2

Algebraic graph theory

The elementary basics of the matrix theory for graphs $G(N, L)$ is outlined. The books by Cvetković *et al.* (1995) and Biggs (1996) are standard works on algebraic graph theory.

2.1 Graph related matrices

1. *Adjacency matrix* A. The adjacency matrix A of a graph G with N nodes is an $N \times N$ matrix with elements $a_{ij} = 1$ only if the pair of nodes (i, j) is connected by a link l of G, otherwise $a_{ij} = 0$. If the graph is undirected, the existence of the link l implies that $a_{ij} = a_{ji}$ and the adjacency matrix $A = A^T$ is a symmetric, zero-one matrix. It is assumed further in this book that the graph G does not contain self-loops ($a_{ii} = 0$) nor multiple links between two nodes. Graphs without self-loops and without multiple links between two nodes are called *simple*.

The complement G^c of the graph G consists of the same set of nodes but with a link l between (i, j) if there is *no* link $l = (i, j)$ in G and vice versa. Thus, $(G^c)^c = G$ and the adjacency matrix A^c of the complement G^c is $A^c = J - I - A$, where J is the all-one matrix ($(J)_{ij} = 1$) and I is the identity matrix. The links in

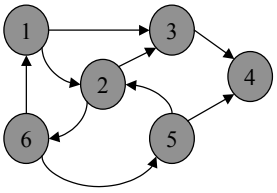

Fig. 2.1. A directed graph with $N = 6$ and $L = 9$. The links are lexicographically ordered, $l_1 = 1 \to 2, l_2 = 1 \to 3, l_3 = 1 \longleftarrow 6, l_4 = 2 \to 3$, etc.

a graph can be numbered in some way, for example, lexicographically as illustrated in Fig. 2.1. Due to different node labeling, the same graph structure can possess many different adjacency matrices (see Section 2.5 below).

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2. *Incidence matrix* B. Information about the direction of the links is specified by the *incidence matrix* B, an $N \times L$ matrix with elements

$$b_{il} = \begin{cases} 1 & \text{if link } l = i \longrightarrow j \\ -1 & \text{if link } l = i \longleftarrow j \\ 0 & \text{otherwise} \end{cases}$$

If e_k is the k-th $N \times 1$ basic vector of the N-dimensional space with $(e_k)_j = 1$ if $k = j$ and otherwise $(e_k)_j = 0$, then the l-th column vector of B, associated to link $l = i \longrightarrow j$, equals $e_i - e_j$. Each column in B has only two non-zero elements. The adjacency matrix and incidence matrix of the graph in Fig. 2.1 are

$$A = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 & 1 & 0 \end{bmatrix}, \quad B = \begin{bmatrix} 1 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 & -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & -1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -1 \\ 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 & 1 \end{bmatrix}$$

An important property of the incidence matrix B is that the sum of each column equals zero,

$$u^T B = 0 \tag{2.1}$$

where $u = (1, 1, \ldots, 1)$ is the all-one vector, also written as an $N \times 1$ matrix $u = \begin{bmatrix} 1 & 1 & \cdots & 1 \end{bmatrix}^T$.

An undirected graph can be represented by an $N \times (2L)$ incidence matrix B, where each link (i, j) is counted twice, once for the direction $i \to j$ and once for the direction $j \to i$. In that case, the degree of each node is just doubled. A link $l = (i, j)$ between node i and j in an undirected graph is also denoted as $l = i \sim j$ or $l = i \leftrightarrows j$. Instead of using the incidence matrix, the unsigned incidence matrix R, defined in **art.** 25, is more appropriate for an undirected graph.

3. *Degree of a node.* By the definition of the adjacency matrix A, the row sum i of A equals the degree d_i of node i,

$$d_i = \sum_{k=1}^{N} a_{ik} \tag{2.2}$$

A neighbor j of a node i is a node in the graph G connected by a link to node i, thus obeying $a_{ij} = 1$. The degree d_i is the number of neighbors of node i and $0 \le d_i \le N - 1$. However, only $N - 1$ degree values are possible in a simple graph, because the existence of $d_k = 0$ for some node k excludes the existence of a degree equal to $N - 1$ and vice versa. Consequently, in any graph G with N nodes, there are at least two nodes with the same degree.

Since $\sum_{i=1}^{N} \sum_{k=1}^{N} a_{ik} = 2L$, where L is the number of links in the graph G, the basic law for the degree follows as

$$\sum_{i=1}^{N} d_i = 2L \tag{2.3}$$

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Probabilistically, when considering an arbitrary nodal degree[1] D, the basic law for the degree becomes

$$E[D] = \frac{2L}{N}$$

meaning that the average degree or expectation of D in a graph G is twice the ratio of the number L of links over the number N of nodes. Especially in large real-world networks, a probabilistic approach is adequate as illustrated in Chapter 8.

The basic law of the degree (2.3) implies that any graph G possesses an *even* (possibly zero) number of nodes with *odd* degree. Indeed, the sum in (2.3) can be split over nodes with even and odd degree so that

$$\sum_{i=1}^{N} d_i^{(o)} = 2L - \sum_{i=1}^{N} d_i^{(e)}$$

where $d_i^{(o)}$ is an odd integer if the degree of node i is odd, otherwise $d_i^{(o)} = 0$ (and similarly for the even degree $d_i^{(e)}$). The right-hand side is always even, which implies that each simple graph must contain an even number of odd degree nodes.

Let us define the degree vector $d = \begin{bmatrix} d_1 & d_2 & \cdots & d_N \end{bmatrix}^T$, then both (2.2) and (2.3) have a compact vector presentation as

$$Au = d \tag{2.4}$$

and

$$u^T A u = u^T d = d^T u = 2L \tag{2.5}$$

For a directed graph, the in-degree d_i^{in} and out-degree d_i^{out} of node i are defined as the number of links entering and leaving, respectively, node i. From the incidence matrix B, the number of "1" elements in row i equals d_i^{out}, while the number of "-1" elements in row i equals d_i^{in}. From an asymmetric adjacency matrix A (where $a_{ij} = 1$ only if there is link from node $i \longrightarrow j$, otherwise $a_{ij} = 0$), we find that

$$Au = d^{\text{out}} \text{ and } u^T A = \left(d^{\text{in}}\right)^T$$

If A is symmetric, then $u^T A = u^T A^T = (Au)^T$ and $d^{\text{out}} = d^{\text{in}} = d$.

4. *Laplacian matrix* Q. The relation between adjacency and incidence matrix is given by the *admittance* matrix or *Laplacian* Q,

$$Q = BB^T = \Delta - A \tag{2.6}$$

where $\Delta = \text{diag}(d_1, d_2, \ldots, d_N)$ is the degree matrix. Indeed, if $i \neq j$ and recalling that each column in the incidence matrix B has precisely two non-zero elements,

$$q_{ij} = \left(BB^T\right)_{ij} = \sum_{k=1}^{L} b_{ik} b_{jk} = \begin{cases} -1 & \text{if } (i,j) \text{ are linked} \\ 0 & \text{if } (i,j) \text{ are not linked} \end{cases}$$

[1] The random variable D of the degree in a graph G is equal to one of the possible realizations or outcomes $d_1, d_2, \ldots, d_N$ of the degrees in G.

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from which the "link decomposition" of the Laplacian, derived in (4.5), follows as

$$Q = \sum_{(i,j)\in\mathcal{L}} (e_i - e_j)\,(e_i - e_j)^T$$

If $i = j$, then $\sum_{k=1}^{L} b_{ik}^2 = d_i$ in (2.6) is the number of links that have node i in common. If self-loops are allowed in a graph, then the right-hand side of definition (2.6) shows that self-loops do not influence the Laplacian Q.

The basic property $u^T B = 0$ in (2.1) of the incidence matrix B leads in (2.6) to

$$Qu = 0$$

Consequently, each row sum $\sum_{j=1}^{N} q_{ij} = 0$, which shows that Q is singular, implying that $\det Q = 0$.

Since BB^T is symmetric, so is Q and A. Hence, although the incidence matrix B specifies the direction of links in the graph, (2.6) loses information about directions and A in (2.6) only reflects the existence of links between a pair of nodes, corresponding to an undirected graph. Consequently, if A is asymmetric and specifies, just like B, the direction of links in a directed graph, then (2.6) does not hold. Moreover, the asymmetric matrix $\Delta - A$ does not define an asymmetric Laplacian, because the row sum of $\Delta - A$ is not everywhere zero. By replacing the degree in Δ by the in-degree or out-degree, either the column sum or the row sum of $\Delta - A$ is zero, so that we may define two different asymmetric "Laplacian" matrices. The arguments illustrate that, generally, directed graphs possess less elegant properties[2] than undirected graphs and give rise to a more complicated analysis.

The Laplace matrix Q can be viewed as a discrete operator acting on a vector. The relation with its continuous counterpart, the Laplacian differential operator, is explained by Merris (1994) for a lattice graph.

5. *Matrices of weighted graphs.* Weighted graphs often appear in practice, where a link between node i and node j in the graph G is specified by one or more real numbers that reflect e.g. a delay, a monetary cost when using the link, the energy needed when traveling over that link, a performance loss, a geographic distance, a quality of service metric in telecommunication networks, like packet loss, jitter, etc.. We call any such real number, that specifies a link characteristic, a weight w_{ij} of the link between node i and j and the $N \times N$ weighted matrix W represents the weights between all pairs (i, j) of adjacent nodes. In most cases, analyses are limited

[2] Perhaps the major disadvantage of directed graphs is that the eigenvalues are not necessarily real (since **art.** 247 does not apply). Even worse, the asymmetric adjacency matrix A may not be diagonalizable and may possess a Jordan canonical form (**art.** 239).
From a physical point of view, flows in networks (**art.** 14) can propagate in either direction, depending on the driving force or potential difference; the incidence matrix B specifies the direction of the flow in the link, while the adjacency matrix $A = A^T$ determines the existence of a link. If the adjaceny matrix is asymmetric, then some links only allow propagation of flows in one direction and forbid the flow in the other direction. Physically, such an asymmetric situation requires non-linear elements (such as diodes in an electrical network or water tubes with directional shutters), which seriously complicate "linear" theory. Nevertheless, asymmetry naturally occurs in www-links, social relations and the Markov graph of a Markov process.

to one link weight, but multiple-parameter routing explained in Van Mieghem and Kuipers (2004) is an example where each entry in the matrix W is a vector, rather than a single real number. The *link weight structure*, the set of all link weights of graph G, is usually specified by a process or a function on the network, so that link weight w_{ij} may depend upon link weight w_{kl}. Since a process on a graph typically introduces directions, W is generally not a symmetric matrix.

We will denote graph matrices of a weighted graph by a tilde to distinguish them from graph matrices of the unweighted graph. For example, the element $\widetilde{a}_{ij}$ of the weighted adjacency matrix $\widetilde{A}$ represents the weight w_{ij} of a link between node i and j and $\widetilde{a}_{jj} = 0$ for all $1 \le j \le N$. Using the Hadamard[3] product $\circ$, the weighted adjacency matrix $\widetilde{A}$ equals $\widetilde{A} = W \circ A$, where $\widetilde{a}_{ij} = w_{ij} a_{ij}$ and a_{ij} is an element of the adjacency matrix A. Hence, the unweighted case can be regarded as a special case where the weighted matrix $W = J$ is the all-one matrix.

A particular class of weighted graphs are undirected weighted graphs, where the corresponding weighted adjacency matrix is symmetric, $\widetilde{A} = \widetilde{A}^T$. The weighted degree of node i is $\widetilde{d}_i = \sum_{j=1}^{N} \widetilde{a}_{ij}$, while the degree vector is $\widetilde{d} = \widetilde{A}u$. Similarly, the corresponding weighted Laplacian can be defined as $\widetilde{Q} = \mathrm{diag}\left(\widetilde{d}\right) - \widetilde{A} = \widetilde{\Delta} - \widetilde{A}$, thus $\widetilde{q}_{ij} = -\widetilde{a}_{ij}$ if $i \neq j$, else, $\widetilde{q}_{jj} = -\sum_{i=1;i\neq j}^{N} \widetilde{q}_{ji}$ and $\widetilde{Q} = \widetilde{Q}^T$.

6. *Walk, path and cycle.* A *walk* of length k from node i to node j is a succession of k links (arcs) or k hops of the form $(r_0 \to r_1)(r_1 \to r_2)\cdots(r_{k-1} \to r_k)$, where node label $r_0 = i$ and $r_k = j$. A *closed walk* of length k is a walk that starts in node $r_0 = i$ and returns, after k hops, to that same node $r_k = i$. A *path* is a walk in which all nodes are different, i.e. $r_l \neq r_m$ for all $0 \le l \neq m \le k$. A *cycle* of length k is a closed walk with different intermediate nodes, i.e. $r_l \neq r_m$ for all $0 \le l \neq m < k$. For an undirected walk, path or cycle, we replace the directed link $r_i \to r_j$ by the undirected link $r_i \sim r_j$. An Eulerian walk (circuit) is a closed walk containing each link of the graph G once, while a Hamiltonian cycle contains each node of G exactly once.

7. *A shortest path.* We consider only additive link weights such that the weight of a path $\mathcal{P}$ is $w(\mathcal{P}) = \sum_{l\in\mathcal{P}} w_l$, i.e., $w(P)$ equals the sum of the weights of the constituent links of the path $\mathcal{P}$. The shortest path $\mathcal{P}^*_{a\to b}$ from node a to node b is the path with minimal weight, thus, $w\left(\mathcal{P}^*_{a\to b}\right) \le w\left(\mathcal{P}_{a\to b}\right)$ for all paths $\mathcal{P}_{a\to b}$. The shortest path weight matrix S has elements $s_{ij} = w\left(\mathcal{P}^*_{i\to j}\right)$. If all link weights are equal to $w_{ij} = 1$ as in an unweighted graph, shortest paths are shortest hop paths and $w\left(P^*_{i\to j}\right) = h_{ij}$ is the hopcount, i.e. the length in hops or links of the shortest path between node i and node j, also called the *distance* between nodes i and j, or sometimes, the length of $\mathcal{P}^*_{i\to j}$. In weighted graphs, the hopcount h_{ij} is generally different from the weight $s_{ij} = w\left(\mathcal{P}^*_{ij}\right)$ of a shortest path.

