Chapter 2
Worth Another Binary Relation: Graphs

In Chap. 1, we have accounted for the different ways we can enumerate elements in a finite set. In particular, we have mentioned that a permutation $\Pi : \mathcal{G} \to \mathcal{G}$ of the finite set $\mathcal{G}$, defines an equivalence relation $\sim$ that partitions $\mathcal{G}$ into a set of equivalence classes $\mathcal{G}/\sim$. In the present chapter, we discuss worth another binary relation,

$$v \smile u, \quad v, u \in \mathcal{G} \tag{2.1}$$

called *adjacency*, and its graph.

2.1 Binary Relations and Their Graphs

A *binary relation* defined on a finite set $\mathcal{G}$ is a collection of ordered pairs $G \subseteq V \times U$ of elements from the arbitrary subsets $V, U \subseteq \mathcal{G}$. The sets $V \subseteq \mathcal{G}$ and $U \subseteq \mathcal{G}$ are called the *domain* and the *codomain* of the relation (2.1), while the collection of ordered pairs G is called its *graph*. In particular, if $V = U = \mathcal{G}$, we simply say that the binary relation (2.1) is defined over $\mathcal{G}$, and its graph is $G = (V, E)$ where V is the set of identical elements called *vertices* (or *nodes*), and $E \subseteq V \times V$ is a collection of pairs of elements from V called *edges*. Graphs are traditionally represented by diagrams in the following way: *vertices are shown by points and edges are the lines connecting vertices if they are related by (2.1).*

Given the two graphs, G and $\bar{G}$, defined on the same set of vertices V, the graph $\bar{G}$ is the *complement* of the graph G if its edge set consists of the edges not present in G.

Given a graph G, we may replace each edge of G by a vertex of some new graph $\mathcal{L}_G$ in such a way that two vertices of $\mathcal{L}_G$ are adjacent if and only if their corresponding edges share a common vertex ("are adjacent") in G. The graph $\mathcal{L}_G$ is called the *line* graph of G. It is obvious that properties of a graph G that depend only on adjacency between edges may be translated into equivalent properties in $\mathcal{L}_G$ that depend on adjacency between vertices. It is worth a mention that taking the line

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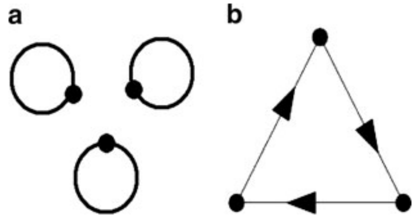


Fig. 2.1 (**a**) A looped graph. (**b**) A cyclic triple

graph twice does not return the original graph G, unless it is a cycle graph, with the cycle length $k \geq 3$.

The graph G is

- *connected directed* if the relation (2.1) is *trichotomous* (for all $v \in \mathfrak{G}$ and $u \in \mathfrak{G}$, exactly one of $v \smile u$, $u \smile v$ or $u = v$ holds).
- *undirected* if the relation (2.1) is *symmetric*: for all $v \in \mathfrak{G}$ and $u \in \mathfrak{G}$, it holds that if $v \smile u$ then $u \smile v$.
- *looped* (its edges connect vertices to themselves, see Fig. 2.1a) if the relation (2.1) is *reflexive* (for all $v \in \mathfrak{G}$, it holds that $v \smile v$) and *coreflexive* (for all $v \in \mathfrak{G}$ and $u \in \mathfrak{G}$, it holds that if $v \smile u$ then $v = u$).
- *non looped* if the relation (2.1) is *irreflexive* (for all $v \in \mathfrak{G}$, it holds that $v \not\smile v$).
- *oriented*, if it has no symmetric pair of directed edges, that is, if the relation (2.1) is *antisymmetric* (for all $v \in \mathfrak{G}$ and $u \in \mathfrak{G}$, it holds that if $v \smile u$ and $u \smile v$ then $v = u$) and *asymmetric* (for all $v \in \mathfrak{G}$ and $u \in \mathfrak{G}$, it holds that if $v \smile u$, then $u \not\smile v$).
- *complete directed*, if the relation (2.1) is *total* (or *linear*) (for all $v \in \mathfrak{G}$ and $u \in \mathfrak{G}$, it holds that either $v \smile u$, or $u \smile v$, or both).
- consisting of a number of *cyclic triples* (or *transitive triples*) if the relation (2.1) is *transitive* (for all $v \in \mathfrak{G}$, $u \in \mathfrak{G}$, and $w \in \mathfrak{G}$, it holds that if $v \smile u$ and $u \smile w$ then $v \smile w$, see Fig. 2.1b).
- *complete* (with self-loops), if (2.1) constitutes an *equivalence* relation, i.e., it is reflexive, symmetric and transitive.
- a *partial order* if the relation (2.1) is reflexive, antisymmetric and transitive.
- a *chain* if it is a total partial order.

2.2 Representation of Graphs by Matrices

Graphs are conveniently represented by matrices. The major advantage of using matrices is that calculations of various graph characteristics can be performed by means of the well known operations with matrices.

For any finite set V of $|V| = N$ vertices, we introduce the canonical orthonormal basis $\{\mathbf{e}_j\}_{j=1}^{N}$ by assigning a unit vector

$$\mathbf{e}_i = (0, 0, \ldots, 1_i, \ldots 0),$$

with 1 at the i-th position, for every vertex $i \in V$. The set of orthonormal vectors constitutes a basis of the space of real functions on V, which we denote as $\mathfrak{F}(V)$. The inner product of two functions f and g from $f, g \in \mathfrak{F}(V)$ is then defined as

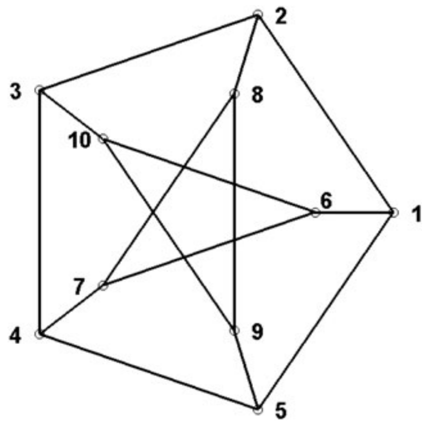
$$(f, g) = \sum_{i \in V} f(i)g(i). \tag{2.2}$$

We introduce the linear *adjacency operator* $\mathcal{A}$ on $\mathfrak{F}(V)$ by

$$(\mathcal{A}f)(i) = \sum_{j \smile i} f(j), \quad f \in \mathfrak{F}(V) \tag{2.3}$$

where $j \smile i$, iff $(i, j) \in E$. Therefore, the adjacency operator is unique for each graph $G(V, E)$, with fixed enumeration of its vertices. The $N \times N-$matrix $\mathbf{A}$ representing the adjacency operator $\mathcal{A}$ with respect to the canonical basis is called the *adjacency matrix* of the graph G. The off-diagonal entry A_{ij}, $i \neq j$, equals the number of edges linking the vertex $i \in V$ to the vertex $j \in V$. The diagonal entry A_{ii} equals the number of loops at the vertex $i \in V$. The adjacency matrix is unique for each graph (up to permuting rows and columns). In the special case of a finite *simple graph*, the adjacency matrix is a (0, 1)-matrix with zeros on its diagonal. The adjacency matrix of a complete graph is all 1's except for 0's on the diagonal. For example, the *Petersen graph* is represented by its adjacency matrix (see Fig. 2.2).

