A tree realization of a distance matrix: the inverse shortest path problem with a demand matrix generated by a tree

P. Van Mieghem*

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Abstract

The general inverse shortest path problem (ISPP) asks to find a weighted adjacency matrix such that the corresponding shortest path weight s_{ij} (i.e. the sum of the link weights over the shortest path) between any pair (i, j) of nodes in the graph satisfies $s_{ij} \leq d_{ij}$, for a given demand d_{ij} . Many variants of ISPP with several additional optimization criteria exist. A specific instance of ISPP is solved here by exploiting the analogy between flow and path networks. In *flow networks*, such as electrical networks where current flows over all paths from source to destination, the inversion of the distance matrix (i.e. effective resistance matrix) directly yields the weighted adjacency matrix by Fiedler's famous block-inverse relation. In *path networks*, where transport follows a single, shortest path as in e.g. telecommunication networks, the corresponding ISPP, subject to end-to-end delays as demands, is a difficult problem. Since transport in a tree can only follow one path, the flow network solution also provides the elegant matrix solution for the corresponding ISPP.

1 Flow and path networks

Design, dimensioning or operation of networks is often constrained by end-to-end limits. For example, a telephone call requires that the digitalized voice packets travels through in a telecommunication network fast enough; the delay between a source and a destination is limited to about 150ms. However, real-time control of systems over the Internet may require a lower end-to-end delay. Thus, different services (voice, video, ftp, email, etc.) typically require a different end-to-end delay. Usually, a telecom operator can determine the demand matrix D containing the maximum tolerably end-to-end delays d_{ij} between nodes i and j in his network. However, given the demand matrix D, a telecom operator is still confronted to dimension his network, both topology and corresponding link weights, so that transport along the "best" path between any pair (i, j) of nodes consumes less time than the maximum tolerable end-to-end delay d_{ij} . Here, we focus on finding a solution to the operator's problem, which we call the "inverse shortest path problem". The inverse shortest path problem (ISPP) appears in

^{*}Faculty of Electrical Engineering, Mathematics and Computer Science, P.O Box 5031, 2600 GA Delft, The Netherlands; *email*: P.F.A.VanMieghem@tudelft.nl

more situations: finding the average travel times in transportation networks [1], seismic tomography (earthquakes) of geologic zones [1], construction of a phylogenetic network (see e.g. [2]), that specifies evolutionary relationships between biological items (molecules, species,...). We also expect applications of ISPP to the human brain, where functional brain regions may be "weighted" from EEG and/or MEG measurements.

Before stating the ISPP in Section 2, we explain the terminology. We consider a graph G that possesses a set \mathcal{N} of N nodes and a set \mathcal{L} of L links. The graph G can be represented [3] by an $N \times N$ adjacency matrix A, with element $a_{ij} = 1$ if there is a link in G between node $i \in \mathcal{N}$ and node $j \in \mathcal{N}$, otherwise $a_{ij} = 0$. Each link $l \in \mathcal{L}$ in the graph G has a weight $w_l > 0$, a positive real number that specifies a property of the link. On the weighted graph G, two different types of transport are possible that lead to either "path networks" or "flow networks". In a path network, the transport of items follows a single path \mathcal{P}_{ij} between a node pair (i, j), whereas in a flow network, the transport propagates over all possible paths from node i to node j. Two typical examples are a communication network, where packets with digitalized information follow most of the time a single path \mathcal{P}_{ij} from source i to destination j, and a power grid, where electrical current flows over all possible paths.

The weight $w(\mathcal{P}_{ij}) = \sum_{l \in \mathcal{P}_{ij}} w_l$ of a path \mathcal{P}_{ij} between a node pair (i, j) consists of the sum of the weights over all links that belong to that path \mathcal{P}_{ij} . We will denote by \mathcal{P}_{ij}^* the shortest path between a node pair (i, j). The shortest path \mathcal{P}_{ij}^* minimizes the path weight over all paths \mathcal{P}_{ij} and obeys $w\left(\mathcal{P}_{ij}^*\right) \leq w\left(\mathcal{P}_{ij}\right)$. Thus, we assume that the link weights are additive. We refer to [4, Chapt. 12] for a discussion of other types of link weights and to [5] for multiple parameter, constraint routing. In most real-world networks, there is only one shortest path \mathcal{P}_{ij}^* , but, in general, there can be many shortest paths between the same node pair (i, j), in particular in unweighted graphs, where each link has the same link weight¹, i.e. $w_{ij} = w$ for all elements of the $N \times N$ link weight matrix W. The weighted adjacency matrix is $\tilde{A} = W \circ A$, where the Hadamard product \circ means a direct elementwise multiplication, $\tilde{a}_{ij} = w_{ij}a_{ij}$ and we use "tilde" notation for weighted graph matrices. In our setting, $\tilde{a}_{ij} = 0$ means that there is no link between node i and j, because we exclude zero link weights, i.e. $w_{ij} > 0$, as in Dijkstra's shortest path algorithm [4, p. 151] and in order to avoid the complication that a zero weight, i.e. $w_{ij} = 0$, would physically mean that node i and j are the same. The separation between link weights, represented by the link weight matrix W, and underlying graph G, represented by the adjacency matrix A, is obvious in unweighted graphs, where W = wJ and J is the all-one matrix. In the unweighted case, the graph is confining. In the other extreme, where link weights are highly variable and where the minimum link weight $w_{\min} > 0$ is orders of magnitude smaller than the maximum link weight $w_{\rm max}$, the underlying graph G is less confining than the link weight structure², which effectively thins out the graph. Indeed, mainly links with small link weights are relevant in a shortest path problem and large link weights may be ignored³ from the onset, especially if link weights are assigned per link independently of the other links (see also [6, Chapter 16], [7, 8, 9]).

Let v_k denote the potential or voltage of node k in the graph G. The effective resistance ω_{ij} between

¹The shortest path does not change if all weights are multiplied by a constant $\alpha > 0$.

²The link weight structure refers to the entire ensemble $\{w_l\}_{l \in \mathcal{L}}$ of all link weights in the graph as one coherent set, possibly generated by a process that takes correlations of weights over links into account. The matrix W can then be considered as one particular realization of the link weight structural process.