In man-made infrastructures, two major types of transport exist: either a packet

[3] The Hadamard product (Horn and Johnson, 1991) is the entrywise product of two matrices: $(A \circ B)_{ij} = A_{ij} B_{ij}$. If A and B are both diagonal matrices, then $A.B = A \circ B$.

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(e.g. car, parcel, IP-packet, container) or a flow (e.g. electric current, water, gas). Transport is either flow-based or path-based. Packets follow a single path from source to destination, whereas a flow spreads over all possible paths. Generally, packets in a weighted network follow shortest paths. The flow analogon of the shortest path weight matrix S is the effective resistance matrix Ω in Chapter 5.

There exist many routing algorithms to compute shortest paths in networks. The most important of these routing algorithms are explained, for example, in Van Mieghem (2010) and Cormen *et al.* (1991).

8. *Graph matrices and distance matrices.* Many other graph-related matrices, in short graph matrices, can be defined and we mention only a few. The effective resistance matrix Ω is studied in Chapter 5. The modularity matrix M is defined and discussed in **art.** 151. The probability transfer matrix $P = \Delta^{-1}A$ of a random walk on a graph is a stochastic matrix, because all elements of P lie in the interval $[0, 1]$ and each row sum is 1. Graph matrices can be scaled or normalized, e.g., normalized Laplacians are $\Delta^{-1}Q$ or $\Delta^{-\frac{1}{2}}Q\Delta^{-\frac{1}{2}}$.

A *distance matrix* D is a non-negative matrix, where element d_{ij} specifies a distance measure between node i and j in a graph. For example, if the distance measure is equal to the hopcount h_{ij}, then $h_{ii} = 0$. Thus, distance matrices possess a zero diagonal and contain the distances between each pair (i, j) of nodes in a graph. Any element of a distance matrix obeys the triangle inequality (**art.** 201): $0 \leq d_{ij} \leq d_{il} + d_{lj}$. The spectrum of distance matrices is reviewed by Aouchiche and Hansen (2014). Both H, S and Ω are distance matrices.

The hopcount matrix H of the directed graph in Fig. 2.1,

$$H = \begin{bmatrix} 0 & 1 & 1 & 2 & 3 & 2 \\ 2 & 0 & 1 & 2 & 2 & 1 \\ \times & \times & 0 & 1 & \times & \times \\ \times & \times & \times & 0 & \times & \times \\ 3 & 1 & 2 & 1 & 0 & 2 \\ 1 & 2 & 2 & 2 & 1 & 0 \end{bmatrix}$$

illustrates asymmetry in directed graphs as well as the possibility of the non-existence, marked by $\times$ in the above matrix, of a path between two nodes, although the graph is connected. For these reasons, we usually confine to undirected, connected graphs. Since $h_{ij} = h_{ji}$ in an undirected, connected graph, the corresponding distance matrix H is symmetric, with positive integer off-diagonal elements and with zero elements on the diagonal.

2.2 The incidence matrix B

The $N \times L$ incidence matrix B in **art.** 2 transforms an $L \times 1$ vector y of the "link"-space to an $N \times 1$ vector x of the "nodal" space by $x = By$. Physically, this transformation is best understood when y is a flow or current vector through links

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in a network, while x is the externally injected current in nodes of the graph G as discussed in **art**. 14 below. We first concentrate on mathematical properties of the incidence matrix B.

9. *Rank of the incidence matrix B.*

Theorem 1 *If the graph G is connected, then rank$(B) = N - 1$.*

Proof: The basic property $u^T B = 0$ in (2.1) implies that $\text{rank}(B) \leq N - 1$. Suppose that there exists a non-zero vector $x \neq \alpha u$ for any real number α such that $x^T B = 0$. Under that assumption, the vector u and x are independent and the kernel (or zero space of B) consisting of all vectors v such that $v^T B = 0$ has at least rank 2, and consequently $\text{rank}(B) \leq N - 2$. We will show that x is not independent, but proportional to u. Consider row j in B corresponding to the non-zero component x_j. All non-zero elements in the row vector $(B)_j$ are links incident to node j. Since each column of B only consists of two elements (with opposite signs), for each link l incident to node j, there is precisely one other row k in B with a non-zero element in column l. In order for the linear relation $x^T B = 0$ to hold, we thus conclude that $x_j = x_k$, and this observation holds for all nodal indices j and k because G is connected. This implies that $x^T B = \alpha u^T B$, which shows that the rank of the incidence matrix cannot be lower than $N - 1$. □

An immediate consequence is that $\text{rank}(B) = N - k$ if the graph has k disjoint but connected components, because then (see also **art.** 116) there exists a relabeling of the nodes such that B can be partitioned as

$$B = \begin{bmatrix} B_1 & O & \dots & O \\ O & B_2 & & \vdots \\ \vdots & & \ddots & \\ O & & \dots & B_k \end{bmatrix}$$

10. *The cycle-space and cut-space of a graph G.* The cycle-space of a graph G consists of all possible cycles in that graph. A cycle (**art**. 6) can have two cycle orientations. This means that the orientation of links in a cycle either coincides with the cycle orientation or that it is the reverse of the cycle orientation. For example, the cycle $(1-2)\,(2-6)\,(6-1)$ in Fig. 2.1 corresponds to the links (columns in B) $1, 6$ and 3 and all links are oriented in the same direction along the cycle. When adding columns $1, 3$ and 6, the sum is zero, which is equivalent to $By = 0$ with $y = (1, 0, 1, 0, 0, 1, 0, 0, 0)$. On the other hand, the triplet $(1-2)\,(2-3)\,(3-1)$, corresponding to the links $1, 4$ and 2, is not a cycle, because not all links are oriented in the same direction such that $y = (1, -1, 0, 1, 0, 0, 0, 0, 0)$ has now negative sign components.

In general, if $By = 0$, then the non-zero components of the vector y are links of a cycle. Indeed, consider the j-th row $(By)_j = x_j$. If node j is not incident with

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links of the cycle, then $x_j = 0$. If node j is incident with some links of the cycle, then it is incident with precisely two links, with opposite sign such that x_j is again zero.

Since the rank of B is $N - k$, where k is the number of connected components, the rank of the kernel (or null space) of B is $L - N + k$. Hence, the dimension of the cycle-space of a graph equals the rank of the kernel of B, which is $L - N + k$. The orthogonal complement of the cycle-space is called the cut-space, with dimension $N - k$. Thus, the cut-space is the space consisting of all vectors y for which $By = x \neq 0$. Since $u^T x = 0$ by (2.1), the non-negative components of x are the nodes belonging to one partition and the negative components define the other partition. These two disjoint sets of nodes thus define a cut in the graph, a set of links whose removal separates the graph G in two disjoint subgraphs. For example in Fig. 2.1, $By = \begin{bmatrix} 1 & 0 & -1 & -2 & 1 & 1 \end{bmatrix}$ defines a cut that separates nodes 3 and 4 from the rest. Section 4.4 further investigates the partitioning of a graph.

11. *Cycles and cuts in a connected graph G.* A spanning tree T in the graph G is a connected subgraph of G that contains all N nodes of G. Any tree on N nodes has $N - 1$ links, whose set is denoted by $\mathcal{T} \subset \mathcal{L}$, and a tree does not contain a cycle.

The definition of a spanning tree $\mathcal{T}$ of the graph G leads to an interesting property: If a link $l \in \mathcal{L}$, but $l \notin \mathcal{T}$, is added to the spanning tree T, then there is a unique cycle in the graph $\mathcal{T} \cup \{l\}$. Indeed, let l be a link between node i and j. Since l does not belong to the spanning tree T, the nodes i and j are not directly connected, but there is a path from node i to node j in spanning tree T, because T is connected. The addition of l to T results in two different paths from node i to node j. By the definition of a cycle, the graph $\mathcal{T} \cup \{l\}$ contains one cycle $cyc\,(T, l)$, which is unique by construction and to which we can associate a vector y_l obeying $By_l = 0$ by **art**. 10. The length of that cycle contains at most N links, because the longest shortest path in the spanning tree has at most $N - 1$ links.

The companion property is: if a link $h \in \mathcal{T}$ (clearly, $h \in \mathcal{L}$) is removed, then there is a unique cut $cut\,(T, h)$, that contains link h and links $e \in \mathcal{L}$, but $e \notin \mathcal{T}$. Similarly, we can associate a vector y_h to the cut $cut\,(T, h)$ that obeys $By_h \neq 0$.

Since there are $L - N + 1$ links of G that do not belong to the spanning tree T, we can construct $L - N + 1$ cycles and the set of cycles $\{cyc\,(T, l)\}_{l \in \mathcal{L} \setminus \mathcal{T}}$ forms an independent set, because a link l belongs to a cycle $cyc\,(T, l)$, but not to another cycle $cyc\,(T, g)$ for $g \neq l$. Moreover, $L - N + 1$ is the dimension of the cycle-space of G (**art.** 10) and the set of vectors y_l, obeying $By_l = 0$, for $l \in \mathcal{L} \setminus \mathcal{T}$ represents a basis for the cycle-subspace of G. Analogously, the set of cuts $\{cut\,(T, h)\}_{h \in \mathcal{T}}$ with associated set of vectors y_h, obeying $By_h \neq 0$, for $h \in \mathcal{T}$ represents a basis for the cut-subspace of G.

12. *Spanning trees and the incidence matrix B.* Consider the incidence matrix B of a graph G and remove an arbitrary row in B, corresponding to a node n. Let M_n be one of the $\binom{L}{N-1}$ square $(N-1) \times (N-1)$ submatrices of B without row n and let G_n denote the subgraph of G on $N - 1$ nodes formed by the links in

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the columns of M_n. Since there are $N-1$ columns in M_n, the subgraph G_n has precisely $N-1$ links, where some links may start or end at node n, outside the node set of G_n. We will now investigate $\det M_n$.

(a) Suppose first that there is no node with degree 1 in G, except possibly for n, in which case G_n is not a tree spanning $N-1$ nodes. Since the number of links is $L(G_n) = N-1$, the basic law of the degree (2.3) shows that there must be a zero degree node in G_n. If the zero degree node is not n, then G_n has a zero row and $\det M_n = 0$. If n is the zero degree node, then each column of M_n contains a 1 and -1. Thus, each row sum of M_n is zero and $\det M_n = 0$.

(b) In the other case, G_n has a node i with degree 1. Then, the i-th row in G_n only has one non-zero element, either 1 or -1. After expanding $\det M_n$ by this i-th row, we obtain a new $(N-2)\times(N-2)$ determinant $M_{n;i}$ corresponding to the graph $G_{n:i}$, formed by the links in the columns of $M_{n;i}$. For $\det M_{n;i}$, we can repeat the analysis: either $G_{n:i}$ is not a tree spanning the $N-2$ nodes of G except for nodes n and i, in which case $\det M_{n;i} = 0$ or $\det M_{n;i} = \pm \det M_{n;i;k}$.

Iterating this process shows that the determinant of any square submatrix M of B is either 0, when the corresponding graph formed by the links, corresponding to the columns in M is not a spanning tree, or ± 1, when that corresponding graph is a spanning tree. Thus, we have shown:

Theorem 2 (Poincaré) *The determinant of any square submatrix of the incidence matrix B is either 0, 1, or -1.*

If the determinant of any square submatrix of a matrix is 0, 1, or -1, then that matrix is said to be *totally unimodular*. Hence, the incidence matrix B is totally unimodular.

13. *The matrix C representing cycles in G.* **Art.** 11 suggests to write the incidence matrix B of the graph G as

$$B = \begin{bmatrix} B_T & B_{G\backslash T} \\ & b_N \end{bmatrix} \tag{2.7}$$

where the $(N-1)\times(N-1)$ square matrix B_T has as columns the (partial[4]) links of the spanning tree T of G, the $(N-1)\times(L-N+1)$ matrix $B_{G\backslash T}$ contains the remaining links of G not belonging to T and the $1\times L$ vector b_N is linearly dependent on the $N-1$ first rows of B, because $\mathrm{rank}(B) = N-1$ by Theorem 1. The $L\times(L-N+1)$ cycle matrix C, in which a column represents a cycle of G, is defined by

$$C = \begin{bmatrix} C_T \\ I_{L-N+1} \end{bmatrix}$$

where the $(N-1)\times(L-N+1)$ matrix C_T contains elements of the vectors y_l, obeying $By_l = 0$, for $l \in \mathcal{L}\backslash\mathcal{T}$. The basic property $By_l = 0$ of a cycle y_l translates to

[4] The row N, corresponding to node N, is not included in B_T and links to or from node N in the columns of B_T only contain a 1 or -1.

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the matrix equation $BC = 0$, from which $B_T C_T + B_{G\setminus T} = 0$. **Art.** 12 demonstrates that $\det B_T = \pm 1$, implying that the inverse of B_T exists, thus

$$C_T = -B_T^{-1} B_{G\setminus T} \tag{2.8}$$

Analogously for the cut-subspace of G, the $L \times (N-1)$ matrix F whose columns contain the $N-1$ vectors y_h, obeying $By_h \neq 0$, for $h \in \mathcal{T}$,

$$F = \begin{bmatrix} I_{N-1} \\ F_T \end{bmatrix}$$

Since each column of F belongs to the orthogonal complement of the cycle-subspace of G, it holds that $C^T F = 0$, from which $C_T^T + F_T = 0$ and, with (2.8),

$$F_T = -C_T^T = \left(B_T^{-1} B_{G\setminus T}\right)^T \tag{2.9}$$

In summary, the basic cycle matrix C_T in (2.8) and the basic cut matrix F_T in (2.9) can be expressed in terms of the incidence matrix B for each spanning tree T in G. The idea to concentrate on a spanning tree T of G originates from Kirchhoff (1847), who found the solution of the current-voltage relations in a resistor network in terms of T.

14. *Electrical resistor network.* The importance of the incidence matrix B and the Laplacian matrix Q of a graph G is nicely illustrated by the current-voltage relations in a resistor network. The flows of currents in a network, steered by forces created by potential differences between nodes, is an example of a linear process, where the dynamic process is proportional to the network's graph. Other examples of processes, that are "linear" in the graph, are water (or fluid or gas) networks, where water flows through pipes and the potential of a node corresponds with its height, heat diffusion in a network, where the nodal potential is its temperature, and mechanical networks where springs connect nodes and nodal displacements are related to potentials.