A *weighted graph* is a graph in which each edge $(i, j) \in E$ has an assigned weight w_{ij}, a real or complex number. The matrix $\mathbf{W}$ of elements w_{ij} describing the weights of all edges in the graph G is called its *affinity matrix*. Clearly, the adjacency matrix is a particular case of the affinity matrix, with all nontrivial weights $w_{ij} = 1$.



$$A_{\text{Petersen}} = \begin{pmatrix} 0&1&0&0&1&1&0&0&0&0 \\ 1&0&1&0&0&0&0&1&0&0 \\ 0&1&0&1&0&0&0&0&0&1 \\ 0&0&1&0&1&0&1&0&0&0 \\ 1&0&0&1&0&0&0&0&1&0 \\ 1&0&0&0&0&0&1&0&0&1 \\ 0&0&0&1&0&1&0&1&0&0 \\ 0&1&0&0&0&0&1&0&1&0 \\ 0&0&0&0&1&0&0&1&0&1 \\ 0&0&1&0&0&1&0&0&1&0 \end{pmatrix}$$

Fig. 2.2 The Petersen graph and its adjacency matrix

The adjacency matrix allows us to formalize the intuitive idea of connectivity of a vertex in a graph. In various applications, higher connectivity vertices play the role of hubs being traversed by more paths between various origin/destination pairs than those with less connectivity. The *degree* of a vertex $i \in V$ is the number of other vertices adjacent to i in the graph G,

$$\begin{aligned} \deg(i) &= \operatorname{card}\{j \in V : i \smile j\} \\ &= \sum_{j \in V} A_{ij}\,. \end{aligned} \tag{2.4}$$

The notion of a vertex degree can be readily generalized for the weighted graph as

$$\deg(i) = \sum_{j \in V} w_{ij}\,. \tag{2.5}$$

The vector of vertex degrees in the unweighted graph G can be calculated with the help of the vector $\mathbf{j} = (1, 1, \ldots, 1)^\top$ as

$$\mathbf{A}_G \mathbf{j} = (\deg(1), \deg(2), \ldots \deg(N))\,. \tag{2.6}$$

The graph is *regular* if each vertex has the same degree. Since each edge is accounted twice while calculating the sum of degrees over all vertices in the graph, it is clear that

$$\sum_{i=1}^{N} \deg(i) = 2|E| \tag{2.7}$$

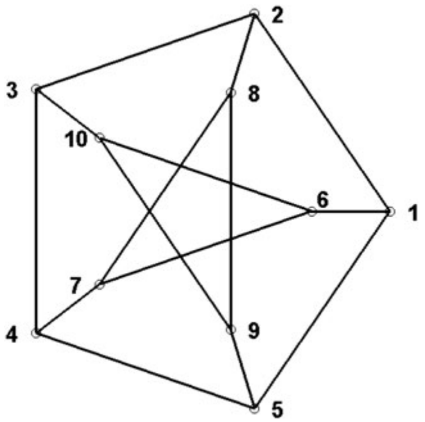
where $|E|$ is the cardinality of the set of edges.

A graph G can be alternatively represented by the *incidence* matrix $\mathbf{B}_G$ that shows the relationship between vertices and edges. The matrix $\mathbf{B}_G$ has one row for each vertex of the graph G and one column for each edge. The entry in the row i and the column j of the incidence matrix $\mathbf{B}_G$ is 1 if the edge j is incident to the vertex i in the graph G and is 0 if it is not. Therefore, the inner product of two columns of the incidence matrix of the graph G is nonzero if and only if the corresponding edges have a common vertex. For example, the incidence matrix of the Petersen graph is given in Fig. 2.3 (right).

The incidence matrix $\mathbf{B}_G$ of a graph G is the rectangular $N \times M$- matrix, and the product $\mathbf{B}_G^\top \mathbf{B}_G$ is a positive symmetric matrix that can be related to the adjacency matrix of the line graph $\mathcal{L}_G$ by

$$\mathbf{A}_{\mathcal{L}_G} = \mathbf{B}_G^\top \mathbf{B}_G - 2 \cdot \mathbf{1}. \tag{2.8}$$

The adjacency matrix of the line graph $\mathbf{A}_{\mathcal{L}_G}$ is the square $M \times M$—matrix describing the line graph that consists of M vertices and



$$B_{\text{Petersen}} = \begin{pmatrix} 1&0&0&1&0&0&0&0&0&0&1&0&0&0&0 \\ 1&0&0&0&1&0&0&1&0&0&0&0&0&0&0 \\ 0&0&0&0&0&1&0&1&1&0&0&0&0&0&0 \\ 0&0&1&0&0&0&0&0&1&1&0&0&0&0&0 \\ 0&0&0&0&0&0&1&0&0&1&1&0&0&0&0 \\ 0&1&0&1&0&0&0&0&0&0&0&1&0&0&0 \\ 0&0&1&0&0&0&0&0&0&0&0&1&1&0&0 \\ 0&0&0&0&1&0&0&0&0&0&0&0&1&1&0 \\ 0&0&0&0&0&0&1&0&0&0&0&0&0&1&1 \\ 0&1&0&0&0&1&0&0&0&0&0&0&0&0&1 \end{pmatrix}$$

Fig. 2.3 The Petersen graph and its incidence matrix

$$M' = \frac{1}{2} \sum_{i \in V} \deg(i)^2 - M \tag{2.9}$$

edges.

2.3 Algebraic Properties of Adjacency Operators

A function $f \in \mathfrak{F}(V)$ is an eigenvector for $\mathbf{A}_G$ if there is a constant θ such that, for each vertex $i \in V$,

$$\theta f(i) = \sum_{j \smile i} f(j), \tag{2.10}$$

that means

$$\mathbf{A}_G f = \theta f.$$

The eigenvalue θ of the eigenfunction f is the root of the characteristic polynomial

$$Q_A = \det(\theta \cdot \mathbf{1} - \mathbf{A}_G). \tag{2.11}$$

It follows from (2.10) that

$$\begin{aligned} |\theta|\,|f(i)| &= \left| \sum_{j \smile i} f(j) \right| \\ &\leq \sum_{j \smile i} |f(j)|\,, \end{aligned} \tag{2.12}$$

and therefore,

$$|\theta| \leq \sum_{j \smile i} \frac{|f(j)|}{|f(i)|}, \tag{2.13}$$

where the equality holds if and only if f is a constant function.

Let us note that the determinant of the adjacency matrix $\mathbf{A}_G$ can be expanded into the sum of contributions from all possible permutations $\Pi \in \mathcal{S}_N$ involving $n = 2, \ldots, N$ nodes of the graph G,

$$\det(\mathbf{A}_G) = \sum_{\Pi \in \mathcal{S}_n} \operatorname{sign}(\Pi) \cdot \prod_{i=1}^{n} A_{i,\Pi(i)} \tag{2.14}$$

where $\operatorname{sign}(\Pi)$ is the sign of the permutation Π. It is obvious that a permutation Π contributes into the sum (2.14) if and only if $(i, \Pi(i)) \in E$. Since any permutation can be decomposed into a product of disjoint cycles (see Sect. 1.2), the permutation Π such that $(i, \Pi(i)) \in E$ induces a *cycle cover* γ of the graph G, the partition of the vertex set into disjoint cycles.