³If their removal does not disconnect the graph.

node *i* and node *j* equals the voltage difference $\omega_{ij} = \frac{v_i - v_j}{I}$ when a unit current I = 1 Ampere is injected in node *i* and leaves the network at node *j*. The $N \times N$ effective resistance matrix Ω with elements ω_{ij} is studied in e.g. [10, 11, 12, 3, 13, 14]. If the graph *G* is connected⁴, then the effective resistance ω_{ij} as well as the path weight $w(\mathcal{P}_{ij})$ is finite for any node pair (i, j) and a shortest path \mathcal{P}_{ij}^* exists between each node pair (i, j). We define the $N \times N$ matrix *S*, that contains all shortest path weights with element $s_{ij} = w\left(\mathcal{P}_{ij}^*\right)$. If the weighted adjacency matrix \widetilde{A} is known, then the matrix *S* is readily found via a shortest path algorithm, like Dijkstra's shortest path algorithm (see e.g. [15, 4]). Dijkstra's shortest path computation is very efficient and only requires $O(N \log N)$ elementary operations. Both the effective resistance matrix Ω and the shortest path weight matrix *S* are distance matrices⁵. Moreover, the effective resistance matrix Ω has rank *N*, implying that det $\Omega \neq 0$, as demonstrated in Theorem 1 in Appendix A that studies the eigenvalues of the the effective resistance matrix Ω .

In the sequel, we limit ourselves to connected, undirected, simple⁶ graphs. Consequently, the $N \times N$ symmetric matrices A, W, \tilde{A}, Ω and S are non-negative with zero diagonal elements.

2 Inverse shortest path problems

After this preparation, we now focus on inverse shortest path problems. The literature abound of variants on the inverse shortest path problem and we can only mention a few variants.

2.1 Inverse shortest path problem without optimization criterion

Inverse Shortest Path Problem (ISPP) Given an $N \times N$ symmetric demand matrix D with zero diagonal elements, but positive off-diagonal elements. Determine a $N \times N$ weighted adjacency matrix \widetilde{A} such that the corresponding shortest path weight matrix S obeys⁷ $S \preccurlyeq D$.

As stated, the ISPP has infinitely many solutions. For example, if $d_{\min} = \min_{ij} D$, then $\tilde{A} = d_{\min} (J - I)$, i.e. the complete graph with link weights equal to the minimum element in the demand matrix, satisfies ISPP. Moreover, suppose that the weighted adjacency matrix \tilde{A} is a solution. If $\alpha = \min_{1 \le i < j \le N} \frac{d_{ij}}{s_{ij}} > 1$, then the solution $\alpha \tilde{A}$ of ISPP is closest possible to D, because $\alpha S \preccurlyeq D$ and at least one element s_{kl} in S satisfies the demand $\alpha s_{kl} = d_{kl}$. Hence, any weighted adjacency matrix $t\tilde{A}$ with $0 < t \le \alpha$ is a solution of ISPP.

A general solution of ISPP is presented in Fig. 1, based on scaling (step 5). Step 1 generates the $N \times N$ adjacency matrix of an arbitrary connected graph, while step 2 chooses an arbitrary $N \times N$ link weight matrix W. Step 5 of GISPA in Fig. 1 illustrates for a given demand matrix D that there

⁴The weighted adjacency matrix \tilde{A} is called irreducible when the graph G is connected (see [6, p. 183]; [3, art. 167 on p. 235]). For a connected graph, the (weighted) Laplacian only has 1 zero eigenvalue and its rank is N - 1.

⁵Any element h_{ij} of a distance matrix H is non-negative $h_{ij} \ge 0$, but $h_{ii} = 0$ and h_{ij} obeys the triangle inequality: $h_{ij} \le h_{ik} + h_{kj}$ for any triple of indices (i, j, k).

⁶A simple graph has no multiple links between a same pair of nodes and also no self-loops, i.e. $a_{ii} = 0$ for each node $i \in \mathcal{N}$.

⁷We use the notation \preccurlyeq in [16, p. 32 and 44] for componentwise inequality, i.e. $S \preccurlyeq D$ means that $s_{ij} \le d_{ij}$ for each i = 1, 2, ..., N and each j = 1, 2, ..., N.

General Inverse Shortest Path Algorithm (D)

- 1. create adjacency matrix A of a connected graph on N nodes
- 2. choose a link weight matrix W
- 3. compute the weighted adjacency matrix $\widetilde{A} = W \circ A$
- 4. compute the shortest path weight matrix S based upon \widetilde{A}
- 5. compute $\alpha = \min_{1 \le i < j \le N} \frac{d_{ij}}{s_{ij}}$ and return $\widetilde{A} \leftarrow \alpha \widetilde{A}$

Figure 1: Metacode of the General Inverse Shortest Path Algorithm (GISPA), with the $N \times N$ demand matrix D as input.

are infinitely many weighted adjacency matrices \widetilde{A} that obey $S \preccurlyeq D$ and with equality $s_{kl} = d_{kl}$ in one element (k, l).

In general, a demand matrix D can be an arbitrary, symmetric non-negative matrix, which is not necessarily a distance matrix, such as the shortest path weight matrix S. Hence, equality in $S \preccurlyeq D$ may not occur. We denote by D' a demand matrix that is also a distance matrix. Any demand matrix D can be transformed into a distance matrix D' with $D' \preccurlyeq D$. Indeed, (a) we require that $d_{ij} > 0$ for each pair (i, j) of nodes. (b) if symmetry is violated, $d_{ij} \neq d_{ji}$, then assign $d'_{ij} = \min(d_{ij}, d_{ji})$. (c) if $d_{ik} + d_{kj} < d_{ij}$ for at least one node $k \in \mathcal{N}$ which violates the triangle inequality of a distance matrix, then we replace $d'_{ij} = \min_{1 \le k \le N} (d_{ik} + d_{kj})$.