The $L \times 1$ flow vector y possesses a component $y_l = y_{ij} = -y_{ji}$, which denotes the electrical current flowing through the link $l = i \sim j$ from node i to node j. Kirchhoff's current law

$$x = By \tag{2.10}$$

is a conservation law. The j-th row in (2.10), $x_j = (By)_j = \sum_{k=1}^{L} B_{jk} y_k$, states that, at each node j in the network G, the current x_j leaving ($x_j \leq 0$) or entering ($x_j \geq 0$) must equal the sum of currents over links incident to j. If current $x_j \geq 0$ is injected at node j, the flow conservation at node j is also written as

$$x_j = \sum_{i \in \text{ neighbors}(j)} y_{ji} = \sum_{i=1}^{N} a_{ij} y_{ji} \tag{2.11}$$

Thus, if no current ($x_j = 0$) is injected nor leaving the node j, then the net current flow, the sum of the flows over links incident at node j, is zero. If $By = 0$, then

art. 10 shows that the non-zero components of y form a cycle. Left-multiplying both sides of $x = By$ in Kirchhoff's current law (2.10) by u^T and using (2.1) yields $u^T x = 0$, which means that the net flow, influx plus outflow, in the network is zero. Thus, $By = x$ reflects a *conservation law*: the demand x_j offered at node j in the network is balanced by the sum of currents or flows at node j and the net demand of influx and outflow to the network is zero.

Each link $l = i \sim j$ between node i and node j contains a resistor with resistance $r_l = r_{ij}$. A flow y_{ij} is said to be physical if there is an associated potential function v on the nodes of the network such that

$$v_i - v_j = r_{ij} y_{ij} \tag{2.12}$$

In electrical networks, the potential function is called the "voltage", whereas in hydraulic networks, it is called the "pressure". The relation (2.12), known as the law of Ohm, reflects that the potential difference $v_i - v_j$ generates a force that drives the current y_{ij} from node i to node j (if $v_i - v_j > 0$, else in the opposite direction) and that the potential difference is proportional to the current y_{ij}. The proportionality constant equals the resistance[5] $r_{ij} > 0$ between node i and j. For other electrical network elements such as capacitors and inductances, the relations between potential and current are more complicated than Ohm's law (2.12) and can be derived from the laws of Maxwell (see e.g. Feynman *et al.* (1963)). We rewrite Ohm's law (2.12) in terms of the current $y_{ij} = \frac{1}{r_{ij}}(v_i - v_j)$ flowing through the link $l = (i, j)$, which becomes in matrix form

$$y_{L\times 1} = \operatorname{diag}\left(\frac{1}{r_{ij}}\right)_{L\times L} \left(B^T\right)_{L\times N} v_{N\times 1} \tag{2.13}$$

where the $N \times 1$ vector v contains as elements the voltage v_j at each node j in G and $\operatorname{diag}\left(\frac{1}{r_{ij}}\right)$ has diagonal elements $\left(\frac{1}{r_1}, \ldots, \frac{1}{r_l}, \ldots, \frac{1}{r_L}\right)$ where $r_l = r_{ij}$ is the resistance of link $l = (i, j)$. Substituting Ohm's law (2.13) into Kirchhoff's conservation law (2.10) yields

$$x = B\operatorname{diag}\left(\frac{1}{r_{ij}}\right) B^T v$$

Similar to the unweighted Laplacian decomposition $Q = BB^T$ in (2.6), we define the $N \times N$ weighted, symmetric Laplacian matrix[6]

$$\widetilde{Q} = B\operatorname{diag}\left(\frac{1}{r_{ij}}\right) B^T \tag{2.14}$$

[5] If $r_{ij} = 0$, then the potential v_i of node i and v_j of node j are the same by Ohm's law (2.12). From an electrical point of view, both nodes cannot be differentiated and we can merge node i and j in the graph to one node. Therefore, we further assume that $r_{ij} > 0$ in the graph G.

[6] Since $r_{ij} > 0$, we can write $\widetilde{Q} = B\operatorname{diag}\left(\frac{1}{r_{ij}}\right) B^T = B\operatorname{diag}\left(\frac{1}{\sqrt{r_{ij}}}\right)\left(B\operatorname{diag}\left(\frac{1}{\sqrt{r_{ij}}}\right)\right)^T$ and may consider the $N \times L$ matrix $\widetilde{B} = B\operatorname{diag}\left(\frac{1}{\sqrt{r_{ij}}}\right)$ as a "weighted incidence" matrix and the unit of the element $\widetilde{B}_{ij}$ is $\frac{1}{\sqrt{\text{Ohm}}}$. The law of Ohm in (2.13) transforms to $y = \operatorname{diag}\left(\frac{1}{\sqrt{r_{ij}}}\right) \widetilde{B}^T v$, so that $\widetilde{B}$ apparently lacks a physical interpretation.

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The weighted Laplacian $\widetilde{Q}$ also generalizes the definition (2.6) of the Laplacian $Q = \Delta - A$ to $\widetilde{Q} = \widetilde{\Delta} - \widetilde{A}$, where the $N \times N$ weighted, symmetric adjacency matrix $\widetilde{A}$ with elements $\widetilde{a}_{ij} = \frac{a_{ij}}{r_{ij}}$ possesses a corresponding weighted degree diagonal matrix $\widetilde{\Delta} = \mathrm{diag}\left(\widetilde{d}_1, \widetilde{d}_2, \ldots, \widetilde{d}_N\right)$ with $\widetilde{d}_j = \left(\widetilde{A}u\right)_j$ introduced in **art.** 8. Alternatively, substitution of Ohm's law $y_{ji} = \frac{1}{r_{ij}}(v_j - v_i)$ into the nodal conservation law (2.11) for node j yields

$$x_j = \sum_{i=1}^{N} \frac{a_{ij}}{r_{ij}}(v_j - v_i) = v_j \sum_{i=1}^{N} \frac{a_{ij}}{r_{ij}} - \sum_{i=1}^{N} \frac{a_{ij}}{r_{ij}} v_i = v_j \sum_{i=1}^{N} \widetilde{a}_{ij} - \sum_{i=1}^{N} \widetilde{a}_{ij} v_i$$

which is, in matrix form, $x = \left(\widetilde{\Delta} - \widetilde{A}\right) v = \widetilde{Q}v$, where the weighted degree is $\widetilde{d}_j = \sum_{j=1}^{N} \widetilde{a}_{ij}$. While link $l = i \sim j$ contains a resistor with resistance $r_l = r_{ij}$, the link weight is $w_l = w_{ij} = \frac{1}{r_l}$.

In summary, we arrive at the fundamental relation between the $N \times 1$ injected current flow vector x into nodes of the network and the $N \times 1$ voltage vector v at the nodes

$$x = \widetilde{Q}v \tag{2.15}$$

Clearly, if all resistances equal $r_{ij} = 1$ Ohm, then the unweighted case with the standard matrices A, B and Q is retrieved. Most properties transfer to the weighted graph related matrices: the weighted Laplacian $\widetilde{Q} = B\mathrm{diag}\left(\frac{1}{r_{ij}}\right) B^T = \widetilde{B}\widetilde{B}^T$ is positive semidefinite (as follows from **art.** 101) and the conservation of total injected flows $u^T x = u^T \widetilde{Q} v = 0$, due to the basic property (2.1) of the incidence matrix B. The power, the energy per unit time (in watts), dissipated in a resistor network is the sum of power dissipated in each resistor, which equals $\mathcal{P} = v^T x$. The fundamental relation (2.15) leads to the quadratic form $\mathcal{P} = v^T \widetilde{Q} v = \sum_{l \in \mathcal{L}} \left(\frac{v_{l+} - v_{l-}}{\sqrt{r_l}}\right)^2$, which will allow us in **art.** 103 to relate the power $\mathcal{P}$ to eigenvalues of the weighted Laplacian $\widetilde{Q}$.

15. *Harmonic functions.* The continuous description of $x = \widetilde{Q}v$ in (2.15) is the Poisson equation $\nabla^2 \phi(r) = -\frac{\rho(r)}{\epsilon_0}$, where the potential $\phi(r)$ is a continuous function of the position $r = (r_1, r_2, \ldots, r_m)$ of a point in an m-dimensional space, the Laplace operator is $\nabla^2 = \frac{\partial^2}{\partial r_1^2} + \frac{\partial^2}{\partial r_2^2} + \cdots + \frac{\partial^2}{\partial r_m^2}$, the charge density $\rho(r)$ specifies the location of electrical charges and the permittivity constant ϵ_0 balances the physical units at the left- and right-hand side. The Poisson equation is related to Gauss's divergence law of the electrical field, that appears as the first Maxwell equation (see, e.g., Feynman *et al.* (1963), Morse and Feshbach (1978)). If the potential $\phi(r)$ is defined at some boundary or surface S that encloses a volume without charges inside, then $\nabla^2 \phi(r) = 0$ for $r \notin S$ and the solution $\phi(r)$ of the Laplace differential equation is called a harmonic function. Harmonic functions possess many nice properties and are the fundamental corner stone, via the Riemann-Cauchy equations, of analytic functions in the complex plane (Titchmarsh, 1964). In the discrete setting, the

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Laplace operator ∇^2 in a continuous space is replaced by a Laplacian matrix $\widetilde{Q}$ on a graph and this powerful association results in more properties of and deeper insight in the Laplacian than the adjacency matrix.

If the current x is injected in some nodes $\mathcal{S} \subset \mathcal{N}$, equivalent with the boundary S, while $x_j = 0$ if $j \notin \mathcal{S}$, then $\left(\widetilde{Q}v\right)_j = 0$ and $v_j = \frac{1}{\widetilde{d}_j} \sum_{i=1}^{N} \widetilde{a}_{ij} v_i$ is a weighted average of the potential of its direct neighbors. The voltage vector v in $x = \widetilde{Q}v$ is called a harmonic at node j if $\left(\widetilde{Q}v\right)_j = 0$. Similar to the continuous setting, known as Dirichlet's boundary problem, Doyle and Snell (1984) prove that a harmonic function $v(j)$, defined on the nodes $j \in \mathcal{N}$ of the graph, achieves its maximum and minimum value at the boundary $\mathcal{S}$. This important property of harmonic functions follows physically from the voltages as potentials in electrical networks (see also Section 5.3.2).

If $x = 0$, then (2.15) indicates that $\widetilde{Q}v = 0$, which is an eigenvalue equation. If the graph G is connected (see **art.** 116), the (weighted) Laplacian has one zero eigenvalue belonging to eigenvector proportional to the all-one vector u, so that the potential or voltage vector $v = \alpha u$, for a non-zero real α. The law of Ohm (2.13) and the basic property (2.1) of the incidence matrix B then show that $y = 0$, thus all currents are zero. Another consequence of the basic property (2.1) of the incidence matrix B is that $\det \widetilde{Q} = 0$ and that the general relation (2.15) *cannot* be directly inverted as $v = \widetilde{Q}^{-1}x$. In Section 4.2, the inversion problem is analyzed and a general method based on the pseudoinverse $\widetilde{Q}^{\dagger}$ of the Laplacian matrix $\widetilde{Q}$ is presented.

16. *Electrical resistor network revisited.* Kirchhoff (1847) considered a variant of the setting in **art.** 14, where the external current vector x is replaced by an external voltage difference vector δv_{ext} over links of G. The law of Ohm in (2.13) becomes $\delta v = \text{diag}(r_{ij})\, y + \delta v_{\text{ext}}$, where the link potential difference vector is $\delta v = B^T v$. If $By = 0$, then **art.** 10 shows that the non-zero components of y form a cycle. Kirchhoff (1847) demonstrated[7] that $C^T \delta v = 0$: the sum of the voltage differences over a cycle is zero, which is Kirchhoff's voltage law.

Considering a spanning tree T as explained in **art.** 10 and 13, we write the link current vector y and potential difference vector δv as

$$y = \begin{bmatrix} y_T \\ y_{G\setminus T} \end{bmatrix} \quad \text{and} \quad \delta v = \begin{bmatrix} \delta v_T \\ \delta v_{G\setminus T} \end{bmatrix}$$

Since there are no external currents, i.e. $x = 0$ and $By = 0$, the link current vector y with (2.7) obeys

$$\begin{bmatrix} B_T & B_{G\setminus T} \\ & b_N \end{bmatrix} \begin{bmatrix} y_T \\ y_{G\setminus T} \end{bmatrix} = B_T y_T + B_{G\setminus T} y_{G\setminus T} = 0$$

[7] More generally, if the magnetic field is time-invariant (see, e.g., Feynman *et al.* (1963)), the Maxwell equation $\nabla \times \overrightarrow{E} = 0$, where $\overrightarrow{E}$ is the electric field vector, and Stokes' theorem then state that $\oint \overrightarrow{E} \overrightarrow{ds} = 0$, implying that any closed contour over the electric field is zero.

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and, invoking (2.8),

$$y_T = -B_T^{-1} B_{G\setminus T} y_{G\setminus T} = C_T y_{G\setminus T}$$

Thus,

$$y = \begin{bmatrix} y_T \\ y_{G\setminus T} \end{bmatrix} = \begin{bmatrix} C_T \\ I_{L-N+1} \end{bmatrix} y_{G\setminus T} = C y_{G\setminus T}$$

illustrating that the whole current vector only depends on those current vector components, associated with links that are not in the spanning tree T. Similar, $C^T \delta v = 0$ leads to $C^T \mathrm{diag}(r_{ij})\, y = -C^T \delta v_{\mathrm{ext}}$. Substituting $y = C y_{G\setminus T}$ then yields

$$\left(C^T \mathrm{diag}\,(r_{ij})\, C\right) y_{G\setminus T} = -C^T \left(\delta v\right)_{\mathrm{ext}}$$

Finally, the $(L-N+1)\times(L-N+1)$ matrix $C^T \mathrm{diag}(r_{ij})\, C$ has rank $L-N+1$ and is invertible,

$$y_{G\setminus T} = -\left(C^T \mathrm{diag}\,(r_{ij})\, C\right)^{-1} C^T \delta v_{\mathrm{ext}}$$

which is Kirchhoff's solution. In fact, Kirchhoff (1847) evaluates the solution further in terms of all spanning trees, reviewed without proof by Schnakenberg (1976). Section 5.6 expresses the effective resistance in terms of spanning trees.