Let us denote the number of connected components in γ as $\operatorname{comp}(\gamma)$, the number of cycles (of the length greater than 2) in that as $\operatorname{cyc}(\gamma)$, and the number of cycles in the cycle cover (including the cycles of length one) as $\operatorname{cyc}(\Pi)$. As the number of odd cycles in Π is congruent (modulo 2) to n, it follows that $n + \operatorname{cyc}(\Pi)$ is congruent (modulo 2) to the number of even cycles in Π. Therefore,

$$\operatorname{sign}(\Pi) = (-1)^{n+\operatorname{cyc}(\Pi)}. \tag{2.15}$$

We also note that since direct and inverse cycles equally contribute into (2.14), there are $2^{\operatorname{cyc}(\gamma)}$ permutations of the same sign in (2.14). Finally, we conclude that for a connected undirected graph G,

$$\det(\mathbf{A}_G) = \sum_{\gamma \subset G} (-1)^{n+\operatorname{cyc}(\Pi)} 2^{\operatorname{cyc}(\gamma)} \tag{2.16}$$

where the summation is over all subgraphs $\gamma \subset G$ of $n = 1, \ldots N$ nodes.

2.4 Perron–Frobenius Theory for Adjacency Matrices

For more information on the spectral properties of adjacency matrices, let us mention that a matrix $\mathbf{A}$ is called *irreducible* if it is not similar to a block upper triangular matrix via a permutation, i.e., there is no any permutation matrix $\boldsymbol{\Pi}$ such that the matrix $\boldsymbol{\Pi}^{-1}\mathbf{A}\boldsymbol{\Pi}$ is of the block upper triangular form. It is worth a mention that if an undirected graph underlying the adjacency matrix $\mathbf{A}$ is connected, then the matrix is always irreducible. Spectral properties of irreducible matrices with non-negative entries are described by the famous *Perron -Frobenius theorem* which asserts that any irreducible real square matrix with non-negative entries has a unique largest real eigenvalue and that the corresponding eigenvector has strictly positive components.

A matrix $\mathbf{A}$ with entries a_{ij} is said to be nonnegative if $a_{ij} \geq 0$, and $\mathbf{A}$ is said to be positive if $a_{ij} > 0$.

Theorem 2.1 (Perron-Frobenius theorem). *Let* $\mathbf{A}$ *be a non-negative irreducible matrix. Then*

1. *The largest eigenvalue* $\nu > 0$
2. *There exists a positive vector* $\mathbf{u} \in \mathbb{R}^n$ *such that* $\mathbf{Au} = \nu\mathbf{u}$,
3. *There exists a positive vector* $\mathbf{v} \in \mathbb{R}^n$ *such that* $\mathbf{A}^\top\mathbf{v} = \nu\mathbf{v}$.
4. *The algebraic multiplicity of* ν *as an eigenvalue of* $\mathbf{A}$ *is equal to one.*

The complete proof of the Perron-Frobenius theorem can be found in many text books such as Bapat and Raghavan (1997) and Dym (2007). Following Ninio (1976), we give below a simple proof of the theorem for positive symmetric matrices $\mathbf{A} = \mathbf{A}^\top$ describing undirected graphs.

Proof. Since the eigenvalues of $\mathbf{A}$ are real and their sum equals Tr $\mathbf{A} > 0$, it follows that the largest eigenvalue $\nu > 0$. Let $\mathbf{u}_i$ be any real normalized eigenvector belonging to ν,

$$\nu u_i = \sum_j a_{ij} u_j, \quad i = 1, 2, \ldots, n, \tag{2.17}$$

and set $x_j = |u_j|$. Then

$$\begin{aligned} 0 < \nu &= \sum_{ij} a_{ij} \mathbf{u}_i \mathbf{u}_j \\ &= \left| \sum_{ij} a_{ij} \mathbf{u}_i \mathbf{u}_j \right| \\ &\leq \sum_{ij} a_{ij} x_i x_j . \end{aligned} \tag{2.18}$$

By the variational theorem, the right-hand side is less than or equal to ν, with equality if and only if x_j is an eigenvector belonging to the largest eigenvalue ν. We therefore have

$$\nu x_i = \sum_j a_{ij} x_j, \quad i = 1, 2, \ldots, n. \tag{2.19}$$

Now if $x_i = 0$ for some i, then on account of $a_{ij} > 0$ for all j, it follows every $x_j = 0$, which cannot be. Thus, every $x_j > 0$. Finally, if ν is a multiple eigenvalue, we can find (since $\mathbf{A}$ is real symmetric) two orthonormal eigenvectors $\mathbf{u}_j$, $\mathbf{v}_j$ belonging to ν. Suppose that $u_i < 0$ for some i. Adding (2.1) and (2.2), we obtain

$$\begin{aligned} 0 &= \nu\,(u_i + |u_i|) \\ &= \sum_j a_{ij}\left(u_j + |u_j|\right), \end{aligned}$$

and as above, it follows that

$$u_j + |u_j| = 0,$$

for every j. In other words, we have either

$$u_j = |u_j| > 0$$

for every j, or

$$u_j = -|u_j| < 0$$

for every j. The same applies to $\mathbf{v}_j$. Hence,

$$\sum_j v_j u_j = \pm \sum_j |v_j u_j| \neq 0$$

so that $\mathbf{u}$ and $\mathbf{v}$ cannot be orthogonal, and therefore ν is non-degenerate. Let now assume that $\mathbf{w}_j$ be a normalized eigenvector belonging to $\mu < \nu$,

$$\sum_j a_{ij} w_j = \mu w_i\,.$$

The variational property and the non-degeneracy of ν then yields

$$\nu > \sum_{ij} a_{ij}\,|w_i| \cdot |w_j| \geq \left|\sum_{ij} a_{ij} w^* w_j\right| = |\mu|. \tag{2.20}$$

□

2.5 Spectral Decomposition of Adjacency Operators

If the graph G is undirected, the corresponding adjacency operator is self-adjoint with respect to the scalar product (2.2), and therefore the adjacency matrix is symmetric; its eigenvalues are real and eigenvectors form an orthogonal basis for $\mathfrak{F}(V)$. For a regular graph G (where each vertex has the same number of neighbors), it is easy to check that the vector $\mathbf{j}$ consisting of all 1's is an eigenvector of the adjacency matrix A, with the eigenvalue $\theta = \deg_G$, the common degree of vertices in that.

A simple complete graph on N nodes also has the eigenvector $\mathbf{j}$ belonging to the eigenvalue $\theta = (N-1)$. Another eigenvalue of the complete graph characterizes those eigenfunctions $f(i) \in \mathfrak{F}(V)$ satisfying

$$\sum_{i \in V} f(i) = 0. \tag{2.21}$$

From (2.21), it is obvious that such the eigenfunctions satisfy the relation

$$\sum_{j \smile i} f(j) = -f(i), \tag{2.22}$$

and therefore $\theta' = -1$ is the correspondent eigenvalue, with the multiplicity $(N-1)$.