Hakimi and Yau [17] have concentrated on finding a weighted graph realization of a distance matrix D', by allowing besides the N nodes (which they call "external" nodes or terminals) also additional nodes (called "interior" nodes). Thus, they allow as solution a $n \times n$ weighted adjacency matrix where $n \geq N$. Their key tool, a triangle-star transform (which they call "elementary reduction cycle") is well known in electrical impedance networks. A triangle K_3 has weights w_{12}, w_{13} and w_{23} and the 3×3 symmetric weighted adjacency matrix $\tilde{A} = W \circ (J - I)$ is

$$\widetilde{A}_{K_3} = \begin{bmatrix} 0 & w_{12} & w_{13} \\ w_{12} & 0 & w_{23} \\ w_{13} & w_{23} & 0 \end{bmatrix}$$

A star $K_{1,3}$ with leave nodes 1, 2, 3 and center node 4 has a 4×4 symmetric weighted adjacency matrix

$$\widetilde{A}_{K_{1,3}} = \begin{bmatrix} 0 & 0 & 0 & x_1 \\ 0 & 0 & 0 & x_2 \\ 0 & 0 & 0 & x_3 \\ x_1 & x_2 & x_3 & 0 \end{bmatrix}$$

If \widetilde{A}_{K_3} is a distance matrix, then $S_{K_3} = \widetilde{A}_{K_3}$. The star $K_{1,3}$, with an additional center node, has the same shortest path weights between its leave nodes if

$$x_1 + x_2 = w_{12}$$
 $x_1 + x_3 = w_{13}$ $x_2 + x_3 = w_{23}$

from which $x_1 = \frac{1}{2} (w_{12} + w_{13} - w_{23}), x_2 = \frac{1}{2} (w_{12} + w_{23} - w_{13})$ and $x_3 = \frac{1}{2} (w_{13} + w_{23} - w_{12})$, where the minus sign corresponds to the complementary or opposite link in the triangle for a node. The

triangle-star transform consists of replacing a weighted triangle in the graph by its corresponding weighted star. The interesting observation of Hakimi and Yau [17] is that the sum of the elements in \widetilde{A}_{K_3} is two times that in $\widetilde{A}_{K_{1,3}}$, thus $u^T \widetilde{A}_{K_3} u = 2u^T \widetilde{A}_{K_{1,3}} u$ (where the all-one vector u is assumed to have the correct dimensions). In other words, the sum of the elements in a distance matrix can be reduced by the triangle-star transform at the expense of added nodes. If a given distance matrix can be realized by a tree, Hakimi and Yau [17] employ the triangle-star transformation repeatedly to deduce the weighted adjacency matrix \widetilde{A}_T of that tree T.

Given an $N \times N$ distance matrix D = D', Culberson and Rudnicki [18] construct a fast algorithm that returns a weighted adjacency matrix of a graph, also possibly with n > N nodes, by neighborjoining, a similar idea as the triangle-star transform, while our exact, matrix solution, presented in Section 3 below, computes the tree on N nodes.

2.2 Optimized inverse shortest path problem

There are numerous variants of the ISPP that ask for a solution that is optimal in some way. A first variant is

Optimized Inverse Shortest Path Problem (OISPP) Given an $N \times N$ symmetric demand matrix D with zero diagonal elements, but positive off-diagonal elements. Determine a $N \times N$ weighted adjacency matrix \widetilde{A} such that the corresponding shortest path weight matrix S obeys $S \preccurlyeq D$ and minimizes a norm ||D - S||.

The requirement $S \preccurlyeq D$ implies that D - S is a non-negative matrix. The norm ||D - S|| can be chosen as the sum of the elements $u^T (D - S) u$, where u is the all-one vector.

If the demand matrix D is a distance matrix D', then S = D' is a solution of OISPP with the complete graph K_N as underlying graph. Indeed, if the shortest path between node i and j is the direct link between node i and j, then $s_{ij} = w_{ij}$ and $w_{ij} \le w_{ik} + w_{kj}$ for any other node k. By choosing $w_{ij} = d_{ij}$, where D = D' is a distance matrix, we find that the shortest path weight $s_{ij} = d_{ij}$ for any pair (i, j) of nodes. In conclusion, when we allow the complete graph as underlying graph, then there is always at least one solution of OISPP. However, Hakimi and Yau [17, Theorem 2] prove that, if the weighted graph G is a realization of the distance matrix D', then G is unique. Their theorem thus implies that, if there is only one solution of OISPP, then it must be a weighted complete graph. If there are more solutions of OISPP, one mostly chooses the solution with minimum norm ||S||, e.g. the minimum sum $u^T S u$ of elements in S.

For a distance matrix D = D' and a given real number r, Winkler [19] has proved that OISPP complemented with the condition that $u^T S u < r$ is NP-hard. Winkler [19] also summarizes the main results up to 1988:

(1) Optimal realizations (with minimum total link weight $u^T S u$) always exist (Hakimi and Yau [17]).

(2) A distance matrix D' is realizable by a weighted tree if and only if every four-tuple (p, q, r, s) of indices satisfies the "four-point condition": namely, the two largest of the three sums $d'_{pq} + d'_{rs}$, $d'_{pr} + d'_{qs}$ and $d'_{ps} + d'_{qr}$ must be equal (Buneman [20]).

(3) If a tree realization exists, then there is only one such realization; it is optimal among all realizations and obtainable in polynomial time.

(4) Several reduction methods (such as the triangle-star transform and compaction explained in [21]) exist to construct an optimal realization in the general case, but none works all the time.