2.3 Connectivity, walks and paths

17. *Connectivity of a graph.* A graph G is connected if there exists a walk (**art**. 6) between each pair of nodes in G.

Theorem 3 *If a graph G is disconnected, then its complement G^c is connected.*

Proof: Since a graph G is disconnected, G possesses at least two connected components G_1 and G_2. There are two situations: (a) If node $i \in G_1$ and node $j \in G_2$, then no link in G connects them. By the definition of the complement of a graph (**art.** 1), there will be a link $i \sim j$ in G^c. (b) If node i and j are in the same connected component in G, then consider any node m in a different connected component. The argument in situation (a) shows that the link $i \sim m$ and the link $j \sim m$ exist in G^c. Consequently, i and j are connected by the path $P = i \sim m \sim j$. Combining the two possible situations demonstrates that any two nodes are reachable in G^c, implying that the graph G^c is connected. □

The converse of Theorem 3, "If G is connected, then its complement G^c is disconnected" is not always true. For example, if G is a tree (except for the star $K_{1,N-1}$), then G^c is connected. Section 4.1.1 gives additional properties of a graph's connectivity.

18. *The number of k-hops walks.* **Art**. 6 has defined a walk. Due to its importance, Lemma 1 is proved in two ways.

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Lemma 1 *The number of walks of length k from node i to node j is equal to the element $\left(A^k\right)_{ij}$.*

Proof by induction: For $k = 1$, the number of walks of length 1 between node i and node j equals the number of direct links between i and j, which is by definition the element a_{ij} in the adjacency matrix A. Suppose the lemma holds for $k-1$. A walk of length k consists of a walk of length $k-1$ from i to some node r which is adjacent to j. By the induction hypothesis, the number of walks of length $k-1$ from i to r is $\left(A^{k-1}\right)_{ir}$ and the number of walks with length 1 from r to j equals a_{rj}. The total number of walks from i to j with length k then equals $\sum_{r=1}^{N}\left(A^{k-1}\right)_{ir} a_{rj} = \left(A^k\right)_{ij}$ (by the rules of matrix multiplication). □

Proof by direct computation: After q iterations in k of the matrix multiplication rule $\left(M^k\right)_{ij} = \sum_{r_{k-1}=1}^{N}\left(M^{k-1}\right)_{ir_{k-1}} m_{r_{k-1}j}$ for any matrix M, we obtain

$$\left(M^k\right)_{ij} = \sum_{r_{k-1}=1}^{N}\sum_{r_{k-2}=1}^{N}\cdots\sum_{r_{k-q}=1}^{N}\left(M^{k-q}\right)_{ir_{k-q}} m_{r_{k-q}r_{k-(q-1)}}\cdots m_{r_{k-2}r_{k-1}} m_{r_{k-1}j}$$

When $q = k-1$, then $\left(M^{k-q}\right)_{ir_{k-q}} = m_{ir_1}$ and it holds for any matrix M that

$$\left(M^k\right)_{ij} = \sum_{r_1=1}^{N}\sum_{r_2=1}^{N}\cdots\sum_{r_{k-1}=1}^{N} m_{ir_1} m_{r_1r_2}\cdots m_{r_{k-2}r_{k-1}} m_{r_{k-1}j}$$

and applied to the adjacency matrix A,

$$\left(A^k\right)_{ij} = \sum_{r_1=1}^{N}\sum_{r_2=1}^{N}\cdots\sum_{r_{k-1}=1}^{N} a_{ir_1} a_{r_1r_2}\cdots a_{r_{k-2}r_{k-1}} a_{r_{k-1}j} \tag{2.16}$$

With the convention $r_0 = i$ and $r_k = j$, (2.16) can be written as

$$\left(A^k\right)_{ij} = \sum_{r_1=1}^{N}\sum_{r_2=1}^{N}\cdots\sum_{r_{k-1}=1}^{N}\prod_{l=0}^{k-1} a_{r_lr_{l+1}} \tag{2.17}$$

where the indicator function $\prod_{l=0}^{k-1} a_{r_lr_{l+1}} = a_{ir_1}a_{r_1r_2}\cdots a_{r_{k-2}r_{k-1}}a_{r_{k-1}j}$ is one if and only if all links in the walk $(i = r_0 \to r_1)(r_2 \to r_3)\cdots(r_{k-1} \to r_k = j)$ exist (i.e. $a_{r_lr_{l+1}} = 1$ for all values of l in $[0, k-1]$), otherwise it is zero. The $(k-1)$-fold multiple summation in the explicit expressions (2.16) and (2.17) ranges over all possible, directed walks $(i = r_0 \to r_1)(r_2 \to r_3)\cdots(r_{k-1} \to r_k = j)$ with k hops (**art**. 6) between node i and j and enumerates, out of all possible walks, the existing walks in the graph, reflected by $\prod_{l=0}^{k-1} a_{r_lr_{l+1}} = 1$. □

The maximum possible number of walks with k hops between two nodes in a graph with N nodes is attained in the complete graph K_N, whose adjacency matrix is $A_{K_N} = J - I$, and equals $(J-I)^k_{ij}$. Invoking Newton's binomium, which is

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allowed because J and I commute, we have

$$(J-I)^k = \sum_{m=0}^{k} \binom{k}{m} J^m (-I)^{k-m}$$

Since $J^m = N^{m-1}J$ for $m > 0$, then $(J-I)^k = (-1)^k I + \sum_{m=1}^{k} \binom{k}{m} N^{m-1}(-1)^{k-m} J$. The binomium gives $(J-I)^k = (-1)^k I + \frac{1}{N}\left((N-1)^k - (-1)^k\right) J$, from which the maximum possible number of walks with k hops between node i and node j in any graph follows as

$$(J-I)^k_{ij} = \begin{cases} \frac{1}{N}\left((N-1)^k - (-1)^k\right) & \text{for } i \neq j \\ \frac{1}{N}\left((N-1)^k - (-1)^k\right) + (-1)^k & \text{for } i = j \end{cases} \tag{2.18}$$

19. *Lower bounds for* $\left(A^k\right)_{ij}$. For any integer $0 \leq n \leq k$, the matrix multiplication form

$$\left(A^k\right)_{ij} = \sum_{q=1}^{N} \left(A^{k-n}\right)_{iq} \left(A^n\right)_{qj} \tag{2.19}$$

reduces, for $n = 1$ and taking into account the absence of self-loops, i.e. $a_{jj} = 0$, to

$$\left(A^k\right)_{jj} = \sum_{q=1;q\neq j}^{N} \left(A^{k-1}\right)_{jq} a_{qj}$$

illustrating for each node j that $\left(A^k\right)_{jj}$ does not depend on $\left(A^{k-1}\right)_{jj}$. For $n = 2$, symmetry in the adjacency matrix, $A = A^T$, yields

$$\left(A^2\right)_{jj} = \sum_{k=1}^{N} a_{jk}a_{kj} = \sum_{k=1}^{N} a_{jk}^2 = \sum_{k=1}^{N} a_{jk} = d_j \tag{2.20}$$

The off-diagonal element $\left(A^2\right)_{ij} = \sum_{k=1}^{N} a_{ik}a_{jk}$ counts the number of nodes k that have a link to both node i and j; i.e. the number of joint neighbors of node i and node j, so that $0 \leq \left(A^2\right)_{ij} \leq \min(d_i, d_j)$. Hence, $\left(A^2\right)_{ij}$ obeys both (A.185) and (A.186) in **art.** 279, because of the basic inequality between the arithmetic and geometric mean of two non-negative real numbers x and y: $\min(x,y) \leq \sqrt{xy} \leq \frac{x+y}{2}$. For $n = 2$ and $k > 2$ in (2.19), we find

$$\begin{array}{ll} \left(A^k\right)_{ij} = \left(A^{k-2}\right)_{ii}\left(A^2\right)_{ij} + \left(A^{k-2}\right)_{ij} d_j + \sum_{q=1;q\neq\{i,j\}}^{N} \left(A^{k-2}\right)_{iq}\left(A^2\right)_{qj} & \text{for } i \neq j \\ \left(A^k\right)_{jj} = \left(A^{k-2}\right)_{jj} d_j + \sum_{q=1;q\neq j}^{N} \left(A^{k-2}\right)_{jq}\left(A^2\right)_{qj} & \text{for } i = j \end{array}$$

The last equation leads to the recursion inequality $\left(A^k\right)_{jj} \geq \left(A^{k-2}\right)_{jj} d_j$ for $k \geq 2$, that, after iteration, results for even $k = 2m$ into

$$\left(A^{2m}\right)_{jj} \geq d_j^m \tag{2.21}$$

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but, for odd $k = 2m + 1$, we can only deduce $\left(A^{2m+1}\right)_{jj} \geq 0$ and equality can occur, e.g. in the path graph, studied in Section 6.4. Similarly, the first equation for $i \neq j$ when $n = 2$ leads, for $k \geq 2$, to the recursion inequality

$$\left(A^k\right)_{ij} \geq \left(A^{k-2}\right)_{ii} \left(A^2\right)_{ij} + d_j \left(A^{k-2}\right)_{ij}$$

After p iterations, we have

$$\left(A^k\right)_{ij} \geq \left(A^2\right)_{ij} \left\{ \sum_{q=0}^{p} \left(A^{k-2(q+1)}\right)_{ii} d_j^q \right\} + d_j^{p+1} \left(A^{k-2(p+1)}\right)_{ij}$$

For odd $k = 2m + 1$ and $p = m - 1$, we can conclude from the lower bound

$$\left(A^{2m+1}\right)_{ij} \geq \left(A^2\right)_{ij} \left\{ \sum_{q=0}^{m-1} \left(A^{2(m-(q+1)+1)}\right)_{ii} d_j^q \right\} + d_j^m a_{ij}$$

that

$$\left(A^{2m+1}\right)_{ij} \geq d_j^m a_{ij}$$

Even $k = 2m$ and $p = m - 1$ give us $\left(A^{2m}\right)_{ij} \geq \left(A^2\right)_{ij} \sum_{q=0}^{m-1} d_j^q \left(A^{2(m-1-q)}\right)_{ii}$. Invoking the lower bound (2.21) yields

$$\left(A^{2m}\right)_{ij} \geq \left(A^2\right)_{ij} \sum_{q=0}^{m-1} d_j^q d_i^{m-1-q} = \left(A^2\right)_{ij} \frac{d_j^m - d_i^m}{d_j - d_i}$$

In conclusion, the properties in the number $\left(A^k\right)_{ij}$ of walks from node i to node j with odd and even length k differ quite significantly, as will be supported by the spectral investigations in **art.** 58. The reason is that A^{2m} is a positive semidefinite matrix (**art.** 278), while A^{2m+1} is not.

20. *The number of k-hops paths.* The number of paths with k hops between node i and node j follows from (2.16) by excluding possible same nodes in the walk,

$$X_k(i, j; N) = \sum_{r_1 \neq \{i,j\}} \sum_{r_2 \neq \{i,r_1,j\}} \cdots \sum_{r_{k-1} \neq \{i,r_1,\ldots,r_{k-2},j\}} a_{ir_1} a_{r_1 r_2} \cdots a_{r_{k-1} j}$$

valid for $k > 1$ and $N > 2$, while the number of paths with $k = 1$ hop between the node pair (i, j) is $X_1(i, j; N) = a_{ij}$. Symmetry of the adjacency matrix A implies that $X_k(i, j; N) = X_k(j, i; N)$. The definition of a path restricts the first index r_1 to $N - 2$ possible values, the second r_2 to $N - 3$, etc., such that the maximum number of k-hop paths, which is attained in the complete graph K_N, where $a_{ij} = 1$ for each link (i, j), equals

$$\prod_{l=1}^{k-1} (N - 1 - l) = \frac{(N-2)!}{(N-k-1)!}$$

whereas the total possible number of walks with k hops is given in (2.18). If we allow self-loops ($a_{jj} \neq 0$), then (2.16) with $\prod_{l=0}^{k-1} a_{r_l r_{l+1}} = 1$ leads to the total possible number of walks with k hops equal to N^{k-1}.

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The total number M_N of paths between two nodes in the complete graph is

$$M_N = \sum_{j=1}^{N-1} \frac{(N-2)!}{(N-j-1)!} = (N-2)! \sum_{k=0}^{N-2} \frac{1}{k!} = (N-2)!e - R$$

where the remainder

$$\begin{aligned} R &= (N-2)! \sum_{j=N-1}^{\infty} \frac{1}{j!} = \sum_{j=0}^{\infty} \frac{(N-2)!}{(N-1+j)!} \\ &= \frac{1}{N-1} + \frac{1}{(N-1)N} + \frac{1}{(N-1)N(N+1)} + \cdots \\ &< \sum_{j=1}^{\infty} \left(\frac{1}{N-1} \right)^j = \frac{1}{N-2} \end{aligned}$$

implying that for $N \geq 3$, the remainder $R < 1$. But M_N is an integer. Hence, the total number of paths in K_N is exactly equal to

$$M_N = [e(N-2)!] \tag{2.22}$$

where $e = 2.718\,281...$ and $[x]$ denotes the largest integer smaller than or equal to x. Since any graph is a subgraph of the complete graph, the maximum total number of paths between two nodes in any graph is upper bounded by $[e(N-2)!]$.