The Petersen graph (see Fig. 2.2) is regular, $\deg_{\mathrm{Pet}} = 3$; its maximal eigenvalue $\theta_{\max} = 3$ corresponds to the normalized eigenvector $\frac{1}{\sqrt{10}}\mathbf{j}$ and express the *mean value property*,

$$f(i) = \frac{1}{3} \sum_{j \smile i} f(j). \tag{2.23}$$

The next eigenvalue, $\theta' = 1$, with multiplicity $m_{\theta'} = 5$, describes the five configurations $f \in \mathfrak{F}(V)$, for which

$$f(i) = \sum_{j \smile i} f(j). \tag{2.24}$$

Let $\mathbf{U}_{\theta'}$ be a $N \times m_{\theta'}$ matrix whose columns form an orthogonal basis for the eigenspace belonging to θ',

$$\mathbf{U}_{\theta'}^{\top} = \begin{pmatrix} -\frac{\sqrt{6}}{6} & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & 0 & 0 & \frac{\sqrt{6}}{6} \\ -\frac{\sqrt{5}\sqrt{2}}{10} & -\frac{\sqrt{5}\sqrt{2}}{10} & 0 & \frac{\sqrt{5}\sqrt{2}}{5} & \frac{\sqrt{5}\sqrt{2}}{10} & -\frac{\sqrt{5}\sqrt{2}}{10} & \frac{\sqrt{5}\sqrt{2}}{10} & 0 & 0 & -\frac{\sqrt{5}\sqrt{2}}{10} \\ -\frac{\sqrt{12}\sqrt{5}}{20} & \frac{\sqrt{12}\sqrt{5}}{30} & \frac{\sqrt{12}\sqrt{5}}{12} & \frac{\sqrt{12}\sqrt{5}}{60} & -\frac{\sqrt{12}\sqrt{5}}{30} & -\frac{\sqrt{12}\sqrt{5}}{20} & -\frac{\sqrt{12}\sqrt{5}}{30} & 0 & 0 & \frac{\sqrt{12}\sqrt{5}}{30} \\ -\frac{\sqrt{9}\sqrt{4}}{36} & -\frac{\sqrt{9}\sqrt{4}}{18} & -\frac{\sqrt{9}\sqrt{4}}{36} & -\frac{\sqrt{9}\sqrt{4}}{36} & \frac{\sqrt{9}\sqrt{4}}{18} & -\frac{\sqrt{9}\sqrt{4}}{36} & -\frac{\sqrt{9}\sqrt{4}}{18} & 0 & \frac{\sqrt{9}\sqrt{4}}{9} & \frac{\sqrt{9}\sqrt{4}}{18} \\ -\frac{\sqrt{2}}{6} & \frac{\sqrt{2}}{6} & -\frac{\sqrt{2}}{6} & -\frac{\sqrt{2}}{6} & -\frac{\sqrt{2}}{6} & -\frac{\sqrt{2}}{6} & \frac{\sqrt{2}}{6} & \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{6} & -\frac{\sqrt{2}}{6} \end{pmatrix}. \tag{2.25}$$

Each column of $\mathbf{U}_{\theta'}$ is an eigenvector of $\mathbf{A}_{\mathrm{Petersen}}$, and therefore

$$\theta' \mathbf{U}_{\theta'} = \mathbf{A}_{\mathrm{Petersen}} \mathbf{U}_{\theta'}.$$

If we denote the i^{th}–row of the matrix $\mathbf{U}_{\theta'}$ by $u_{\theta'}(i)$, then the above equation can be rewritten in the following form,

$$\theta u_{\theta'}(i) = \sum_{j \smile i} u_{\theta'}(j), \tag{2.26}$$

which allow us to interpret the function $u_{\theta'}(i) : V \to \mathbb{R}^{m_{\theta'}}$ as a *low-dimensional representation* of the vertex $i \in V$ belonging to the eigenvalue θ'.

Columns of the matrix $\mathbf{U}_{\theta'}$ are the orthonormal vectors, so that

$$\mathbf{U}_{\theta'}^{\top} \mathbf{U}_{\theta'} = \mathbf{1} \in \mathbb{R}^{m_{\theta'}}, \tag{2.27}$$

while another product,

$$\boldsymbol{\mathcal{P}}_{\theta'} = \mathbf{U}_{\theta'}\mathbf{U}_{\theta'}^{\top}, \tag{2.28}$$

is the symmetric matrix, $\boldsymbol{\mathcal{P}}_{\theta'} = \boldsymbol{\mathcal{P}}_{\theta'}^{\top}$, an orthogonal projection onto the column space of $\mathbf{U}_{\theta'}$, independent upon the orthonormal basis of vectors $\mathbf{U}_{\theta'}$, as being an *invariant* of the eigenspace belonging to the eigenvalue θ'.

Analogously, the remaining eigenvalue of the adjacency matrix of the Petersen graph, $\theta'' = -2$, with multiplicity $m_{\theta''} = 4$, describes the configurations $f \in \mathfrak{F}(V)$, for which

$$f(i) = -\frac{1}{2}\sum_{j \smile i} f(j). \tag{2.29}$$

The eigenspace belonging to this eigenvalue has the orthogonal basis

$$\mathbf{U}_{\theta''}^{\top} = \begin{pmatrix} -\frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & -\frac{\sqrt{6}}{6} & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \\ \frac{\sqrt{6}}{6} & 0 & \frac{-\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{-\sqrt{6}}{6} & \frac{-\sqrt{6}}{6} & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \\ \frac{\sqrt{9}\sqrt{2}}{18} & \frac{-\sqrt{9}\sqrt{2}}{9} & \frac{\sqrt{9}\sqrt{2}}{18} & \frac{-\sqrt{9}\sqrt{2}}{18} & \frac{\sqrt{9}\sqrt{2}}{18} & \frac{-\sqrt{9}\sqrt{2}}{18} & 0 & \frac{\sqrt{9}\sqrt{2}}{9} & \frac{-\sqrt{9}\sqrt{2}}{9} & \frac{\sqrt{9}\sqrt{2}}{18} \\ \frac{\sqrt{5}\sqrt{2}}{30} & \frac{\sqrt{5}\sqrt{2}}{30} & \frac{\sqrt{5}\sqrt{2}}{30} & \frac{-2\sqrt{5}\sqrt{2}}{15} & \frac{\sqrt{5}\sqrt{2}}{30} & \frac{-2\sqrt{5}\sqrt{2}}{15} & \frac{\sqrt{5}\sqrt{2}}{5} & \frac{-2\sqrt{5}\sqrt{2}}{15} & \frac{\sqrt{5}\sqrt{2}}{30} & \frac{\sqrt{5}\sqrt{2}}{30} \end{pmatrix}. \tag{2.30}$$

Let us denote the orthogonal projection onto the column space of $\mathbf{U}_{\theta''}$ as

$$\boldsymbol{\mathcal{P}}_{\theta''} = \mathbf{U}_{\theta''}\mathbf{U}_{\theta''}^{\top}. \tag{2.31}$$

It is obvious that

$$\boldsymbol{\mathcal{P}}_{\theta}\boldsymbol{\mathcal{P}}_{\tau} = \boldsymbol{\mathcal{P}}_{\theta}\delta_{\theta\tau}, \tag{2.32}$$

and $\boldsymbol{\mathcal{P}}_{\theta'}\boldsymbol{\mathcal{P}}_{\theta''} = 0$, in particular. Generalizing this example, we conclude that

$$\mathbf{A}_G\boldsymbol{\mathcal{P}}_{\theta} = \theta\boldsymbol{\mathcal{P}}_{\theta}, \tag{2.33}$$

and therefore, there is a *spectral decomposition* for the adjacency matrix $\mathbf{A}_G$,

$$\mathbf{A}_G = \sum_{\theta} \theta\boldsymbol{\mathcal{P}}_{\theta} \tag{2.34}$$

where the summation is over all eigenvalues of $\mathbf{A}_G$.