2.3 OISPP subject to constraints on the adjacency matrix A

A second class of variants asks to find the weighted adjacency matrix \tilde{A} that minimizes a norm ||D - S||, confined to a certain class of graphs (i.e. constraints on the adjacency matrix A) and/or to a certain link weight structure (i.e. constraints on the link weight matrix W). Suppose that the adjacency matrix A is given, then we can compute each possible path \mathcal{P}_{ij} between a node pair (i, j) and require that its corresponding weight obeys

$$w\left(\mathcal{P}_{ij}\right) = \sum_{l \in \mathcal{P}_{ij}} w_l \le d_{ij}$$

This procedure will lead to huge set of linear inequalities in L unknowns $\{w_1, w_2, \ldots, w_L\}$ for each pair (i, j), that surely can be reduced because of the massive overlap in links of the set P_{ij} of all possible paths \mathcal{P}_{ij} between the node pair (i, j). By choosing the Euclidean (or least mean squares) norm $\|D - S\|_2^2 = \sum_{i=1}^N \sum_{j=1}^N (d_{ij} - s_{ij})^2$, Burton and Toint [1] have proposed a quadratic linear programming algorithm to solve OISPP, given the adjacency matrix A. They have applied and fine-tuned the Goldfarb-Idnani method for convex quadratic programming, which has a polynomial computational complexity.

Finally, Fortz and Thorup [22] have investigated a related problem, where the demand d_{ij} is the traffic from node *i* to node *j*, i.e. the amount of packets that are injected in node *i*, follow the shortest path \mathcal{P}_{ij}^* and leave the network at node *j*. The objective of Fortz and Thorup [22] is to minimize the maximum link utilization or traffic by optimizing the assignment of link weights. The difference with the ISPP lies in the additivity of the $w(\mathcal{P}_{ij}) = \sum_{l \in \mathcal{P}_{ij}} w_l$ of a path \mathcal{P}_{ij} : the traffic does not increase over each link of the path \mathcal{P}_{ij} and is independent of the number of links in path \mathcal{P}_{ij} . The current in flow networks, which is the analogon of traffic in [22], also does not change, but the voltage difference $v_i - v_j$ and the effective resistance ω_{ij} do increase by adding a link weight in a single path (e.g. on a tree).

3 Exact solution of the flow analogon of ISPP

Although many problems rely on shortest paths in a path network, there does not exist a clear relation between the shortest path weight matrix S and the underlying weighted adjacency matrix \tilde{A} . The shortest path computation is beyond the realm of linear algebra: entirely algorithmic and non-linear, in the sense that min-max operations appear [15, Chap. 26].

In undirected flow networks, on the other hand, Fiedler [23, 24] has derived a remarkable block matrix relation, from which we can deduce [13, 25, 14],

$$\begin{pmatrix} 0 & u^T \\ u & \Omega \end{pmatrix}^{-1} = \begin{pmatrix} -2\sigma^2 & p^T \\ p & -\frac{1}{2}\widetilde{Q} \end{pmatrix} \quad \text{with } \Omega p = 2\sigma^2 u \tag{1}$$

where $\widetilde{Q} = \widetilde{\Delta}_F - \widetilde{A}_F$ is the weighted Laplacian and the variance $\sigma^2 = \frac{\zeta^T \widetilde{Q}\zeta}{4} + R_G$, where $R_G = \frac{1}{2}u^T \Omega u = \frac{1}{2}\sum_{i=1}^N \sum_{j=1}^N \omega_{ij}$ is the effective graph resistance [12]. The diagonal matrix is $\widetilde{\Delta}_F = \text{diag}(\widetilde{A}_F u)$,

where u is the all-one vector. The vector ζ contains the diagonal elements of pseudoinverse Q^{\dagger} of the Laplacian \tilde{Q} and is equally important as the weighted degree vector $\tilde{d} = \tilde{A}_F u$, whose components are the diagonal elements of the weighted Laplacian \tilde{Q} . We emphasize the subscript F for a flow network in \tilde{A}_F , which is different from the weighted adjacency matrix \tilde{A} of the path network. Indeed, if we use the resistance (in Ohm) $r_l = w_l$ as the weight of link l between node i and j implying that $a_{ij} = 1$, then the weighted Laplacian \tilde{Q} in the flow network has elements $\tilde{q}_{ij} = -\frac{1}{r_{ij}}$ for $i \neq j$ (see [13]) and $(\tilde{a}_F)_{ij} = \frac{1}{r_{ij}}$, whereas $\tilde{a}_{ij} = w_{ij} \circ a_{ij} = r_{ij}$ in the path network. In both path and flow network, the entries are zero if there is no link link between node i and node j, i.e. $(\tilde{a}_F)_{ij} = a_{ij} = 0$; in particular, there are no self-loops, i.e. $(\tilde{a}_F)_{ii} = a_{ii} = 0$. Fiedler's block matrix (1) indicates the one-to-one relation between the effective resistance matrix Ω and the weighted Laplacian \tilde{Q} , and thus, the weighted adjacency matrix \tilde{A}_F (whose non-zero elements are the inverse of those of \tilde{A}). Applying block inverse formulae to Fiedler's block matrix identity (1), as demonstrated in the second proof of Theorem 1 in Appendix A, indicates that $2\sigma^2 = \frac{1}{u^T\Omega^{-1}u}$ and the vector $p = \frac{1}{u^T\Omega^{-1}u}\Omega^{-1}u$, while the inverse of the effective resistance matrix is

$$\Omega^{-1} = \frac{1}{2\sigma^2} p \cdot p^T - \frac{1}{2} \widetilde{Q}$$
⁽²⁾

Hence, the weighted adjacency matrix follows from (2) and $\tilde{Q} = \tilde{\Delta}_F - \tilde{A}_F$ as

$$\widetilde{A}_F = \widetilde{\Delta}_F + 2\Omega^{-1} - \frac{1}{\sigma^2} p \cdot p^T$$
(3)

Fiedler's powerful block matrix inverse (1) does not only hold for the effective resistance matrix Ω , but (1) also holds for squared Euclidean distance matrices H for which $h_{ij} = ||r_i - r_j||^2$ for some set of points $\{r_1, r_2, \ldots, r_n\}$ in the Euclidean space, which are the vertices of a simplex [26]. As demonstrated in [26], any undirected, weighted graph can be uniquely represented by a simplex in the (N-1) dimensional Euclidean space. Assuming that the given demand matrix D is a distance matrix of the inverse simplex [26] (i.e. conform to an effective resistance matrix), we can replace Ω by D in (3). In summary, for flow networks, we find the weighted adjacency matrix \tilde{A}_F in (3) such that the corresponding effective resistance matrix Ω obeys $\Omega = D$, which is the flow analogon of ISSP with minimization of $||D - \Omega||$.