21. *Hopcount h_{ij} in a connected graph.* A graph G is connected if there exists a walk between each pair of nodes in G. Lemma 1 shows that connectivity is equivalent to the existence of some integer $k > 0$ for which $\left(A^k\right)_{ij} \neq 0$ for each nodal pair (i, j). The lowest integer $k = h_{ij}$, where $i \neq j$, for which $\left(A^k\right)_{ij} \neq 0$, but $\left(A^m\right)_{ij} = 0$, for all $0 \leq m < k$, equals the number of hops in the shortest walk – which is then a path – from node i to node j. Thus, for $i \neq j$, the vector $\left(A_{ij}, \left(A^2\right)_{ij}, \ldots, \left(A^{k-1}\right)_{ij}, \left(A^k\right)_{ij}\right)$ with $k = h_{ij}$ components equals $\left(A^k\right)_{ij} e_k$, where e_k is the k-th basic vector of the k-th dimensional space. If $i = j$, then we define the hopcount of the shortest path to be $h_{ii} = 0$. Hence, the element h_{ij} in the distance matrix H, defined in **art.** 8, equals $h_{ij} = k1_{\left\{\min_k : \left(A^k\right)_{ij} \neq 0\right\}}$ for $i \neq j$ and $h_{ii} = 0$. The hopcount h_{ij} of the shortest path $\mathcal{P}^*_{ij}$ between node i and node j is a unique integer, although there can be multiple shortest paths between node i and node j, so that $\left(A^{h_{ij}}\right)_{ij} \geq 1$.

Each off-diagonal $(i \neq j)$ element in the hopcount matrix H obeys

$$h_{ij} = \min_{1 \leq r \leq N} \left(\frac{1}{a_{ir}} + h_{rj} \right) \tag{2.23}$$

Indeed, if node r is a direct neighbor of node i, then $a_{ir} = 1$ and the hopcount of the remaining path from node r to node j equals h_{rj}. The minimum-hop (or shortest) path travels over that neighbor r of node i with the minimum remaining hops to the destination node j. If $r = j$ and $a_{ij} = 1$, then we find, with $h_{jj} = 0$, hopcount 1 for the direct neighbor path. If r is not a neighbor of i, then $\frac{1}{a_{ir}} = \infty$, which

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removes the index $q = r$ entry $\frac{1}{a_{ir}} + h_{rj}$ from the minimal set $\left\{\frac{1}{a_{iq}} + h_{qj}\right\}_{1\le q\le N}$ in (2.23). Since G is connected, thus excluding isolated nodes, there is at least one element $a_{ir} = 1$ in that minimal set. The non-linear recursion (2.23) can also be written as

$$h_{ij} = 1 + \min_{r\in \text{ neighbors}(i)} h_{rj}$$

22. *Diameter of a graph.* The *diameter* of the graph G, denoted by ρ and sometimes by ρ_G or $\rho(G)$, is the number of hops in the longest shortest path in G and equals $\rho = \max_{1\le i\le N; 1\le j\le N} h_{ij}$. In a connected graph, the diameter is upper bounded by $\rho \le N-1$, the hopcount $N-1$ of the longest possible shortest path in any connected graph on N nodes. The maximal diameter $\rho = N-1$ occurs in a path on N nodes. The diameter of a connected graph G is lower bounded by $\rho \ge 1$ and the minimal diameter $\rho = 1$ only occurs in the complete graph K_N. If G is disconnected, the diameter is not defined, but sometimes put as $\rho > N$ or $\rho \to \infty$ or, even $\rho = 0$; in principle, any integer outside the interval $[1, N-1]$ can serve as an indication of the non-existence of the diameter. We remark that $A^\rho - J$ is not necessarily a non-negative matrix, because $\left(A^{h_{ij}+1}\right)_{ij}$ can be zero[8], even though $\left(A^{h_{ij}}\right)_{ij} \ge 1$.

Lemma 2 *Let $f_k > 0$ for any $k \ge 0$ and A be the adjacency matrix of a connected graph G, then all elements of the matrix $\sum_{k=0}^m f_k A^k$ are positive for $m \ge \rho$. If $m < \rho$, the non-negative matrix $\sum_{k=0}^m f_k A^k$ contains at least one zero element.*

Proof: The definition of the diameter implies that, for each node pair (i,j) in a connected graph G, there exists a path with hopcount at most equal to ρ. This means that $\left(A^k\right)_{ij}$ is non-zero for at least one integer $k \in [0,\rho]$. In addition, there exists a pair (r,q), separated by the longest shortest path in G, for which $\left(A^k\right)_{rq} = 0$ for all $k < \rho$. Since each coefficient $f_k > 0$, it follows that $\sum_{k=0}^\rho f_k \left(A^k\right)_{ij} > 0$ for each node pair (i,j), but $\sum_{k=0}^m f_k A^k$ with $m < \rho$ contains at least one zero element, namely $\sum_{k=0}^m f_k \left(A^k\right)_{rq} = 0$. □

When $f_k = \alpha^{\rho-k}\binom{\rho}{k}$ with $\alpha > 0$, then $\sum_{k=0}^\rho f_k A^k = \sum_{k=0}^\rho \binom{\rho}{k}\alpha^{\rho-k}A^k = (\alpha I + A)^\rho$, which leads to the known result that the diameter ρ is the smallest integer for which the matrix $(I+A)^\rho$ has positive elements. Since $\left(A^k\right)_{ij}$ are integers, it also follows that $(I+A)^\rho - J$ is a non-negative matrix (see Section 10.6).

We infer from Lemma 2 that, for each node pair (i,j), at least one of the matrices in the sequence $\{A^m\}_{0\le m\le\rho} = \left\{I, A, A^2, \ldots, A^\rho\right\}$ contains a non-zero (i,j) element,

[8] For example, in a path graph, studied in Section 6.4, with $N = 3$ and adjacency matrix $A = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$, there is not a walk with length 2 (nor any even number) between node 1 and node 2 (i.e. $\left(A^{2k}\right)_{12} = 0$ for $k > 1$), while there is a walk of odd length, thus $\left(A^{2k+1}\right)_{12} > 0$ for $k > 0$. The diameter $\rho = 2$, but $A^2 - J$ contains negative elements.

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while there is at least one node pair (r, q), corresponding to the longest shortest path in G with ρ hops, whose entries in the sequence $\{A^m\}_{0\leq m<\rho}$ are zero. The next Lemma generalizes this observation.

Lemma 3 *For any diagonal matrix M and for each node pair (i, j), at least one of the matrices in the sequence $\{(A+M)^m\}_{0\leq m\leq\rho}$ contains a non-zero (i, j) element.*

Proof: Let G and G' denote the graph represented by the adjacency matrix A without self-loops ($a_{jj} = 0$ for any node j) and the same graph with weighted self-loops (equal to m_{jj} for node j), respectively. As explained in **art.** 21, the smallest integer $k = h_{ij}$, where $i \neq j$, for which $\left(A^k\right)_{ij} \neq 0$, but $\left(A^m\right)_{ij} = 0$, for all $0 \leq m < k$, is the hopcount of the shortest *path* in G from node i to node j. The expression (2.16) indicates that $\left(A^{h_{ij}}\right)_{ij} \neq 0$ does not depend on any diagonal element of A, because a path is a walk with all nodes different. This means that $\left((A+M)^{h_{ij}}\right)_{ij} = \left(A^{h_{ij}}\right)_{ij} \neq 0$. In addition, for $m < h_{ij}$, there is no path in G from i to j with m hops. Since a diagonal element, associated to a self-loop in G', cannot help to reach node j from i if there is no path from i to j in the graph G and thus also not in G', there also holds that $\left((A+M)^m\right)_{ij} = \left(A^m\right)_{ij} = 0$ for $m < h_{ij}$. These facts demonstrate Lemma 3. Only when $m > h_{ij}$, then $(A+M)^m_{ij}$ can differ from $\left(A^m\right)_{ij}$. □

An interesting consequence of Lemma 3 is that, also for the Laplacian $Q = \Delta - A$, one of the matrices in the sequence $\{Q^m\}_{0\leq m\leq\rho}$ contains a non-zero (i, j) element. Finally, combining Lemma 2 and 3 leads to the statement that there exists a matrix polynomial $p_m(A+M)$ of degree $m \in [0, \rho]$, whose (i, j)-th element is non-zero.

23. *h-hops adjacency matrix.* Analogous to Estrada (2012), who defines a path-Laplacian, we define the h-hops graph ${}_hG$ on N nodes as the graph that contains a link between i and j if their distance in an original graph G is h hops. The corresponding h-hops adjacency matrix ${}_hA$ has elements

$$\left({}_hA\right)_{ij} = 1_{\{h_{ij}=h\}} \tag{2.24}$$

We define ${}_0A = I$ and, clearly, ${}_1A = A$. **Art.** 21 shows that a walk with $h = \min_k \left\{\left(A^k\right)_{ij} \neq 0\right\}$ is also the shortest path between i and j and that, for $i \neq j$,

$$\left({}_hA\right)_{ij} = 1_{\left\{\left\{\forall m\in[1,h):\left(A^m\right)_{ij}=0\right\}\cap\left\{\left(A^h\right)_{ij}>0\right\}\right\}} \tag{2.25}$$

while the diagonal elements $\left({}_hA\right)_{jj}$ in (2.24) are zero for $h > 0$. **Art.** 22 illustrates that the composed event $\left\{\forall m \in [1, h) : \left(A^m\right)_{ij} = 0\right\}$ is also equal to the event $\left\{\sum_{m=1}^{h-1}\left(A^m\right)_{ij} = 0\right\}$, because all elements in A^k are non-negative. For the same reason, the last event is also equal to the event $\left\{\sum_{m=1}^{h-1} c_m\left(A^m\right)_{ij} = 0\right\}$, where $c_m > 0$ for each index m. Hence, the number of conditions to be checked in (2.25)

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is reduced to two in

$$({}_hA)_{ij} = 1_{\left\{\left\{\sum_{m=1}^{h-1} c_m (A^m)_{ij}=0\right\} \cap \left\{(A^h)_{ij}>0\right\}\right\}} = 1_{\left\{\sum_{m=1}^{h-1} c_m (A^m)_{ij}=0\right\}} 1_{\left\{(A^h)_{ij}>0\right\}} \tag{2.26}$$

Finally, we can choose $c_m = \binom{h}{m}$ so that $\sum_{m=1}^{h} c_m (A^m)_{ij} = \left((A+I)^h\right)_{ij}$ for $i \neq j$ and (2.26) simplifies to

$$({}_hA)_{ij} = 1_{\left\{\left((A+I)^{h-1}\right)_{ij}=0\right\}} 1_{\left\{(A^h)_{ij}>0\right\}}$$

Lemma 2 states that $\sum_{m=0}^{h} c_m (A^m)_{ij} > 0$ for all $h \geq \rho$ and, consequently, (2.26) implies that ${}_hA = O$ for all $h > \rho$ as well as

$$\sum_{h=0}^{N-1} {}_hA = \sum_{h=0}^{\rho} {}_hA = J$$

The relation with the distance matrix H in **art.** 8 and **art**. 21 is

$$H = \sum_{h=1}^{\rho} h \; {}_hA$$

The number of links $\frac{1}{2} u^T \; {}_hAu$ in the graph ${}_hG$ equals the number of node pairs connected by an h-hop shortest path.

The sequence of h-hops adjacency matrices $\{{}_hA\}_{1 \leq h \leq \rho} = \{{}_1A, {}_2A, \ldots, {}_\rho A\}$ defines a multi-layer network where, in each xy-plane, the graph ${}_hG$ is depicted and along the z-axis, the number h of hops is varied. Such multi-layer network may visualize how the links $({}_hA)_{ij}$ around node i to any other node j in G vary with hop h and it allows to construct the levelset (Van Mieghem, 2014, Sec. 16.2.2), the set containing the number of nodes $({}_hAu)_i$ at each level h in a shortest path tree rooted at node i of G and depicted in Fig. 6.4.

24. *Effects of link removals on the diameter.* Schoone *et al.* (1987) have derived bounds for the maximum diameter of a still connected graph G_k, obtained from an original graph G with diameter ρ after the removal of k links. For undirected graphs G, Schoone *et al.* (1987) prove an upper bound for the diameter in G_k of $(k+1)\rho$ and a lower bound of $(k+1)\rho - k$, for even ρ, and of $(k+1)\rho - 2k + 2$, for odd $\rho \geq 3$. For the special cases of $k = 2$ and $k = 3$, the exact bounds are $\rho(G_2) \leq 3\rho - 1$ and $\rho(G_3) \leq 4\rho - 2$, respectively. In addition, Schoone *et al.* (1987) prove that the problem of finding G_k by removing k links in G so that $\rho(G_k)$ is at least m as well as the related problem of finding the graph G_l by adding l links to G so that $\rho(G_l) \leq m$ is NP-complete.

2.4 The line graph

25. The line graph $l(G)$ of the graph $G(N, L)$ has as set of nodes the links of G and two nodes in the line graph $l(G)$ are adjacent if and only if they have, as links

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in G, one node of G in common. Given the graph G, the definition thus specifies the line graph operator $l\,(.)$. The line graph $l\,(G)$ of G is sometimes called the "dual" or "interchanged" or "derived" graph of G. For example, the line graph of the star $K_{1,n}$ is the complete graph K_n and the line graph of the example graph in Fig. 2.1 is drawn in Fig. 2.2. When G is connected, then also $l\,(G)$ is connected as follows from the definition[9] of the line graph $l\,(G)$.

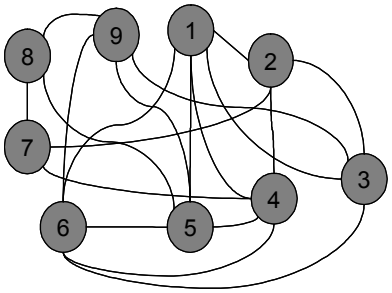

Fig. 2.2. The line graph of the undirected variant of the graph drawn in Fig. 2.1.

We denote by R the absolute value of the incidence matrix B, i.e., $R_{ij} = |b_{ij}|$. In other words, $R_{ij} = 1$ if node i and link j are incident, otherwise $R_{ij} = 0$. Hence, the unsigned incidence matrix R ignores the direction of links in the graph, in contrast to the incidence matrix B. Analogously to the definition of the Laplacian in **art.** 4, we may verify that the $N \times N$ adjacency matrix A of the graph G is written in terms of the unsigned $N \times L$ node-link incidence matrix R as

$$A = RR^T - \Delta \tag{2.27}$$

The $L \times L$ adjacency matrix of the line graph $l\,(G)$ is similarly written in terms of R as

$$A_{l(G)} = R^T R - 2I \tag{2.28}$$

The matrix $B^T B$ is generally a $(-1, 0, 1)$-matrix. Taking the absolute value of its entries equals $R^T R$, whereas the Laplacian matrix $Q = 2\Delta - RR^T = BB^T$.

