{W^TW}$, originally defined to avoid fractions, gives $\mathbf{nI}$ as the product with $\mathbf{SS^T}$, it is necessary to divide by n. For example for $C(4)$

$\mathbf{W^T}$						$\mathbf{W^TW}$			triangular decomposition square roots		
1	1	1	0	0	0	3	2	1	3/4		
0	1	1	1	1	0	2	4	1	1/3	2/3	
0	0	1	0	1	1	1	2	3	1/12	1/6	1/2

The diagonal elements of the quadratic form $\mathbf{W^TW}$ give resistance distances of the vertices from the root.[2,6] They can be calculated directly as $(1/d_l + 1/d_r)^{-1}$, where d_l and d_r are left and right distances from the root, respectively. The third possibility, how they can be calculated, is the assymmetric triangular decomposition. This is instructive with cycles. It shows how fractions in the triangular decomposition can be reached from the path matrix, e.g., for $C(5)$

4/5				1	3/4	2/4	1/4
3/5	3/4				1	2/3	1/3
2/5	2/4	2/3				1	1/2
1/5	1/4	1/3	1/2				1

The elements of the matrices are $(n-i)/(n-j+1)$ and $(n-j)/(n-i)$, respectively.

Multiple bonds can be expressed in the incidence matrices **S** by repeating rows. This multiplicity k of an arc will decrease the code of the vertex, the arc is going in, as $1/k$. This corresponds to conductivity, e.g., 1,2-propene has three codes (square roots are now shown) corresponding to roots 1, 2, and 3, respectively

1			1			1		
1	1/2		1	1/2		1	1	
1	1/2	1	1	0	1	1	1	1/2

ROOTED UNORIENTED BIPARTITE GRAPHS

The incidence matrices of rooted unoriented trees **G** have elements $g_{ij} = 1$ if the edge i is incident with the vertex j, $g_{ij} = 0$ otherwise. They can be formulated in the lower triangular form, when on the diagonal the unit matrix **I** is, too. Therefore, they have the inverses with the same elements[5] as the corresponding oriented trees, but negative signs appear. The sign at 1 is negative, if the preceding sign on the walk going in the same direction was positive. All neighbors of a vertex have opposite signs. For example

$\mathbf{G^TG}$					$\mathbf{W}$					
2	1	0	0	0	1					
1	3	1	1	0	−1	1				
0	1	1	0	0	1	−1	1			
0	1	0	2	1	1	−1	0	1		
0	0	0	1	1	−1	1	0	−1	1	

The existence of these inverses is allowed by the possibility that all tree edges can be oriented head to tail. Therefore, such oriented trees in the quadratic form $\mathbf{SS^T}$ have all positive elements, and this matrix cannot be distinguished from the quadratic form $\mathbf{GG^T}$ of the same tree with edges instead arcs. Both matrices have the same sets of eigenvalues and eigenvectors. Since this is a property of all bipartite graphs, the existence of rooted inverses of $\mathbf{G^TG}$ can be expected for all bipartite graphs.

Table 1. Boiling Points of Some Alcohols

alcohol	descriptors					calcd °C	exper °C
distance	1	2	3	CH	4		
weights °C	64.6	13.4	19.0	−9.0	20.7		
MeOH	1	0	0	0	0	64.6	64.6
EtOH	1	1	0	0	0	78.0	78.0
1-PrOH	1	1	1	0	0	97.0	97.0
2-PrOH	1	2	0	1	0	82.4	82.4
1-BuOH	1	1	1	0	1	117.7	117.7
1-i-BuOH	1	1	2	1	0	107	108
2-BuOH	1	2	1	1	0	101.4	98
2-PeOH	1	2	1	1	1	122.1	118.5
3-PeOH	1	2	2	1	0	120.4	116

ROOTED PHYSICOCHEMICAL PROPERTIES

Some physicochemical properties of molecules are connected with specific atoms. They are rooted in them, and the property is determined by the surrounding of the atoms.

The ^{13}C chemical shift is an example. Grant and Paul[7] correlated ^{13}C chemical shift of carbon atoms in alkanes with the number of carbon atoms in distances 1−5 from the root. This raw correlation was improved by corrective terms for C-valencies of neighbor atoms. Lindenman and Adams[9] ammended the result inversing the role of the descriptors.

If the chemical shift of all atoms is determined positively by the first and second neighbors and negatively by the third neighbor, then the sum will show roughly the same trend[9] as an index combining their numbers.

Boiling points of alkanes are physicochemical properties of whole molecules. They correlate well with the sum of distances, the Wiener index. This index fails for monosubstituted alkanes, e.g., alcohols.[10]

An explanation could be that all carbon atoms of alkanes have equivalent weights as roots. A hydroxyl group is a dominant root and has the greatest effect on the boiling point. This hypothesis can be checked by simple calculations (in Table 1), exploiting walks to carbon atoms from the hydroxyl group as descriptors. The corrective term is formed by the CH group in any position in the chain (difference between experimental and calculated value for isopropyl alcohol).

The results are inferior to the results obtained by sophisticated techniques[10,11] but are better than with the Wiener index, even after it was split into the Altenburg polynomial and was inserted in the analogical matrix as in Table 1.

DISCUSSION

There are $n(n-1)$ paths from n roots to other vertices of connected graphs. In the walk matrices **W**, only half of them were used, the second half being redundant. The walk (path) matrices **W** can be differentiated, like graphs themselves, by choosing a vertex as the root. Walk (path) matrices **W** can be formulated in the space of bonds as well as in the space of vertices. They are rooted in the space of vertices by the unit element.

Each of n partial differences determines some properties of the graph and the corresponding molecule. The quadratic

rooted form gives a perturbed Laplace−Kirchhoff matrix which has a true inverse. Its eigenvalues correlate with undisturbed Laplace−Kirchhoff matrices, as preliminary checks show. In large graphs, the induced error will be relatively small, and a rooted inverse could replace the sum of all n partial inverses, the Eichinger matrix **E**, which eigenvalues are inverted eigenvalues of the corresponding Laplace−Kirchhoff matrix (except the zero eigenvalue). The inverse has resistance distances (plus 1 as the perturbation) on its diagonal.

The distances of nodes from the roots are evaluated in the DARC topological analysis, of course (e.g., refs 12 and 13). The reported results are not new, and they give a better insight as to how different elements of the topological space are related. Since the mathematical techniques used are elementary, they can help students to understand associations.

If topological distances are inverse elements of the Laplace−Kirchhoff matrices, then geometrical distances must be related with valences in molecules, especially in crystals. This task remains as an open problem.

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