A constrained system can never reach a lower global minimum of the system dynamics than a system without constraints. Hence, transport restricted to a single path is never more efficient than unrestricted transports over all possible paths, which implies that the weight of the shortest path $w\left(\mathcal{P}_{ij}^*\right)$ is lower bounded by the effective resistance $\omega_{ij} \leq s_{ij} = w\left(\mathcal{P}_{ij}^*\right)$ and, thus, $\Omega \preccurlyeq S$. Only if G is a tree, then $S = \Omega$, because transport in trees follows a single path. Incidentally, we have found for any tree the exact solution of the OISPP: If the demand matrix D = D' is a distance matrix on a tree, then the weighted adjacency matrix \widetilde{A} is deduced from (3) with $\Omega = D$, after transforming \widetilde{A}_F to \widetilde{A} .

In contrast to the available algorithms, our solution via (3) provides a closed form matrix solution for the OISPP on underlying trees, in which the properties of effective resistance matrix play a crucial role. Extending the flow analogon towards path networks and the ISPP for other graphs than trees or the complete graph seems difficult and stands on the agenda of future research. If the demand matrix D is not a proper distance matrix of the inverse simplex, then matrix elements of \tilde{A}_F in (3) can be negative. Acknowledgements I am grateful to Lieven Vandenberghe, Karel Devriendt, Rogier Noldus and Siyu Tang for useful discussions and input. Zhihao Qiu and Xiaowei Duan have suggested improvements to the initial text.

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A Eigenvalues of the effective resistance matrix Ω

The effective resistance matrix Ω is defined [3, p. 206] by

$$\Omega = \zeta . u^T + u . \zeta^T - 2Q^\dagger \tag{4}$$

where Q^{\dagger} is the pseudoinverse of the Laplacian [13] and the vector $\zeta = \left(Q_{11}^{\dagger}, Q_{22}^{\dagger}, \dots, Q_{NN}^{\dagger}\right)$ with non-negative components $Q_{jj}^{\dagger} \geq 0$. All diagonal elements of Ω are zero and all other elements of Ω are non-negative. We further assume that the graph G is connected so that all elements of effective resistance matrix Ω are finite. The explicit form of the matrix $\zeta . u^T + u.\zeta^T$ is

$$\zeta.u^{T} + u\zeta^{T} = \begin{bmatrix} 2\zeta_{1} & \zeta_{1} + \zeta_{2} & \zeta_{1} + \zeta_{3} & \cdots & \zeta_{1} + \zeta_{N} \\ \zeta_{1} + \zeta_{2} & 2\zeta_{2} & \zeta_{2} + \zeta_{3} & \cdots & \zeta_{2} + \zeta_{N} \\ \zeta_{1} + \zeta_{3} & \zeta_{2} + \zeta_{3} & 2\zeta_{3} & \cdots & \zeta_{3} + \zeta_{N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \zeta_{1} + \zeta_{N} & \zeta_{2} + \zeta_{N} & \zeta_{3} + \zeta_{N} & \cdots & 2\zeta_{N} \end{bmatrix}$$

Let us denote the eigenvalue equation of the $N \times N$ symmetric, non-negative matrix Ω by

$$\Omega v_k = \rho_k v_k$$

where ρ_k is the k-th eigenvalue belonging to the normalized eigenvector v_k , i.e. $v_k^T v_k = 1$. The real eigenvalues are ordered as usual, $\rho_1 \ge \rho_2 \ge \cdots \ge \rho_N$. The eigenvalue decomposition in matrix form is

$$\Omega = V R V^T \tag{5}$$

where V is an orthogonal matrix, $R = \text{diag}(\rho)$ and the $N \times 1$ vector $\rho = (\rho_1, \rho_2, \dots, \rho_N)^T$ with eigenvalues of Ω . Invoking the definition (4) leads to

$$\zeta . u^T v_k + u . \zeta^T v_k - 2Q^{\dagger} v_k = \rho_k v_k$$

Taking into account that $u^T Q^{\dagger} = 0$, we obtain

$$u^T \zeta . u^T v_k + u^T u . \zeta^T v_k = \rho_k u^T v_k$$

The definition of the effective graph resistance $R_G = \frac{1}{2}u^T \Omega u$, complemented by $u^T \zeta = \frac{R_G}{N}$, shows that

$$\rho_k = \frac{R_G}{N} + N \frac{\zeta^T v_k}{u^T v_k} \tag{6}$$

Theorem 1 In a connected graph, the effective resistance matrix Ω has full rank, i.e. det $\Omega \neq 0$.

We give two proofs.

Proof 1: Consider the vector $z = \alpha u + \beta y$, where the vector y is orthogonal to the all-one vector u, i.e. $y^T u = 0$, and where α and β are real numbers. The definition (4) of Ω and $u^T \zeta = \frac{R_G}{N}$ show that

$$\Omega z = \alpha N \zeta + \left(\alpha \frac{R_G}{N} + \beta \zeta^T y \right) u - 2\beta Q^{\dagger} y$$

We compute two quadratic forms,

$$u^T \Omega z = 2\alpha R_G + \beta N \zeta^T y$$

and, using $y^T u = 0$,

$$y^T \Omega z = \alpha N y^T \zeta - 2\beta y^T Q^{\dagger} y$$

which we write in matrix form,

$$\begin{bmatrix} 2R_G & N\zeta^T y \\ N\zeta^T y & -2y^T Q^{\dagger} y \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} u^T \Omega z \\ y^T \Omega z \end{bmatrix}$$

Since the determinant

$$\det \begin{bmatrix} 2R_G & N\zeta^T y \\ N\zeta^T y & -2y^T Q^{\dagger} y \end{bmatrix} = -4R_G y^T Q^{\dagger} y - (N\zeta^T y)^2 < 0$$

is never zero because Q^{\dagger} is positive semidefinite, the inverse matrix exists and there is a unique solution of the vector

$$\begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} 2R_G & N\zeta^T y \\ N\zeta^T y & -2y^T Q^{\dagger} y \end{bmatrix}^{-1} \begin{bmatrix} u^T \Omega z \\ y^T \Omega z \end{bmatrix}$$

If $\Omega z = 0$, then $\alpha = \beta = 0$ and, consequently, z = 0. In other words, there does not exist a non-zero vector z for which $\Omega z = 0$, implying that $\rho = 0$ is not an eigenvalue of Ω . Equivalently, Ω is of full rank.