In a graph G, where multiple links with the same direction between two nodes are excluded, we consider

$$\left(B^T B\right)_{ij} = \sum_{n=1}^{N} b_{ni} b_{nj} = \begin{cases} 1 & \text{if both link } i \text{ and } j \text{ either start or end in node } n \\ -1 & \text{if either link } i \text{ or } j \text{ starts or ends in node } n \\ -2 & \text{if link } i \text{ and } j \text{ have two nodes in common} \end{cases}$$

The latter case, where $\left(B^T B\right)_{ij} = -2$, occurs for a bidirectional link between two nodes. If the links at each node of the graph G either all start or all end, then

[9] In a connected graph G, each node is reachable from any other node via a path (a sequence of adjacent links, **art.** 6). Similarly, in the dual setting corresponding to the line graph, each link in G is reachable from any other link via a path (a sequence of adjacent nodes or neighbors).

we observe that $\left(B^T B\right)_{ij} = 1$ for all links i and j and, in that case, it holds that $B^T B = R^T R$. An interesting example of such a graph is the general bipartite graph, studied in Section 6.8, where the direction of the links is the same for each node in the set $\mathcal{M}$ to each node in the other set $\mathcal{N} \backslash \mathcal{M}$.

26. *Basic properties of the line graph.* The number of nodes in the line graph $l\,(G)$ equals the number L of links in G. The number of links in the line graph $l\,(G)$ is computed from the basic law of the degree (2.5) and (2.28) with the $L \times 1$ all-one vector u as

$$\begin{aligned} L_{l(G)} &= \frac{1}{2} u^T A_{l(G)} u = \frac{1}{2} u^T R^T R u - u^T u \\ &= \frac{1}{2} \left\| R u \right\|_2^2 - L \end{aligned}$$

It follows from the definition of the unsigned incidence matrix R that $u_{1\times N}^T R = 2u_{L\times 1}^T$ or

$$R^T u = 2u \tag{2.29}$$

which is the companion of (2.1), and that

$$Ru = d \tag{2.30}$$

because the row sum of $\sum_{l=1}^{L} R_{il} = d_i$, the number of links in G incident to node i. Hence, we find that the number of links in the line graph $l\,(G)$ equals

$$L_{l(G)} = \frac{1}{2} d^T d - L = \frac{1}{2} \sum_{i=1}^{N} d_i^2 - L \tag{2.31}$$

Alternatively, each node i in G with degree d_i generates in the line graph $l\,(G)$ precisely d_i nodes that are all connected to each other as a clique, corresponding to $\binom{d_i}{2}$ links. The number of links in $l\,(G)$ is thus also

$$L_{l(G)} = \sum_{i=1}^{N} \binom{d_i}{2}$$

Art. 4 indicates that the average degree of a node in the line graph $l\,(G)$ is

$$E\left[D_{l(G)}\right] = \frac{2L_{l(G)}}{N_{l(G)}} = \frac{1}{L} \sum_{i=1}^{N} d_i^2 - 2$$

The degree vector of the line graph $l\,(G)$ follows from (2.4) as

$$\begin{aligned} d_{l(G)} &= A_{l(G)} u_{L\times 1} = R^T R u - 2u \\ &= R^T d - 2u \end{aligned}$$

Each column of R (as in the incidence matrix B) contains only two non-zero elements and the vector component $\left(R^T d\right)_l = d_{l^+} + d_{l^-}$, where l_+ denotes the node

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at the start and l_- the node at the end of the link l. Hence, the maximum (and similarly minimum) degree of the line graph $l(G)$ equals

$$\max d_{l(G)} = \max_{1\le l\le L} (d_{l^+} + d_{l^-} - 2) \le d_{(1)} + d_{(2)} - 2$$

where $d_{(k)}$ denotes the k-th largest degree in G and $d_{(k-1)} \ge d_{(k)}$ for $2 \le k \le N$.

Example The degree vector of a regular graph with degree r is $d = r u_{N\times 1}$. The degree vector of the corresponding line graph is $d_{l(G)} = R^T d - 2u = r R^T u - 2u$ and with (2.29), we find $d_{l(G)} = 2(r-1) u_{L\times 1}$. The line graph of a regular graph with degree r is also a regular graph with degree $2(r-1)$. The total number of links follows from $L_{l(G)} = \sum_{i=1}^N \binom{d_i}{2} = N\frac{r(r-1)}{2}$ or from the basic law of the degree (2.5), $L_{l(G)} = \frac{1}{2} d_{l(G)}^T u = (r-1) L = (r-1)\frac{r}{2} N$.

The sum of all off-diagonal elements in A^2 equals

$$\begin{aligned}\sum_{i=1}^N \sum_{j=1;j\ne i}^N (A^2)_{ij} &= \sum_{i=1}^N \sum_{j=1;j\ne i}^N \sum_{k=1}^N a_{ik} a_{kj} = \sum_{k=1}^N \sum_{i=1}^N a_{ki} \sum_{j=1;j\ne i}^N a_{kj} \\ &= \sum_{k=1}^N \sum_{i=1}^N a_{ki}(d_k - a_{ki}) = \sum_{k=1}^N \left(d_k \sum_{i=1}^N a_{ki} - \sum_{i=1}^N a_{ki} \right)\end{aligned}$$

and, thus

$$\sum_{i=1}^N \sum_{j=1;j\ne i}^N (A^2)_{ij} = \sum_{k=1}^N d_k (d_k - 1) = 2L_{l(G)} \tag{2.32}$$

where the last equality follows from (2.31) and $\sum_{i=1}^N \sum_{j=1;j\ne i}^N (A^2)_{ij}$ equals twice the total number of two-hop walks with different source and destination nodes. In other words, the total number of connected triplets of nodes in G, which is half of (2.32), equals the number of links in the line graph $l(G)$.

The $L \times L$ Laplacian matrix $Q_{l(G)}$ of the line graph $l(G)$ is, by definition (2.6),

$$\begin{aligned}Q_{l(G)} &= \operatorname{diag}\left(d_{l(G)}\right) - A_{l(G)} \\ &= \operatorname{diag}\left(R^T d\right) - R^T R\end{aligned}$$

which illustrates that the relation between the Laplacian Q of the graph G and the Laplacian $Q_{l(G)}$ of its line graph $l(G)$ is less obvious.

27. Since $R^T R$ is a Gram matrix (**art.** 280), all eigenvalues of $R^T R$ are non-negative. Hence, it follows from (2.28) that the eigenvalues of the adjacency matrix of the line graph $l(G)$ are not smaller than -2.

The adjacency spectra of the line graph $l(G)$ and of G are related by Lemma 11 in **art.** 284 since

$$\det\left(\left(R^T R\right)_{L\times L} - \lambda I\right) = \lambda^{L-N} \det\left(\left(R R^T\right)_{N\times N} - \lambda I\right)$$

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Using the definitions (2.28) and (2.27) in **art.** 25 yields

$$\det\left(A_{l(G)} - (\lambda - 2)\, I\right) = \lambda^{L-N} \det\left(\Delta + A - \lambda I\right)$$

or

$$\det\left(A_{l(G)} - \lambda I\right) = (\lambda + 2)^{L-N} \det\left(\Delta + A - (\lambda + 2)\, I\right) \tag{2.33}$$

The eigenvalues of the adjacency matrix of the line graph $l\,(G)$ are those of the unsigned Laplacian $\Delta + A$ in **art**. 30 shifted over -2 and an eigenvalue at -2 with multiplicity $L - N$.

If $B^T B = R^T R$, then Lemma 11 indicates that

$$\det\left(\left(B^T B\right)_{L\times L} - \lambda I\right) = \lambda^{L-N} \det\left(\left(B B^T\right)_{N\times N} - \lambda I\right)$$

from which

$$\det\left(Q - \lambda I\right) = \lambda^{N-L} \det\left(A_{l(G)} - (\lambda - 2)\, I\right)$$

or

$$\det\left(A_{l(G)} - \lambda I\right) = (\lambda + 2)^{L-N} \det\left(Q - (\lambda + 2)\, I\right) \tag{2.34}$$

In graphs G, where $B^T B = R^T R$, the eigenvalues of the adjacency matrix of the line graph $l\,(G)$ are those of the Laplacian $Q = \Delta - A$ shifted over -2 and an eigenvalue at -2 with multiplicity $L - N$.

The restriction, that all eigenvalues of an adjacency matrix are not less than -2, is not sufficient to characterize line graphs (Biggs, 1996, p. 18). The state-of-the-art knowledge about line graphs is reviewed by Cvetković *et al.* (2004), who treat the characterization of line graphs in detail. Referring for proofs to Cvetković *et al.* (1995, 2004), we mention here only:

Theorem 4 (Krausz) *A graph is a line graph if and only if its set of links can be partitioned into "non-trivial" cliques, namely (i) two cliques have at most one node in common and (ii) each node belongs to at most two cliques.*

Theorem 5 (Van Rooij and Wilf) *A graph is a line graph if and only if (i) it does not contain the star $K_{1,3}$ as an induced subgraph and (ii) the remaining (or opposite) nodes in any two triangles with a common link must be adjacent and each of such triangles must be connected to at least one other node in the graph by an odd number of links.*

28. *Inverse line graph.* Given a line graph $l\,(G)$, it is possible to reconstruct the original graph G by the inverse line graph operation $l^{-1}\,(.)$, so that $l^{-1}\,(l\,(G)) = G$ returns the original graph G.

Each link l in G connects two nodes i and j and is transformed in the line graph $l\,(G)$ to a node l that belongs to two cliques $\widehat{K}_{d_i}$ and $\widehat{K}_{d_j}$, where a clique, denoted by $\widehat{K}_n$, contains the complete graph K_n and additional links to other nodes outside

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the complete graph K_n. If a line graph $l(G)$ can be partitioned into cliques (Krausz' Theorem 4), then the number of those cliques equals the number N of nodes in G and each node l in $l(G)$, belonging to two cliques i and j, corresponds to a link l in G between two nodes i and j. Apart from the line graph $l(G) = K_3$, that has two original graphs, the triangle K_3 and the star $K_{1,3}$ on four nodes, the reconstruction or inverse line graph $l^{-1}(G)$ is unique by a theorem of Whitney (1932).

Algorithms to compute the original graph G from the line graph $l(G)$ are presented by Lehot (1974) and Roussopoulos (1973). Our inverse line graph algorithm ILIGRA complements and has advantages over Lehot's and Roussopoulos' algorithm, as explained in Liu *et al.* (2015).

29. *Repeated line graph transformations.* The Cauchy-Schwarz inequality (A.72), $\left(\sum_{i=1}^{N} d_i\right)^2 \leq N \sum_{i=1}^{N} d_i^2$ with equality only for regular graphs where $d_j = r$ for each node j, the basic law of the degree (2.3) and (2.31) indicate that

$$L_{l(G)} \geq L\left(\frac{2L}{N} - 1\right) \tag{2.35}$$

The number $L_{l(G)}$ of links in the line graph can only be equal to the number L of links in the original graph if the average degree $\frac{2L}{N} = 2$ and the graph is regular. Hence, the line graph of a cycle C_N on N nodes is again the cycle C_N, i.e. $l(C_N) = C_N$.

For $k \geq 1$, van Rooij and Wilf (1965) have constructed the sequence $G_0, G_1, \ldots, G_k$ of graphs, where the graph $G_k = l(G_{k-1})$ has N_k nodes and L_k links and where the original graph G_0 is possibly the only non-line graph. The k-th line graph iterate $\underbrace{l.l\ldots l}_{k \text{ times}}(G_0)$ is denoted by $G_k = l^k(G_0)$. The line graph of the path P_N on N nodes is $l(P_N) = P_{N-1}$. Hence, the k-th iterate $l^k(P_N) = P_{N-k}$ becomes the empty graph for $k = N - 1$, while the cycle, obeying $l^k(C_N) = C_N$, is invariant under a line graph transformation.

The basic property (**art.** 26) of the line graph shows that $N_k = L_{k-1}$ and (2.35) becomes

$$\frac{N_{k+1}}{N_k} \geq 2\frac{N_k}{N_{k-1}} - 1$$

Let $\nu_k = \frac{N_{k+1}}{N_k}$, then $\nu_{k+1} \geq 2\nu_k - 1$, equivalent to $\nu_{k+1} - 1 \geq 2(\nu_k - 1)$ and after p iterations, we obtain

$$\nu_k - 1 \geq 2(\nu_{k-1} - 1) \geq 2^2(\nu_{k-2} - 1) \geq \ldots \geq 2^p(\nu_{k-p} - 1)$$

If $k - p = 0$, then, with $\nu_0 = \frac{L}{N}$, we find that $\nu_k = \frac{N_{k+1}}{N_k} \geq 2^k\left(\frac{L}{N} - 1\right) + 1$. With $\xi = \frac{L}{N} - 1$, iterating $N_{k+1} = \nu_k N_k$ downwards yields

$$N_k \geq N\prod_{j=0}^{k-1}\left(1 + 2^j\xi\right) = N\xi^k 2^{\frac{k(k-1)}{2}}\prod_{j=0}^{k-1}\left(1 + \frac{1}{2^j\xi}\right) \tag{2.36}$$

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If G_j is regular, then all G_k with $k > j$ are also regular graphs (**art.** 26), in which case the equality sign in (2.36) holds. Hence, if G_0 is a regular graph with degree r, then $\xi = \frac{r}{2} - 1$ and equality holds in (2.36) so that $N_k = N\prod_{j=0}^{k-1}\left(1 + 2^j\left(\frac{r}{2} - 1\right)\right)$. Since the degree of a node in any graph with $N > 3$ is smaller than or equal to $r = N - 1$ in the complete graph, we find an upper bound

$$N_k \leq N \prod_{j=0}^{k-1} \left(1 + 2^j \left(\frac{N-1}{2} - 1\right)\right)$$

In summary, for any graph with $\xi = \frac{L}{N} - 1 > 0$, $N > 3$ (but excluding the star $K_{1,3}$, because $l(K_{1,3}) = K_3$) and at least one nodal degree $d_i \geq 3$, the number N_k of nodes in G_k is increasing in k rapidly[10] as $O\left(N\xi^k 2^{\frac{k(k-1)}{2}}\right)$.