2.6 Adjacency and Walks on a Graph

A *walk* W_ℓ of length $\ell \geq 1$ in a graph G is an ordered sequence of vertices of G,

$$W_\ell = \{v_0, v_1, \ldots v_\ell\},$$

such that $v_{k-1} \smile v_k$, $k = 1, \ldots, \ell$. If the first and the last vertices of the walk coincide, then W_ℓ is a cycle.

The nonnegative integer powers of a matrix $\mathbf{A}_G$ of order N are defined by

$$\mathbf{A}_G^0 = \mathbf{1}, \quad \mathbf{A}_G^1 = \mathbf{A}_G,$$

and

$$\mathbf{A}_G^k = \mathbf{A}_G \cdot \mathbf{A}_G^{k-1},$$

for $k > 1$. Provided $\mathbf{A}_G$ is the adjacency matrix of the graph G, the elements of its positive integer power, $A_{G\,ij}^k$, equal the numbers of walks of length k connecting the vertices $i \in V$ and $j \in V$ in the graph G. This is obviously true for $k = 1$ since the graph G has precisely one walk connecting i and j if $A_{G\,ij} = 1$, but the vertices are not connected if $A_{G\,ij} = 0$. For $k > 1$, we can justify the above statement by the inductive assumption. Namely, let us assume that $A_{G\,ij}^k$ equals the number of all walks of length k connecting the two vertices i and j in G. For the elements of the forthcoming matrix, we have

$$\begin{aligned} A_G^{k+1}{}_{ij} &= A_{i1} \cdot A_{G\,1j}^k + \ldots + A_{iN} \cdot A_{G\,Nj}^k \\ &= \sum_{l \smile i} A_{g\,lj}^k \end{aligned} \tag{2.35}$$

where the latter sum is nothing else but the *total number of all walks* of length k between the vertex j and all vertices $l \in V$ directly connected to i in the graph G. Hence, $A_G^{k+1}{}_{ij}$ equals the number of all walks of length $k+1$ connecting the vertices i and j, completing the induction.

The number of closed walks of length k in G equals the sum of diagonal elements in the matrix $\mathbf{A}_G^k$,

$$\mathrm{Tr}\ \mathbf{A}^k = \sum_\theta \theta^k, \tag{2.36}$$

where the last sum is over all eigenvalues θ, with the account of their multiplicity. Hence we get the following simple results:

$$\mathrm{Tr}\ \mathbf{A}_G = 0 \quad \text{iff} \quad G \quad \text{is} \quad \text{simple}; \tag{2.37}$$

$$\mathrm{Tr}\ \mathbf{A}_G^2 = 2E, \tag{2.38}$$

where E is the number of edges,

$$\mathrm{Tr}\ \mathbf{A}_G^k = k!\mathrm{cyc}_k(G), \tag{2.39}$$

where $\mathrm{cyc}_k(G)$ is the number of cycles of length k in the graph G.

Let $\mathbf{U}$ is the orthogonal matrix of eigenvectors of the adjacency matrix $\mathbf{A_G}$. Then

$$A_{G\,ij}^k = \sum_{l=1}^n \theta_l^k u_{il} u_{jl}.$$

The number of all walks of length k in G equals

$$\begin{aligned} N_k(G) &= \sum_{i,j\in V} A^k_{Gij} \\ &= \sum_{l=1}^{N}\left(\sum_{i=1}^{N} u_{il}\right)^2 \theta_l^k \\ &= \sum_{l=1}^{N} \xi_l \theta_l^k \end{aligned}$$

where $\xi_l \equiv \left(\sum_{i=1}^N u_{il}\right)^2$. The generating function for the numbers $N_k(G)$ is

$$\begin{aligned} H(t) &= \sum_{k=0}^{\infty} N_k t^k \\ &= \sum_{l=1}^{N} \frac{\xi_l}{1 - t\theta_l}. \end{aligned}$$

2.7 Principal Invariants of the Graph Adjacency Matrix

An *isomorphism* between the two undirected non-weighted graphs G_1 and G_2 is an edge-preserving bijection f between their vertex sets. Namely, any two vertexes $v \smile u$ adjacent in G_1, are mapped by f into the two vertexes $f(v) \smile f(u)$, adjacent in G_2. Isomorphic graphs are said to have the same structure, as sharing all *graph invariants* which depend on neither a labeling of the graph vertexes, nor a drawing. The important structural characteristics of a graph, such as the order of the graph N, the number of 1-loops in the graph $N_\circ$, the size of the graph E, the number of triangles $N_\triangle$, and, in general, the number of the k–cycles $\mathrm{cyc}_k(G)$, for all $k = 1, \ldots, N$, are the graph invariants, as they are preserved under the action of graph isomorphisms, but changed if the graph transformation is not an isomorphism. It is then obvious that the values of polynomials in the above structural characteristics are also preserved under the action of graph isomorphisms, though in the common case they could be the same even for two non-isomorphic graphs.

In the present section, we show that for each undirected graph there are some polynomials in the structural characteristics which remains invariant under the graph isomorphisms. They are related to the *principal invariants* of the graph adjacency matrix $\mathbf{A}_G$, that are the coefficients $I_k(\mathbf{A}_G)$, $k = 1, \ldots, N$, of its characteristic polynomial,

$$\begin{aligned} \det\left(\mathbf{A}_G - \theta \cdot \mathbf{1}\right) &= \sum_{k=0}^{N} I_k(\mathbf{A}_G)(-\theta)^{N-k} \\ &= 0, \end{aligned} \tag{2.40}$$

where θ is an eigenvalue of $\mathbf{A}_G$. The principal invariants $I_k(\mathbf{A}_G)$, can be expressed, in terms of the moments Tr $\mathbf{A}_G^k$ (see Gantmacher 1959, Chap. 4), with the use of Newton's identities resulting in the k-th symmetric polynomials,

$$I_k\left(\mathbf{A}_G\right) = \frac{(-1)^{k-1}}{k}\sum_{l=0}^{k-1}(-1)^l I_l(\mathbf{A}_G)\mathrm{Tr}\ \mathbf{A}_G^l, \tag{2.41}$$

where we assume that $I_0 = 1$. In particular, accordingly to (2.38, 2.39)

$$\begin{aligned} I_1\left(\mathbf{A}_G\right) &= \mathrm{Tr}\ \mathbf{A}_G \\ &= N_\circ, \end{aligned} \tag{2.42}$$

$$\begin{aligned} I_2\left(\mathbf{A}_G\right) &= \frac{1}{2}\left((\mathrm{Tr}\ \mathbf{A}_G)^2 - \mathrm{Tr}\ \mathbf{A}_G^2\right) \\ &= \frac{N_\circ^2}{2} - E, \end{aligned} \tag{2.43}$$

$$\begin{aligned} I_3\left(\mathbf{A}_G\right) &= \frac{1}{3}\left((\mathrm{Tr}\ \mathbf{A}_G)^3 - 3\mathrm{Tr}\ \mathbf{A}_G^2\mathrm{Tr}\mathbf{A}_G + 2\mathrm{Tr}\ \mathbf{A}_G^3\right) \\ &= \frac{N_\circ^3}{3} - 2E\cdot N_\circ + 4N_\triangle, \end{aligned} \tag{2.44}$$

etc. It can be shown that the expressions (2.41) correspond to the non-negative integer partitions of the number k,

$$k = 1\cdot m_1 + 2\cdot m_2 + \ldots + k\cdot m_k, \tag{2.45}$$

in which m_i is the number of subsets containing precisely i elements in the corresponding partition, as each such a partition contributes into (2.41) by the product of moments,