Proof 2: Another proof of Theorem 1 relies on the Merger matrix and Fiedler's block matrix relation (1), that only holds if Ω^{-1} exists. Applying the block inverse [3]

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \begin{bmatrix} (A - BD^{-1}C)^{-1} & -(A - BD^{-1}C)^{-1} BD^{-1} \\ -D^{-1}C (A - BD^{-1}C)^{-1} & D^{-1} + D^{-1}C (A - BD^{-1}C)^{-1} BD^{-1} \end{bmatrix}$$
(7)

yields

$$\begin{bmatrix} 0 & u^{T} \\ u & \Omega \end{bmatrix}^{-1} = \begin{bmatrix} -(u^{T}\Omega^{-1}u)^{-1} & (u^{T}\Omega^{-1}u)^{-1} u^{T}\Omega^{-1} \\ \Omega^{-1}u (u^{T}\Omega^{-1}u)^{-1} & \Omega^{-1} - \Omega^{-1}u (u^{T}\Omega^{-1}u)^{-1} u^{T}\Omega^{-1} \end{bmatrix}$$

and comparison with the right-hand side of Fiedler's block matrix relation (1) indicates that $2\sigma^2 = \frac{1}{u^T \Omega^{-1} u}$, $p = \frac{1}{u^T \Omega^{-1} u} \Omega^{-1} u$, while

$$-\frac{1}{2}\widetilde{Q} = \Omega^{-1} - \Omega^{-1}u \left(u^T \Omega^{-1}u\right)^{-1} u^T \Omega^{-1} = \Omega^{-1} - \frac{1}{2\sigma^2} p \cdot p^T$$

The latter, rewritten as (2), illustrates that Ω^{-1} exists. Using the definition of weighted Laplacian $\widetilde{Q} = \widetilde{\Delta} - \widetilde{A}$ in terms of the weighted adjacency matrix \widetilde{A} in (2) yields

$$\widetilde{\Delta} - \widetilde{A} = \frac{1}{\sigma^2} p \cdot p^T - 2\Omega^{-1}$$

from which the weighted degree at node *m* follows as $\widetilde{d}_m = \frac{p_m^2}{\sigma^2} - 2\left(\Omega^{-1}\right)_{mm} \ge 0.$

We rewrite Fiedler's block matrix relation (1) as

$$\begin{pmatrix} 1 & 0 \\ 0 & I \end{pmatrix} = \begin{pmatrix} -2\sigma^2 & p^T \\ p & -\frac{1}{2}\widetilde{Q} \end{pmatrix} \begin{pmatrix} 0 & u^T \\ u & \Omega \end{pmatrix} = \begin{pmatrix} p^T u & -2\sigma^2 u^T + p^T \Omega \\ 0 & p u^T - \frac{1}{2}\widetilde{Q}\Omega \end{pmatrix}$$

Using $\Omega p = 2\sigma^2 u$ and $p = \frac{1}{u^T \Omega^{-1} u} \Omega^{-1} u$, we arrive at

$$pu^T - \frac{1}{2}\widetilde{Q}\Omega = I$$

This matrix relation was earlier deduced in a different way in [13, eq. (20)].

Theorem 2 In a connected graph, the effective resistance matrix Ω has only one positive eigenvalue.

Proof⁸: For any vector z, definition (4) of Ω indicates that

$$z^{T}\Omega z = 2\left(z^{T}\zeta\right)\left(z^{T}u\right) - 2z^{T}Q^{\dagger}z \tag{8}$$

If $z^T u = 0$ or $z^T \zeta = 0$, then $z^T \Omega z \leq 0$, because Q^{\dagger} is positive semidefinite. In other words, for any vector z orthogonal to the all-one vector u or to the vector ζ , the quadratic form $z^T \Omega z$ is negative, but $\frac{1}{2}u^T \Omega u = 2R_N > 0$ and $\zeta^T \Omega \zeta > 0$. Theorem 1 states that Ω is of full rank N and has no zero eigenvalue, which implies that there are (N-1) negative eigenvalues and one positive eigenvalue. \Box

A consequence of Theorem 2 and the zero diagonal in Ω lead to

$$\rho_1 = -\sum_{k=2}^{N} \rho_k \text{ and } \rho_1 = \sum_{k=2}^{N} |\rho_k|$$

while the Perron-Frobenius theorem (see e.g. [3]) tells us that $|\rho_N| < \rho_1$. Hence, apart from the largest, positive eigenvalue ρ_1 , all other eigenvalues ρ_k in Ω with $2 \le k \le N$ lie in the interval $(-\rho_1, 0)$, excluding both end points. Since $(N-1) |\rho_2| \le \sum_{k=2}^{N} |\rho_k| \le (N-1) |\rho_N|$, we have that $-\frac{\rho_1}{(N-1)} \le \rho_2 < 0$ and $-\rho_1 < \rho_N \le -\frac{\rho_1}{(N-1)}$.