Xiong (2001) has shown for a connected graph G_0 different from a path that $l^n(G_0)$ is Hamiltonian if $n \leq \rho - 1$, where ρ is the diameter (**art.** 22) of G_0, while Harary and Nash-Williams (1965) prove that, if G_0 is Eulerian (**art.** 6), then $l^3(G_0)$ is Hamiltonian and conversely.

30. *Unsigned Laplacian.* The unsigned or signless Laplacian $\overline{Q} = \Delta + A$, studied by Cvetković *et al.* (2007), possesses a number of interesting properties. The definition (2.27) shows that $\overline{Q} = RR^T$ is a positive semidefinite matrix and all its eigenvalues are non-negative (**art.** 27). The smallest eigenvalue of $\overline{Q}$ of a connected graph is only equal to zero if the graph is bipartite. Indeed, $\overline{Q}x = 0$ implies that $Rx = 0$, which is only possible if $x_i = -x_j$ for every link $l = i \sim j$ in the graph, i.e. only if G is bipartite (**art.** 25). Cvetković *et al.* (2007) show that this zero eigenvalue is simple in a connected graph and that the multiplicity of the zero eigenvalue of $\overline{Q}$ in any graph equals the number of bipartite components. The smallest eigenvalue of the signless Laplacian can be regarded as a measure of the non-bipartiteness of a graph. Stanić (2015) devotes a chapter on inequalities of the signless Laplacian.

[10] The fundamental cornerstone in the theory of Gaussian polynomials, defined as

$$\begin{bmatrix} k \\ l \end{bmatrix}(q) = \frac{\prod_{j=1}^{k}(1-q^j)}{\prod_{j=1}^{l}(1-q^j)\,\prod_{j=1}^{k-l}(1-q^j)} = \prod_{j=1}^{l}\frac{(1-q^{k-j+1})}{(1-q^j)} \tag{2.37}$$

is

$$Q_k(z,x) = \prod_{m=0}^{k-1}(x + q^m z) = \sum_{m=0}^{k}\begin{bmatrix} k \\ m \end{bmatrix}(q)\, q^{m(m-1)/2}\, z^m\, x^{k-m} \tag{2.38}$$

which bears a striking resemblance to Newton's binomium (Rademacher, 1973; Goulden and Jackson, 1983) for $q = 1$ so that $\begin{bmatrix} k \\ l \end{bmatrix}(1) = \binom{k}{l}$. We define $Q_k(-x,x) = \delta_{0k}$ in correspondence to the first factor for $m = 0$ in the product. The so-called q-analog (2.38) of Newton's binomium is derived via induction from the recursion $Q_k(z,x) = (x + q^{k-1}z)\,Q_{k-1}(z,x)$ for $k > 0$ and $Q_0(x,z) = 1$. When k tends to infinity, (2.38) leads for $|q| < 1$ to

$$\prod_{m=0}^{\infty}(1 + q^m z) = \sum_{m=0}^{\infty}\frac{q^{m(m-1)/2}}{\prod_{j=1}^{m}(1-q^j)}\, z^m \tag{2.39}$$

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2.5 Permutations, partitions and the quotient graph

31. *Permutation matrix P.* Consider the set $\mathcal{N} = \{n_1, n_2, \ldots, n_N\}$ of nodes of G, where n_j is the label of node j. The most straightforward way is the labeling $n_j = j$. Suppose that the nodes in G are relabeled. This means that there is a permutation, often denoted by π, that rearranges the node identifiers n_j as $n_i = \pi(n_j)$. The corresponding permutation matrix P has, on row i, element $p_{ij} = 1$ if $n_i = \pi(n_j)$, and $p_{ij} = 0$ otherwise. Thus, in each row there is precisely one non-zero element equal to 1 and, consequently, it holds that

$$Pu = u$$

For example, the set of nodes $\{1, 2, 3, 4\}$ is permuted to the set $\{2, 4, 1, 3\}$ by the permutation matrix

$$P = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

If the vector $v = (1, 2, 3, 4)$, then the permuted vector $w = Pv = (2, 4, 1, 3)$. Next, $z = Pw = P^2v = (4, 3, 2, 1)$, then $y = Pz = P^3v = (3, 1, 4, 2)$, and, finally, $Py = P^4v = v$. Thus, $P^4 = I$. The observation $P^N = I$ holds in general for each $N \times N$ permutation matrix P: each node can be relabeled to one of the $\{n_1, n_2, \ldots, n_N\}$ possible labels and the permutation matrix maps each time a label $n_j \to \pi(n_j) = n_i$, where, generally, $n_i \neq n_j$, else certain elements are not permuted[11]. After N relabelings, we arrive again at the initial labeling and $P^N = I$. The definition (A.27) of the determinant shows that $\det P = \pm 1$, because in each row there is precisely one non-zero element equal to 1.

Another example of a permutation matrix is the unit-shift relabeling transformation in Section 6.2.1.

32. *A permutation matrix P is an orthogonal matrix.* Since a permutation matrix P relabels a vector v to a vector $w = Pv$, both vectors v and w contain the same components, but in a different order (provided $P \neq I$), such that their norms (**art.** 201) are equal, $\|v\| = \|w\|$. Using the Euclidean norm $\|x\|_2^2 = x^T x$, the equality $v^T v = w^T w$ implies that $P^T P = I$, such that P is an orthogonal matrix (**art.** 247).

If G_1 and G_2 are two directed graphs on the same set of nodes, then they are called *isomorphic*[12] if and only if there is a permutation matrix P such that $P^T A_{G_1} P = A_{G_2}$. Since permutation matrices are orthogonal, $P^{-1} = P^T$, the spectra of G_1 and G_2 are identical (**art.** 247) : the spectrum (set of eigenvalues) is an invariant of the isomorphism class of a graph. However, the converse "if the spectrum (set of eigenvalues) is the same, then the graph is isomorphic" is not true

[11] The special permutation $P = I$ does not, in fact, relabel nodes.
[12] The word "isomorphism" stems from $\iota\sigma o\varsigma$ (isos: same) and $\mu o\rho\varphi\eta$ (morphei: form).

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in general. There exist nonisomorphic graphs that have precisely the same set of eigenvalues and such graphs are called *cospectral graphs*.

33. *A permutation matrix P is a doubly-stochastic matrix.* Left-multiplying both sides of $Pu = u$ with P^T and using $P^T P = I$ in **art.** 32 leads to $P^T u = u$. Since each element $p_{ij} \in [0, 1]$ and the row sum of P equals 1, i.e. $Pu = u$, we conclude that P is a stochastic matrix and property $P^T u = u$ makes P a doubly-stochastic matrix.

34. *Automorphism.* We investigate the effect of a permutation π of the nodal set $\mathcal{N}$ of a graph on the structure of the adjacency matrix A. Suppose that $n_i = \pi(n_j)$ and $n_k = \pi(n_l)$, then we have with the definition of P in **art.** 31,

$$(PA)_{il} = \sum_{m=1}^{N} p_{im} a_{ml} = a_{jl}$$

$$(AP)_{il} = \sum_{m=1}^{N} a_{im} p_{ml} = a_{ik}$$

In order for A and P to commute, i.e. $PA = AP$, we observe that, between each node pair (n_j, n_l) and its permutation $(\pi(n_j), \pi(n_l))$ there must be a link such that $a_{jl} = 1 = a_{ik}$. An *automorphism* of a graph is a permutation π of the nodal set $\mathcal{N}$ such that (n_i, n_j) is a link of G if and only if $(\pi(n_i), \pi(n_j))$ is a link of G. Hence, if the permutation π is an automorphism, then A and P commute. In fact, an automorphism is an isomorphism of the graph G to itself and represents a form of symmetry that maps the graph onto itself. A classical example is the Peterson graph in Fig. 2.3: by rotating the five nodes (both inner as outer ring) over 72 degrees, we obtain again a Peterson graph. All possible such permutations, that preserve all details of its structure, constitute the automorphism group of a graph G, denoted by $\mathrm{Aut}(G)$. A graph is called *symmetric* if there are non-trivial, i.e. excluding $P = I$, automorphisms ($|\mathrm{Aut}(G)| > 1$), and *asymmetric* if the trivial permutation $P = I$ is the only automorphism ($|\mathrm{Aut}(G)| = 1$). Determining $\mathrm{Aut}(G)$ or testing whether a graph has a non-trivial automorphism is a "hard" problem, likely NP-complete, but its hardness class is still unknown, just as the graph isomorphism problem (**art.** 38).

The consequences of the commutation $PA = AP$ for the spectrum of the adjacency matrix A are interesting. Suppose that x is an eigenvector of A belonging to the eigenvalue λ, then

$$APx = PAx = P\lambda x = \lambda Px$$

which implies that Px is also an eigenvector of A belonging to eigenvalue λ. If x and Px are linearly independent, then λ cannot be a simple eigenvalue. Thus, an automorphism produces multiple eigenvectors belonging to a same eigenvalue.

35. *Enumeration of graphs.* The total number of undirected graphs $G(N, L)$ with

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N nodes and L links equals

$$n_{G(N,L)} = \binom{\binom{N}{2}}{L} \tag{2.40}$$

which is the number of ways that we can distribute the L ones, corresponding to the L links, in the upper (or lower) triangular part of an $N \times N$ symmetric adjacency matrix, containing $\binom{N}{2}$ possible positions. The total number of undirected graphs with N nodes then follows by summing (2.40) over all possible number of links, $0 \leq L \leq \binom{N}{2}$, as

$$n_{G(N)} = 2^{\binom{N}{2}} \tag{2.41}$$

The enumeration has implicitly assumed that all nodes are distinguishable. For example, each node has a certain characteristic property (i.e. a label, a color, a size, etc.). In many cases, the nodes of a graph are all of the same type and indistinguishable, which means that, if we relabel two nodes, the resulting graph is still the same or isomorphic to the former. The number of ways in which we can relabel the N nodes is $N!$. However, the number of graphs isomorphic to a given graph G is $N!/|\mathrm{Aut}(G)|$. Therefore, for any class C of graphs closed under isomorphism (e.g. all graphs, or all regular graphs), the number of isomorphism classes is $\overline{|Aut(C)|}/N!$, where $\overline{|Aut(G)|}$ is the average size of the automorphism group of a graph in G. Hence, the total number of undirected, nonisomorphic graphs is

$$n_{\text{nonisomorphic } G(N)} = \frac{2^{\binom{N}{2}}}{N!}\overline{|Aut(G\,(N))|} \tag{2.42}$$

where $\overline{|Aut(G\,(N))|}$ is the average number of automorphisms among all graphs on N nodes and the complicating factor in (2.42).

In some cases, the enumeration of graph properties (such as the number of walks (**art.** 59), the number triangles in (3.8) and spanning trees (**art.** 117)) can be efficiently computed from the spectrum of the graph, while in other cases, enumeration leads to a challenging combinatorial problem (such as the number of regular or cospectral graphs (**art.** 40)). Techniques for enumeration of graph properties, including a proof of (2.42), are discussed in depth in the book by Harary and Palmer (1973).

36. *Partitions.* A generalization of a permutation is a partition that separates the nodal set $\mathcal{N}$ of a graph in disjoint, non-empty subsets of $\mathcal{N}$, whose union is $\mathcal{N}$. The $k \in \{1, 2, \ldots, N\}$ disjoint, non-empty subsets generated by a partition are sometimes called cells, and denoted by $\{C_1, C_2, \ldots, C_k\}$. If $k = N$, the partition reduces to a permutation. We also denote a partition by π.

Let $\{C_1, C_2, \ldots, C_k\}$ be a partition of the set $\mathcal{N} = \{1, 2, \ldots, N\}$ of nodes and let

A be a symmetric matrix, that is partitioned as

$$A = \begin{bmatrix} A_{1,1} & \cdots & A_{1,k} \\ \vdots & & \vdots \\ A_{k,1} & \cdots & A_{k,k} \end{bmatrix}$$

where the block matrix $A_{i,j}$ is the submatrix of A formed by the rows in C_i and the columns in C_j. For example, the partition $C_1 = \{1, 3\}$, $C_2 = \{2, 4, 6\}$ and $C_3 = \{5\}$ of the nodes in Fig. 2.1 leads to the partitioned adjacency matrix

$${}_{\pi}A = \begin{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} & \begin{bmatrix} 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix} & \begin{bmatrix} 0 \\ 0 \end{bmatrix} \\ \begin{bmatrix} 1 & 1 \\ 0 & 1 \\ 1 & 0 \end{bmatrix} & \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} & \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \\ \begin{bmatrix} 0 & 0 \end{bmatrix} & \begin{bmatrix} 1 & 1 & 1 \end{bmatrix} & [0] \end{bmatrix}$$

which is obtained from the matrix A on p. 16 by relabeling nodes according to $1 = \pi(1), 2 = \pi(3), 3 = \pi(2), 4 = \pi(4), 5 = \pi(6), 6 = \pi(5)$. The characteristic matrix S of the partition, also called the community matrix S, is the $N \times k$ matrix whose columns are the vectors C_k labeled in accordance with ${}_{\pi}A$. Thus, in the example, the partition $C_1 = \{1, 3\}$, $C_2 = \{2, 4, 6\}$ and $C_3 = \{5\}$, translates after relabeling into ${}_{\pi}C_1 = \{\pi(1) = 1, \pi(3) = 2\}$, ${}_{\pi}C_2 = \{\pi(2) = 3, \pi(4) = 4, \pi(6) = 5\}$ and ${}_{\pi}C_3 = \{\pi(5) = 6\}$, respectively, with corresponding matrix S

$$S = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} u_2 & 0 & 0 \\ 0 & u_3 & 0 \\ 0 & 0 & u_1 \end{bmatrix}$$

where u_j is the all one vector of dimension j. Clearly, $S^T S = \mathrm{diag}(2, 3, 1)$.