$$\begin{aligned} T_{m_1,\ldots,m_k} &\equiv \mathrm{Tr}\left(\mathbf{A}_G^{m_1}\right)\ldots\mathrm{Tr}\left(\mathbf{A}_G^{m_k}\right) \\ &= m_1!\ldots m_k! N_\circ\cdot E\cdot N_\triangle\cdot N_\square\ldots\mathrm{cyc}_k(G) \end{aligned} \tag{2.46}$$

where $\mathrm{cyc}_k(G)$ is the number of the k-cycles in the graph G. We have used (2.39) to derive the last equality in (2.46). Since the partition labels a conjugate class in the symmetric group of permutations of k elements $\mathcal{S}_k$, we conclude from (1.18) that the number of elements in the conjugate class is equal to

$$C_{m_1,\ldots,m_k} = \frac{k!}{m_1!\ldots m_k! 1^{m_1}\ldots k^{m_k}}, \tag{2.47}$$

and taking into account the parities of partitions, we derive the combinatorial expression for the principal invariants of the graph,

$$I_k\left(\mathbf{A}_G\right) = \frac{1}{k!} \sum_{\left\{\sum_i i m_i = k\right\}} (-1)^{\sum_i (i-1) m_i} C_{m_1,\ldots,m_k} T_{m_1,\ldots,m_k}, \tag{2.48}$$

in which the summation is defined over all nonnegative–integer partitions (2.45).

Alternatively, in order to obtain the expressions (2.48) we can use the generating function approach proposed by Zhang et al. 2008. Let us define the two generating functions $\mathfrak{F}(z)$ and $\mathfrak{G}(z)$ for the infinite sequences $\{I_k\}_{k=1}^{\infty}$ and $\left\{\mathrm{Tr}\ \mathbf{A}_G^k\right\}_{k=1}^{\infty}$ respectively,

$$\mathfrak{F}(z) = \sum_{k=0}^{\infty} z^k I_k, \quad I_0 = 1, \tag{2.49}$$

and

$$\mathfrak{G}(z) = \sum_{k=0}^{\infty} z^k \mathrm{Tr}\ \mathbf{A}_G^k. \tag{2.50}$$

Analyzing the recursive relations (4.15) between the principal invariants I_k, we can conclude that the generating functions (2.49) and (2.50) satisfy the differential equation

$$\frac{d}{dz}\mathfrak{F}(z) = -\mathfrak{F}(z)\mathfrak{G}(z) \tag{2.51}$$

supplied by the initial condition $\mathfrak{F}(0) = 1$. The solution of (2.51) is

$$\begin{aligned}
\mathfrak{F}(z) &= \exp\left(-\int_0^z \mathfrak{G}(z) dz\right) \\
&= \exp\left(-\sum_{k=1}^{\infty} \frac{z^k}{k} \mathrm{Tr}\ \mathbf{A}_G^k\right) \\
&= \prod_{k=1}^{\infty} \exp\left(-\frac{z^k}{k} \mathrm{Tr}\ \mathbf{A}_G^k\right) \\
&= \sum_{k=0}^{\infty} z^k \cdot \sum_{\left\{\sum_{l=1}^k l m_l = k\right\}} \prod_{l=1}^{k} \frac{(-1)^{m_l}}{m_l!} \left(\frac{\mathrm{Tr}\ \mathbf{A}_G^l}{l}\right)^{m_l}.
\end{aligned} \tag{2.52}$$

Thus, we obtain, for the principal invariants of the graph adjacency matrix, the expression equivalent to (2.48):

$$I_k\left(\mathbf{A}_G\right) = \sum_{\left\{\sum_{l=1}^k l \cdot m_l = k\right\}} \prod_{l=1}^{k} \frac{(-1)^{m_l}}{m_l!} \left(\frac{\mathrm{Tr}\ \mathbf{A}_G^l}{l}\right)^{m_l}, \tag{2.53}$$

where the summation is defined over all partitions (2.45).

Plugging the expressions (2.46) and (2.47) back into (2.48), we obtain the general expression for the principal invariants of the adjacency matrix $\mathbf{A}_G$ in terms of the numbers of l–cycles in the graph G,

$$I_k\left(\mathbf{A}_G\right) = \sum_{\{\sum_i i m_i = k\}} (-1)^{\sum_i (i-1) m_i} \prod_{l=1,\dots,k;m_l \neq 0} \frac{\mathrm{cyc}_l(G)}{l^{m_l}}. \tag{2.54}$$

2.8 Euler Characteristic and Genus of a Graph

Any graph can be drawn as a set of points in $\mathbb{R}^3$ and of continuous arcs connecting some pairs of them. Aiming at a convenient visualization of certain graph's properties, we can draw the graph in many different ways supposing that good graph drawing algorithms allow for as few edge crossings as possible. Those graphs which can be drawn on a plane without edge crossings are called *planar*, as they can be embedded in the plane. As the arcs of a planar graph can be drawn without edge crossings, they divide that plane into some number of regions called *faces*.

The relations between the order (the number of vertices) N, the size (the number of edges) E, and the number of faces F in a planar polygon

$$N - E + F = 1, \tag{2.55}$$

and its direct generalization to a convex polyhedron, a geometric solid in three dimensions with flat faces and straight edges,

$$N - E + F = 2 \tag{2.56}$$

have been known since Descartes (1639). Leonard Euler was published the formula (2.56) in 1751, while proving that there are exactly five Platonic solids. The remarkable fact is that the result of the sign alternating sums in (2.55, 2.56) called the *Euler characteristic* is independent of both the particular figure and the way it is bent, as being sensitive merely to its topological structure: any change to the graph that creates an additional face would keep the value $N - E + F = 2$ an invariant.

For a general connected graph, the Euler characteristic χ can be defined axiomatically as its unique additive characteristic over its subgraphs,

$$\chi(X \cup Y) = \chi(X) + \chi(Y) - \chi(X \cap Y), \tag{2.57}$$

normalized in such a way that $\chi(\emptyset) = 0$ and $\chi(\mathrm{Polygon}) = 1$, for any polygon. It can be considered as a version of the inclusion-exclusion principle and meets the sieve formula (1.23). In particular, the Euler characteristic can be defined for a finite connected graph G by the alternating sum,

$$\chi(G) = \sum_{k=1}^{k_{\max}} (-1)^{k-1} q_k, \tag{2.58}$$

in which $k_{\max}$ is the maximal degree of vertices in the graph G, $q_1 = E$ is the number of edges in G, q_2 is the number of couples of incident edges (sharing a common vertex), q_3 is the number of triples of incident edges, etc., until $q_{k_{\max}}$ is the number of $k_{\max}$−tuples of incident edges. It can be demonstrated readily that the definition (2.58) coincides with

$$\chi(G) = N - E \tag{2.59}$$

where N is the number of vertices and E is the number of edges in G. To prove the formula (2.59), let us classify vertices of the graph G accordingly to their degrees,

$$c_k = \{v \in V : \deg(v) = k\}, \quad k = 1, \dots, k_{\max}, \tag{2.60}$$

where $k_{\max}$ is the maximal degree of nodes in the graph G and note that

$$\sum_{k=1}^{k_{\max}} k \cdot |c_k| = 2E. \tag{2.61}$$

Let us calculate the number q_2 of couples of edges sharing a common vertex in G. Clearly, each vertex of degree 2 corresponds to a pair of edges contributing to q_2. Moreover, each vertex of degree 3 corresponds to the $\binom{3}{2}$ pairs of edges accounted in q_2. Analogously, each vertex of degree 4 corresponds to the $\binom{4}{2}$ pairs of edges accounted in q_2, etc. Consequently, we obtain

$$q_2 = \sum_{m=2}^{k_{\max}} \binom{m}{2} |c_m|. \tag{2.62}$$

Similarly, we conclude that

$$q_3 = \sum_{m=3}^{k_{\max}} \binom{m}{3} |c_m|, \dots, \quad q_{k_{\max}} = \binom{k_{\max}}{k_{\max}} |c_{k_{\max}}|. \tag{2.63}$$