In addition, (6) implies for k > 1 that

$$-\frac{1}{N}\left(|\rho_k| + \frac{R_G}{N}\right) = \frac{\zeta^T v_k}{u^T v_k}$$

Since $\frac{\zeta^T v_k}{u^T v_k} = \frac{\|\zeta\|_2 \|v_k\|_2 \cos(\theta_{\zeta, v_k})}{\|u\|_2 \|v_k\|_2 \cos(\theta_{u, v_k})} = \frac{\sqrt{\zeta^T \zeta} \cos(\theta_{\zeta, v_k})}{\sqrt{N} \cos(\theta_{u, v_k})}$, where $\theta_{a,b}$ is the angle between vector a and b, we have $|\rho_k| + \frac{R_G}{N} = \cos(\theta_{\zeta, v_k})$

$$\frac{|\rho_k| + \frac{n_G}{N}}{\sqrt{N\zeta^T\zeta}} = \frac{\cos\left(\theta_{\zeta, v_k}\right)}{\cos\left(\theta_{u, v_k}\right)}$$

⁸This proof is due to Karel Devriendt.

indicating that either θ_{ζ,v_k} or $\theta_{u,v_k} \in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right)$, but not both! Since $N \operatorname{Var}[\zeta] = \sum_{j=1}^{N} \left(Q_{jj}^{\dagger} - \frac{R_G}{N^2}\right)^2 = \zeta^T \zeta - \frac{R_G^2}{N^3} \ge 0$ as shown in [13, Section V.A],

$$-\frac{\cos\left(\theta_{\zeta,v_k}\right)}{\cos\left(\theta_{u,v_k}\right)} \le 1 + \frac{|\rho_k|}{\sqrt{N\zeta^T\zeta}}$$

If $\theta_{\zeta,v_k} \in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right)$, then $-\cos\left(\theta_{u,v_k}\right) = \cos\left(\pi - \theta_{u,v_k}\right)$ and $\pi - \theta_{u,v_k} \ge \theta_{\zeta,v_k}$. If $\theta_{\zeta,v_k} \in \left(\frac{\pi}{2}, \frac{3\pi}{2}\right)$, then $\pi - \theta_{\zeta,v_k} \le \theta_{u,v_k}$. In words, the angle θ_{ζ,v_k} is smaller than the angle θ_{u,v_k} .

Gerschgoring's theorem [3, p. 212] states that each eigenvalue ρ_k lies in circle around the origin (because each diagonal element of Ω is zero) with radius $(\Omega u)_i$ for $1 \leq i \leq N$. It follows from the definition (4) and $\zeta^T u = \frac{R_G}{N}$ that

$$\Omega u = \zeta N + u \frac{R_G}{N}$$

and Gerschgoring's theorem becomes, for a certain k and i,

$$|\rho_k| \le \frac{R_G}{N} + N\zeta_i$$

while (6) indicates that $\rho_k = \frac{R_G}{N} + N \frac{\zeta^T v_k}{u^T v_k}$. In particular, Gerschgoring's theorem [3, p. 212] provides the upper bound

$$\rho_1 \le \frac{R_G}{N} + N \max_i \zeta_i \tag{9}$$

while the Rayleigh inequality $\rho_1 \geq \frac{z^T \Omega z}{z^T z}$ for any vector z shows that, for z = u,

$$\rho_1 \ge \frac{u^T \Omega u}{u^T u} = \frac{2R_G}{N} \tag{10}$$

Since $\frac{R_G}{N} = u^T \zeta = \sum_{j=1}^N \zeta_j = NE[\zeta]$, the lower and upper bound are written as

$$2E\left[\zeta\right] \le \frac{\rho_1}{N} \le E\left[\zeta\right] + \zeta_{\max}$$

Combining both and Theorem 2 implies that there exists a component i in ζ so that, for k > 1,

$$\frac{\left|\zeta^T v_k\right|}{\left|u^T v_k\right|} \le \frac{2R_G}{N^2} + \zeta_i$$

Since the principal eigenvector components are non-negative, the corresponding inequality for v_1 also follows from a general inequality

$$\frac{\zeta^T v_1}{u^T v_1} = \frac{\sum_{j=1}^N \zeta_j v_j}{\sum_{j=1}^N v_j} \le \max_i \zeta_i$$

where equality only holds if $\zeta = \alpha u$; thus, with $\zeta^T u = \frac{R_G}{N}$, if $\zeta = \frac{R_G}{N^2} u$. If $\zeta = \frac{R_G}{N^2} u$, then we also find that $\rho_1 = \frac{2R_G}{N}$ and $v_1 = \frac{u}{\sqrt{N}}$ and that $v_k^T u = 0$ for k > 1 (which perhaps only holds for the complete graph K_N).

In summary, we can bound three eigenvalues of the effective resistance matrix Ω : the largest eigenvalue and only positive one, the second largest eigenvalue and the smallest eigenvalue,

$$\begin{cases} \frac{2R_G}{N} \le \rho_1 \le \frac{R_G}{N} + N \max_i \zeta_i \\ -\frac{\rho_1}{(N-1)} \le \rho_2 < 0 \\ -\rho_1 < \rho_N \le -\frac{\rho_1}{(N-1)} \end{cases}$$

The last bounds for ρ_N are not tight. The second bound can be written as $-\frac{N}{N-1} (E[\zeta] + \zeta_{\max}) \leq \rho_2 < 0$ and illustrates with the vector $\zeta = \left(Q_{11}^{\dagger}, Q_{22}^{\dagger}, \dots, Q_{NN}^{\dagger}\right)$ that, for sufficiently large N, the interval $(-2\zeta_{\max}, 0)$ in which ρ_2 – the eigenvalue closest to zero – lies, is intimately connected to the diagonal elements of the pseudoinverse of the Laplacian. Theses bounds may be sharpened by computations⁹ of trace $(\Omega^m) = \sum_{k=1}^m \rho_k^m$.

 $^9\mathrm{We}$ can show that

trace
$$(\Omega^2) = \sum_{j=1}^{N} \rho_j^2 = 2N\zeta^T \zeta + 2\left(\sum_{k=1}^{N-1} \frac{1}{\mu_k}\right)^2 + 4\sum_{k=1}^{N-1} \frac{1}{\mu_k^2}$$

where $\mu_1 \ge \mu_2 \ge \cdots \ge \mu_{N-1} \ge \mu_N = 0$ are the eigenvalues of the Laplacian matrix Q.

B Perturbation of the effective resistance matrix Ω

Since the sum of two distance matrices is also a distance matrix, we consider $\Omega = \Omega_1 + \varepsilon \Omega_2$, where $\varepsilon \geq 0$ is a real number that can be chosen arbitrarily small. We are interested to deduce the effect of perturbing the effective resistance matrix Ω_1 by $\varepsilon \Omega_2$ on the weighted Laplacian \tilde{Q} . By scaling Ω with ε , the relations $2\sigma^2 = \frac{1}{u^T \Omega^{-1} u}$ and the vector $p = \frac{1}{u^T \Omega^{-1} u} \Omega^{-1} u$ indicate that only σ^2 is multiplied by ε , but not the vector p.