In general, $S^T S = \mathrm{diag}(|C_1|, |C_2|, \ldots, |C_k|)$, where $|C_k|$ equals the number of elements in the set C_k. Each row of S only contains one non-zero element, which follows from the definition of a partition: a node can only belong to one cell or community of the partition and the union of all cells is again the complete set $\mathcal{N}$ of nodes. Thus, the elements of the $N \times k$ community matrix S after relabeling are

$$S_{ij} = \begin{cases} 1 & \text{if node } i \text{ belongs to the community } {}_{\pi}C_j \\ 0 & \text{otherwise} \end{cases}$$

or compactly, $S_{ij} = 1_{\{\pi^{-1}(i) \in C_j\}}$. The columns of S are orthogonal and $\mathrm{trace}\left(S^T S\right) = N$.

37. *Quotient matrix.* The quotient matrix corresponding to the partition specified

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by $\{C_1, C_2, \ldots, C_k\}$ is defined as the $k \times k$ matrix

$$A^{\pi} = \left(S^T S\right)^{-1} S^T \left({}_{\pi}A\right) S \tag{2.43}$$

where $\left(S^T S\right)^{-1} = \text{diag}\left(\frac{1}{|C_1|}, \frac{1}{|C_2|}, \ldots, \frac{1}{|C_k|}\right)$. The quotient matrix of the matrix A of the example in **art.** 36 is

$$A^{\pi} = \begin{bmatrix} 1 & 2 & 0 \\ \frac{4}{3} & \frac{2}{3} & 1 \\ 0 & 3 & 0 \end{bmatrix}$$

We can verify that $(A^{\pi})_{ij}$ denotes the average row sum of the block matrix $({}_{\pi}A)_{i,j}$. An example of the quotient matrix Q^{π} of a Laplacian Q is given in Section 6.13.

If the row sum of each block matrix $A_{i,j}$ is equal to the same constant, then the partition π is called *equitable* or regular. In that case, $A_{i,j}u = ({}_{\pi}A)_{i,j}\, u$ or ${}_{\pi}AS = SA^{\pi}$. Also, a partition π is equitable if, for any i and j, the number of neighbors that a node in C_i has in the cell C_j does not depend on the choice of a node in C_i.

For example, consider a node v in the Petersen graph shown in Fig. 2.3 and construct the three cell partitions as $C_1 = \{v\}$, C_2 is the set of the neighbors of v and C_3 is the set of nodes two hops away from v. The number of neighbors of v in

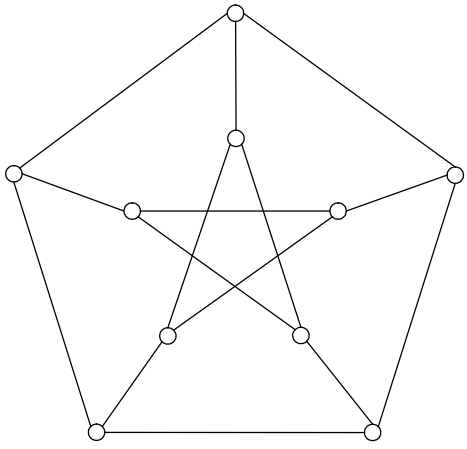

Fig. 2.3. The Petersen graph.

C_2 is three and zero in C_3, while the number of neighbors of a node in C_2 with C_3 is two such that

$$A^{\pi} = \begin{bmatrix} 0 & 3 & 0 \\ 1 & 0 & 2 \\ 0 & 1 & 2 \end{bmatrix}$$

A distance partition with respect to node v is the partition of $\mathcal{N}$ into the sets of

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nodes in G at distance r from a node v. A distance partition is, in general, not equitable.

If v is an eigenvector of A^π belonging to the eigenvalue λ, then Sv is an eigenvector of ${}_\pi A$ belonging to the same eigenvalue λ. Indeed, left-multiplication of the eigenvalue equation $A^\pi v = \lambda v$ by S yields

$$\lambda S v = S A^\pi v = ({}_\pi A)\, S v$$

This property makes equitable partitions powerful.

For example, the adjacency matrix of the complete bipartite graph $K_{m,n}$ (see Section 6.7) has an equitable partition with $k = 2$. The corresponding quotient matrix is $A^\pi = \begin{bmatrix} 0 & m \\ n & 0 \end{bmatrix}$ whose eigenvalues are $\pm\sqrt{mn}$, which are the non-zero eigenvalues of $K_{m,n}$. The quotient matrix of the complete multipartite graph is derived in Section 6.9. Exact solutions of the epidemic mean-field equations in Prasse *et al.* (2021) rely on equitable partitions.

The quotient graph of an equitable partition, denoted by G^π, is the directed graph with the cells of the partition π as its nodes and with $(A^\pi)_{ij}$ links going from cell/node C_i to node C_j. Thus, $(A^\pi)_{ij}$ equals the number of links that join a node in the cell C_i to the nodes in cell C_j. In general, the quotient graph contains multiple links and self-loops. The subgraph induced by each cell in an equitable partition is necessarily a regular graph because each node in cell C_i has the same number of neighbors in cell C_j.

2.6 Cospectral graphs

Cospectral graphs are nonisomorphic graphs that possess the same set of eigenvalues, as earlier defined in **art.** 32. Since the spectrum of graphs is the main theme in this book, we cannot avoid devoting some attention to cospectral graphs.

38. Checking whether two graphs have the same adjacency eigenvalues is a polynomial, thus "easy" problem. However, determining whether two cospectral graphs are isomorphic can be non-polynomial, thus "hard", but it is currently unknown (McKay and Piperno, 2014) whether the graph isomorphism problem is NP-hard.

Almost all non-star-like trees are *not* determined by the spectrum of the adjacency matrix (van Dam and Haemers, 2003). Godsil and Royle (2001) start by the remark that the spectrum of a graph does not determine the degrees, nor whether the graph is planar and that there are many graphs that are cospectral, i.e., although graphs are different (nonisomorphic), their spectrum is the same. Cvetković *et al.* (2009) devote a whole chapter on the characterization of graphs by their spectrum. They list theorems on graphs that are determined by their spectrum such as regular graphs with degree $r = 2$ and complete bipartite graphs, but they also present counter examples. Finally, van Dam and Haemers (2003) conjecture that sufficiently large graphs are determined by their spectrum, roughly

speaking because the probability of having cospectral graphs becomes vanishingly small when the number of nodes N increases. A major tool to construct cospectral graphs is Godsil-McKay switching.

39. *Godsil-McKay switching for cospectral graph construction.* Godsil and McKay (1982) have invented an ingenious way to construct cospectral graphs by using a certain partitioning π of a graph and by rewiring a specific set of links, which is called "switching". They start by proposing the partition $\pi = \{C_1, C_2, \ldots, C_k, F\}$, where (a) any two nodes in C_i have the same number of neighors in C_j, for $1 \leq i, j \leq k$ and i can be the same as j; (b) a node $v \in F$ has either zero, $n_i/2$ or n_i neighbors in C_i, where the number of nodes in C_i is $n_i = |C_i|$. Any graph G with N nodes can be partitioned in this way, in particular, if $C_j = \{j\}$ and $F = \{N\}$. Of course, the interest lies in finding non-trivial partitions where $n_i > 1$, for at least some i. The adjacency matrix corresponding to this partition π is denoted as a block matrix

$$ {}_\pi A = \begin{bmatrix} A_{1,1} & A_{1,2} & \cdots & A_{1,k} & A_{F_1} \\ A_{1,2}^T & A_{2,2} & \cdots & A_{2,k} & A_{F_2} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ A_{1,k}^T & A_{2,k}^T & \cdots & A_{k,k} & A_{F_k} \\ A_{F_1}^T & A_{F_2}^T & \cdots & A_{F_k}^T & A_F \end{bmatrix} $$

where $A_{j,j}$ is the $n_j \times n_j$ adjacency matrix of the set of nodes belonging to C_j and the adjacency matrix $A_{i,j}$ and A_{F_j} describe the interlinking between the sets C_i and C_j and between the sets C_j and F, respectively. By construction, the row sum of each block matrix $A_{i,j}$ is constant, thus $A_{i,j}u = d_{ij}u$, where d_{ij} denotes the number of neighbors in C_j that each node in C_i has. The row sum of A_{F_j}, i.e. $A_{F_j}u = f_j u$, where f_j is either 0, $n_j/2$ or n_j. Since all block matrices of ${}_\pi A$ are adjacency matrices and symmetric, the column sums are constant as well. Next, Godsil and McKay (1982) introduce the $m \times m$ matrix $V_m = \frac{2}{m} J_{m\times m} - I_m$, where the all-one $r \times m$ matrix $J_{r\times m} = u_r . u_m^T$. The matrix V_m features interesting properties, because V_m is a Householder reflection (see **art.** 197). First, using $J_{l\times q} J_{q\times k} = u_l u_q^T u_q u_k^T$ and $u_q^T u_q = q$ so that $J_{l\times q} J_{q\times k} = q J_{l\times k}$, we find that

$$ V_m^2 = I_m \tag{2.44} $$

Next, for an $m \times n$ matrix X with constant row sum r and column sum c, it holds that

$$ V_m X V_n = X \tag{2.45} $$

Indeed, $V_m X = \frac{2}{m} u_m u_m^T X - X = \frac{2c}{m} u_m u_n^T - X$ from which

$$ \begin{aligned} V_m X V_n &= \left(\frac{2c}{m} u_m u_n^T - X \right) \left(\frac{2}{n} u_n u_n^T - I_n \right) \\ &= \left(\frac{2c}{m} - \frac{2r}{n} \right) u_m u_n^T + X \end{aligned} $$

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The sum of all elements in X equals $rm = cn$, from which $\frac{c}{m} = \frac{r}{n}$, demonstrating (2.45). Finally, if the $2m \times 1$ vector x contains m zero elements and m one elements, then the definition $V_m = \frac{2}{m} u_m u_m^T - I_m$ directly shows that

$$V_{2m} x = u_{2m} - x \tag{2.46}$$

This last property (2.46) motivates the Godsil-McKay construction of the graph G^* obtained from G with adjacency matrix ${}_\pi A$ as follows. For all those sets C_i, where each node $v \in F$ is connected to $n_i/2$ nodes in C_i, these $n_i/2$ links are deleted and each node $v \in F$ is reconnected to the other $n_i/2$ nodes in the set C_i. The fascinating relation between G and G^* is that G^* and G, as well as their complements G^{*c} and G^c, have the same adjacency eigenvalues. Hence, G and G^* are cospectral with cospectral complement. The proof is surprisingly easy, the adjacency matrix of G^* satisfies

$${}_\pi A^* = V \, ({}_\pi A) \, V \tag{2.47}$$

where the block-diagonal matrix $V = \mathrm{diag}\big(V_{n_1}, V_{n_2}, \ldots, I_{|F|}\big)$. Property (2.45) illustrates that ${}_\pi A^*$ is the same as ${}_\pi A$, except for the last block row and block column. Property (2.46) switches in A_{F_j} all zero entries into one and vice versa. Finally, left-multiplying both sides of (2.47) by V and invoking property (2.44) shows that the eigenvalue equation ${}_\pi A^* y = \lambda y$ is equivalent to ${}_\pi A \, (Vy) = \lambda \, (Vy)$. Hence, ${}_\pi A^*$ and ${}_\pi A$ possess the same eigenvalues with the corresponding eigenvectors y and Vy. Since the adjacency matrix of the complement G^c is also a block matrix with constant row and column sums and of similar block structure as ${}_\pi A$, the same arguments also demonstrate that G^{*c} and G^c are cospectral.

The Godsil-McKay construction of the cospectral graph G^* illustrates that the main difficulty lies in finding a non-trivial Godsil-MacKay partition π with corresponding adjacency matrix ${}_\pi A$. The useful properties of V_m for cospectral graph constructions result from the fact that the labeling of nodes in any cell C_i and F does not influence a sum as $u_m^T z_m = \sum_{k=1}^m z_k$, so that only constant row (and column) sums are required in the Godsil-McKay construction.

40. Although cospectral graphs are not easy to construct, they should not be ignored. The following theorem, due to Brendan McKay, implies that the probability to draw a regular graph (**art.** 55) out of the set of all nonisomorphic graphs with N nodes is substantially lower than randomly choosing a cospectral graph.

Theorem 6 (McKay) *For sufficiently large N, the number of cospectral graphs exceeds the number of regular graphs.*

Proof[13]**:** The number of pairs of cospectral graphs, conjectured by Godsil and McKay (1982) and proved by Haemers and Spence (2004, Theorem 3), is at least $\left(\frac{1}{24} - o\,(1)\right) N^3 g_{N-1}$, where $g_N = n_{\text{nonisomorphic } G(N)}$ in (2.42) is the number of

[13] Private communication with Brendan McKay.

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nonisomorphic graphs with N nodes (**art.** 35). Since pairs of cospectral graphs are a subset of all cospectral graphs and since most graphs are asymmetric (**art.** 34), we find with (2.42), for large N, that the number of cospectral graphs is lower bounded by $n_{\text{cospectral graph}} \geq cN^4 \frac{2^{\binom{N-1}{2}}}{N!}$, where c is a constant. The total number of regular graphs was determined, for large N, by McKay and Wormald (1990, Corollary 1),

$$n_{\text{regular graphs}} \sim \sqrt{2e}\beta_N \frac{2^{\frac{N^2}{2}}}{(\pi N)^{\frac{N}{2}}}$$

where β_N, specified in McKay and Wormald (1990, Corollary 1), has a different value depending on whether N is even, $1 \bmod 4$ or $3 \bmod 4$. Let the constant $b = \max_N \sqrt{2e}\beta_N$ so that $b \approx 4.2$. Most regular graphs are shown in Krivelevich *et al.* (2001) to be asymmetric. The total number of nonisomorphic regular graphs is, for large N, at most

$$n_{\text{nonisomorphic regular graphs}} \leq b' \frac{2^{\frac{N^2}{2}}}{(\pi N)^{\frac{N}{2}}\, N!}$$

where the constant b' is slightly larger than b. The ratio

$$\frac{n_{\text{nonisomorphic regular graphs}}}{n_{\text{cospectral graph}}} \leq \frac{b'}{c} \frac{1}{(\pi N)^{\frac{N}{2}}\, N^4 2^{-\frac{3}{2}N+1}} = O\left(\frac{e^{-\frac{N}{2}(\ln N + \ln \pi - 3\ln 2)}}{N^4}\right)$$

rapidly tends to zero with N. □

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