The above equations establish a duality between the cardinalities of degree classes of vertices in a finite undirected graph and their analogs for edges by means of the linear transformation involving the matrix of binomial coefficients,

$$\begin{pmatrix} q_2 \\ q_3 \\ \vdots \\ q_{k_{\max}-1} \\ q_{k_{\max}} \end{pmatrix} = \begin{pmatrix} 1 & \binom{3}{2} & \ldots\ldots & & \binom{k_{\max}}{2} \\ 0 & 1 & \ldots\ldots & & \binom{k_{\max}}{3} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & 1 & \binom{k_{\max}}{k_{\max}-1} \\ 0 & 0 & \ldots & 0 & 1 \end{pmatrix} \begin{pmatrix} |c_2| \\ |c_3| \\ \vdots \\ |c_{k_{\max}-1}| \\ |c_{k_{\max}}| \end{pmatrix}. \tag{2.64}$$

Now, if we substitute the above relations back into (2.58) and take into account that for any $n \in \mathbb{N}$,

$$\sum_{l=1}^{n} (-1)^{l-1} \binom{n}{l} = 1, \tag{2.65}$$

we obtain the formula (2.59).

A natural generalization of planar graphs are graphs which can be drawn on a surface of a given *genus* that is the number of non-intersecting cycles on the graph. Genera are used in topological theory for classifying surfaces, as two surfaces can be deformed one into the other if and only if they have the same genus; surfaces of higher genus have correspondingly more holes. Spheres have genus zero, as having no holes. Surfaces of genus one are tori. Surfaces of genus two and higher are associated with the hyperbolic plane. The genus $g(G)$ of a graph G can be defined in terms of the Euler characteristic (2.58) via the relationship

$$\chi(G) = 2 - g(G). \tag{2.66}$$

It is easy to check that planar graphs have genus one, and convex polyhedra have genus zero.

2.9 Euler Characteristics and Genus of Complex Networks

In many real-world networks represented by large highly inhomogeneous graphs the distribution describing the fractions $P(k)$ of nodes having precisely k connections to other nodes exhibit a heavy tail (Newman 2003a). The well-known example is a *scale-free network*, in which the degree distribution (asymptotically) follows a power law,

$$P(k) \propto k^{-\gamma},$$

for some $\gamma > 1$. Scale-free graphs noteworthy ubiquitous to many empirically observed networks (Albert and Barabási 2002). It is important to note that the Euler characteristic of a graph defined by (2.58, 2.59) is simply related to the *mean degree* of nodes calculated with respect to the degree statistics. Provided the degree distribution in the graph is $P(k)$, we note that the number of vertices having precisely k neighbors equals

$$|c_k| = N \cdot P(k),$$

so that the relation (2.61) reads as

$$N \cdot \sum_{k=1}^{k_{\max}} k \cdot P(k) = N \langle k \rangle \\ = 2E. \tag{2.67}$$

where $k_{\max}$ is the maximal node degree in the graph G and $\langle \ldots \rangle$ denotes the mean degree in the graph, with respect to the given degree distribution $P(k)$. Then, it follows from the definition of the Euler characteristic (2.59) that for such a graph

$$\frac{\chi(G)}{N} = 1 - \frac{\langle k \rangle}{2}. \tag{2.68}$$

If the mean degree of a node in the network is $\langle k \rangle > 2$, it follows from (2.68) that $\chi(G) < 0$. In particular, the genus of the graph underlying a complex network in such a case equals to

$$g(G) = 2 - \frac{N}{2}\left(2 - \langle k \rangle\right) > 2 \tag{2.69}$$

indicating that the graph can rather be embedded into a surface associated with a hyperbolic geometry. In Krioukov et al. (2009), it has been found that the Internet represented on the level of autonomous systems exhibits a remarkable congruency with the Poincaré disc model of hyperbolic geometry.

2.10 Coloring a Graph

Graph coloring is an assignment of colors to vertices of a graph subject to such a constraint that no two adjacent vertices share the same color. The most famous result in the graph coloring theory know as the *four color map theorem* states that given any separation of a plane into contiguous regions, called a map, the regions can be colored using at most four colors so that no two adjacent regions have the same color. The number of graph colorings $\mathcal{P}_G(z)$ as a function of the number of colors z (known as the *chromatic polynomial* of a graph) was originally defined by G.D. Birkhoff for planar graphs, in an attempt to prove the four color map theorem. The Birkhoff's chromatic polynomial has been generalized to the case of general graphs by Whitney (1932).

Following his work, we consider coloring of N vertices in a graph G in such a way that any two vertices which are joined by an arc are of different colors. It is clear that there are $n = z^N$ possible colorings, formed by giving each vertex in succession any one of z colors at our disposal. Accordingly to the inclusion-exclusion principle (1.23), the cardinality of the set of admissible colorings is

$$\begin{aligned} \mathcal{P}_G(z) = z^N & \\ & -\left[n(e_{ij}) + \ldots + n(e_{kl})\right] \\ & +\left[n(e_{ij}e_{kl} + \ldots)\right] \\ & -\ldots \\ & +(-1)^E n(e_{ij}\ldots e_{kl}), \end{aligned} \tag{2.70}$$

where e_{ij} denotes those colorings with the property that i and j are of the same color (associated with the arc e_{ij} in G), and $n(\ldots)$ denotes the cardinality of those colorings. The first term in (2.70) corresponds to the subgraph containing no arcs, the second term stands for the subgraph of disjoint arcs, eventually the last term corresponds to the whole graph G.

A typical term $n(e_{ij}\ldots e_{kl})$ in (2.70) is the number of ways of coloring G in z or fewer colors in such a way that i and j are of the same color, k and l are of the same color, etc. Since any two vertices that are joined by an arc in the corresponding subgraph must be of the same color, all the vertices in a single connected piece of the subgraph are of the same color. Consequently, if there are p connected pieces in that, the absolute value of the correspondent typical term is therefore z^p. Moreover, if the subgraph contains b arcs in p connected pieces, its contribution into (2.70) is

$$(-1)^b n(e_{ij}\ldots e_{kl}) = (-1)^b z^p. \tag{2.71}$$

Let (p, b) denote the number of subgraphs of b arcs in p connected pieces, summing over all values of p and b, we obtain the chromatic polynomial in z,

$$\mathcal{P}_G(z) = \sum_{p,b}(-1)^b (p, b) z^p. \tag{2.72}$$

If we assume that the graph G is connected and for any $G' \subseteq G$ let

$$r(G') = |G'| - p(G'),$$

where $p(G')$ is the number of connected components in G', we further transform (2.72) to

$$\mathcal{P}_G(z) = \sum_{G'\subseteq G}(-1)^{|G'|-r(G')}(-z)^{r(G)-r(G')} \tag{2.73}$$

that is usually written in the form of the two variable polynomial,

$$\mathcal{R}_G(u, v) = \sum_{G'\subseteq G} u^{|G'|-r(G')} v^{r(G)-r(G')}, \tag{2.74}$$

called the *Whitney rank generating function*.