After combining (2) with $\Omega = \Omega_1 + \varepsilon \Omega_2$, we find

$$\Omega^{-1} = (\Omega_1 + \varepsilon \Omega_2)^{-1} = (\Omega_1 (I + \varepsilon \Omega_1^{-1} \Omega_2))^{-1}$$
$$= (I + \varepsilon \Omega_1^{-1} \Omega_2)^{-1} \Omega_1^{-1}$$

where $(AB)^{-1} = B^{-1}A^{-1}$ (see e.g. [27, p. 93]) is used. Invoking $(I + \varepsilon R)^{-1} = \sum_{k=0}^{\infty} (-1)^k \varepsilon^k R^k$ for sufficiently small $\varepsilon < \frac{1}{\lambda_{\max}(R)}$,

$$\Omega^{-1} = \left(I + \sum_{k=1}^{\infty} \left(-1\right)^{k} \varepsilon^{k} \left(\Omega_{1}^{-1} \Omega_{2}\right)^{k}\right) \Omega_{1}^{-1}$$

and ignoring higher order terms $O(\varepsilon^2)$ yields

$$\Omega^{-1} \approx \Omega_1^{-1} - \varepsilon \Omega_1^{-1} \Omega_2 \Omega_1^{-1}$$

Then

$$\frac{1}{2\sigma^2} = u^T \Omega^{-1} u \approx u^T \Omega_1^{-1} u^T - \varepsilon u^T \Omega_1^{-1} \Omega_2 \Omega_1^{-1} u = \frac{1}{2\sigma_1^2} \left(1 - \frac{\varepsilon}{2\sigma_1^2} p_1^T \Omega_2 p_1 \right)$$

and

$$p = 2\sigma^{2}\Omega^{-1}u \approx 2\sigma^{2}\Omega_{1}^{-1}u - \varepsilon 2\sigma^{2}\Omega_{1}^{-1}\Omega_{2}\Omega_{1}^{-1}u$$

$$= \frac{\sigma^{2}}{\sigma_{1}^{2}} \left(p_{1} - \varepsilon \Omega_{1}^{-1}\Omega_{2}p_{1}\right)$$

$$\approx \frac{1}{1 - \frac{\varepsilon}{2\sigma_{1}^{2}}p_{1}^{T}\Omega_{2}p_{1}} \left(p_{1} - \varepsilon \Omega_{1}^{-1}\Omega_{2}p_{1}\right) \approx \left(1 + \frac{\varepsilon}{2\sigma_{1}^{2}}p_{1}^{T}\Omega_{2}p_{1}\right) \left(p_{1} - \varepsilon \Omega_{1}^{-1}\Omega_{2}p_{1}\right)$$

$$= p_{1} + \varepsilon \left(\frac{p_{1}^{T}\Omega_{2}p_{1}}{2\sigma_{1}^{2}} - \Omega_{1}^{-1}\Omega_{2}\right) p_{1}$$

Finally, to first order in ε , we have with $\Omega^{-1} = \frac{1}{2\sigma^2} p \cdot p^T - \frac{1}{2} \widetilde{Q}$

$$\begin{split} \widetilde{Q} &\approx \frac{1}{\sigma^2} p p^T - 2\Omega_1^{-1} + 2\varepsilon \Omega_1^{-1} \Omega_2 \Omega_1^{-1} \\ &\approx \frac{1}{\sigma_1^2} \left(1 - \frac{\varepsilon}{2\sigma_1^2} p_1^T \Omega_2 p_1 \right) \left(p_1 + \varepsilon \left(\frac{p_1^T \Omega_2 p_1}{2\sigma_1^2} - \Omega_1^{-1} \Omega_2 \right) p_1 \right) \left(p_1 + \varepsilon \left(\frac{p_1^T \Omega_2 p_1}{2\sigma_1^2} - \Omega_1^{-1} \Omega_2 \right) p_1 \right)^T \\ &- 2\Omega_1^{-1} + 2\varepsilon \Omega_1^{-1} \Omega_2 \Omega_1^{-1} \\ &= \frac{1}{\sigma_1^2} \left(1 - \frac{\varepsilon}{2\sigma_1^2} p_1^T \Omega_2 p_1 \right) p_1 p_1^T + \frac{\varepsilon}{\sigma_1^2} \left\{ \frac{p_1^T \Omega_2 p_1}{\sigma_1^2} p_1 p_1^T - \Omega_1^{-1} \Omega_2 p_1 p_1^T - p_1 p_1^T \Omega_2^T \left(\Omega_1^{-1} \right)^T \right\} - 2\Omega_1^{-1} + 2\varepsilon \Omega_1^{-1} \Omega_2 \Omega_1^{-1} \\ &= \frac{1}{\sigma_1^2} p_1 p_1^T - 2\Omega_1^{-1} + \frac{\varepsilon}{\sigma_1^2} \left\{ \frac{p_1^T \Omega_2 p_1}{2\sigma_1^2} p_1 p_1^T - \Omega_1^{-1} \Omega_2 p_1 p_1^T - p_1 p_1^T \Omega_2^T \left(\Omega_1^{-1} \right)^T \right\} + 2\varepsilon \Omega_1^{-1} \Omega_2 \Omega_1^{-1} \end{split}$$

and

$$\widetilde{Q} \approx \widetilde{Q}_1 + \varepsilon \left\{ \frac{p_1^T \Omega_2 p_1}{2\sigma_1^4} p_1 p_1^T - \frac{1}{\sigma_1^2} \left(\Omega_1^{-1} \Omega_2 p_1 p_1^T + p_1 p_1^T \Omega_2^T \left(\Omega_1^{-1} \right)^T \right) + 2\Omega_1^{-1} \Omega_2 \Omega_1^{-1} \right\}$$

which is fairly complicated.