A root of a chromatic polynomial (a *chromatic root*) is a value z where $\mathcal{P}_G(z) = 0$. It is obvious that $z = 0$ is always a chromatic root for any graph, as no graph can be 0-colored. Furthermore, $z = 1$ is a chromatic root for every graph with at least an edge, as only edgeless graphs can be 1-colored. An edge e can be colored only with two colors, therefore

$$\mathcal{P}_e(z) = z(z-1).$$

The triangle K_3 can be colored with three colors, so that

$$\mathcal{P}_{K_3}(z) = z(z-1)(z-2),$$

etc. In general, for a connected graph G on N vertices, the chromatic polynomial $\mathcal{P}_G(z)$ is a polynomial of degree N. Although, for some basic graph classes, recurrent formulas for the chromatic polynomials are known, computational problems associated with the finding the chromatic polynomial for a given graph often require nondeterministic polynomial time to be solved. The *chromatic number*, the smallest number of colors needed to color the vertices of the graph so that no two adjacent vertices share the same color, is obviously the smallest positive integer that is not a chromatic root. Under a simple change of variables, the Whitney rank generating function (2.74) is transformed into the *Tutte polynomial* in two dual variables, $x = u - 1$ and $y = 1 - v$,

$$\begin{aligned} \mathcal{R}_G(u-1, v-1) &\equiv \mathcal{T}_G(x, y) \\ &= \sum_{G' \subseteq G} (x-1)^{p(G')-p(G)} (y-1)^{p(G')+N'-N} \end{aligned} \tag{2.75}$$

where $p(G')$ denotes the number of connected components in the graph G', N' is the order of the graph G', and N is the order of G. The Tutte polynomial of a graph is its invariant that factors into graph's connected components: given $G = G' \bigcup G''$,

$$\mathcal{T}_G(x, y) = \mathcal{T}_{G'}(x, y) \times \mathcal{T}_{G''}(x, y).$$

2.11 Shortest Paths in a Graph

A connected graph is called a *tree* if it contains no cycles. A *spanning tree* of a connected, undirected graph G is a connected tree composed of all the vertices of G. Much of the research in the various applications such as communications, road network design, and engineering has involved problems in which the network to be designed is a tree connecting a collection of sites and satisfying the different optimization criteria. For instance, one can mention the *travelling salesman problem*, in which the cheapest round-trip route is searched such that the salesman visits each city exactly once and then returns to the starting city (Dantzig et al. 1954). The algorithms for constructing the minimum spanning trees and searching the shortest path originated in 1926 for the purpose of efficient electrical coverage of Bohemia (Nesetril et al. 2000). It is clear that a single connected graph G can have many different spanning trees. The number $t(G)$ of spanning trees of the graph G is its important invariant, which can be calculated using *Kirchhoff's matrix-tree theorem*.

Kirchhoff's theorem relies on the notion of the *canonical Laplace matrix* of a graph G (de Verdiére 1998),

$$\mathbf{L}_{\mathrm{c}} = \mathbf{D} - \mathbf{A}_G, \tag{2.76}$$

where $\mathbf{D}$ is the diagonal graph's degree matrix and its adjacency matrix $\mathbf{A}_G$. The matrix (2.76) has the property that the sum of its entries across any row and any column is 0, so that the vector of all ones $\mathbf{j}$ spans the null-space of $\mathbf{L}_{\mathrm{c}}$,

$$\mathbf{L}_{\mathrm{c}}\mathbf{j} = 0. \tag{2.77}$$

The Laplacian matrix (2.76) can be factored into the product of the incidence matrix and its transpose,

$$\mathbf{L}_{\mathrm{c}} = \mathbf{B}_G \mathbf{B}_G^{\top}. \tag{2.78}$$

Let $\mathbf{B}'_G$ be the incidence matrix with its first row deleted, so that

$$\mathbf{B}'_G \mathbf{B}'^{\top}_G = \mathrm{Minor}$$

where Minor is a minor of the Laplace operator (2.76) (let us note that all minors of the Laplace operator are equal, as its null-space is one dimensional). Then, using the Cauchy-Binet formula (see, for example, Roman 2005; Shores 2006) we can write

$$\begin{aligned} \det(\mathrm{Minor}) &= \sum_{\mathfrak{S}} \det(\mathbf{B}'_{\mathfrak{S}}) \det(\mathbf{B}'^{\top}_{\mathfrak{S}}) \\ &= \sum_{\mathfrak{S}} \det(\mathbf{B}'_{\mathfrak{S}})^2 \end{aligned} \tag{2.79}$$

where $\mathbf{B}'_{\mathfrak{S}}$ denotes the $(N-1)\times(N-1)$ matrix whose columns are those of $\mathbf{B}'_G$ with index in the $(N-1)$-subset $\mathfrak{S}$. Since any of such subsets specifies $(N-1)$ edges of the original graph, and any set of edges forming a cycle gives zero contribution into the determinant (2.79), those edges induce a spanning tree, with the determinant $\det(\mathbf{B}'_{\mathfrak{S}}) = \pm 1$. Summing over all possible subsets $\mathfrak{S}$ in (2.79), we conclude that the total number of spanning trees $\mathcal{T}(G)$ of the connected graph G is

$$\begin{aligned} \mathcal{T}(G) &= \det(\mathrm{Minor}) \\ &= \frac{1}{N} \prod_{\lambda_k \neq 0} \lambda_k \end{aligned} \tag{2.80}$$

where the product is over all the non-zero eigenvalues of the Laplacian matrix (2.76). The result (2.80) is known as Kirchhoff's matrix tree theorem.

In graph theory, the *shortest path problem* consists of finding the quickest way to get from one location to another on a graph. The number of edges in a shortest path connecting two vertices, $i \in V$ and $j \in V$, in the graph is the *shortest path distance* between them, d_{ij}. It is obvious that $d_{ij} = 1$ if $i \sim j$. We may find the shortest path from the node to any other node by performing a breadth first search of eligible arcs on a graph spanning tree. It is obvious that the shortest path can be not unique, as there might be many spanning trees for the graph. However, we can choose one shortest path for each node, so that the resulting graph of eligible arcs for a breadth first search of all shortest paths from the node forms a tree.

There are a number of other graph properties defined in terms of distance. The diameter of a graph is the greatest distance between any two vertices,

$$\mathfrak{D}_G = \max_{i,j \in V} d_{ij}.$$

The radius of a graph is given by

$$\mathfrak{R}_G = \min_{i \in V} \max_{j \in V} d_{ij}.$$

The distance would determine the relative importance of a vertex within the graph. The *mean shortest path distance* from vertex i to any other vertex in the graph is

$$\ell_i = \frac{1}{N-1} \sum_{j \in V} d_{ij}. \tag{2.81}$$

In graph theory, the relation (2.81) expresses the *closeness* being a *centrality measure* of the vertex within a graph. *Betweenness* is another centrality measure of a vertex within a graph. It captures how often in average a vertex may be used in journeys from all vertices to all others in the graph. Vertices that occur on many shortest paths between others have higher betweenness than those that do not. Betweenness is estimated as the ratio

$$\text{Betweenness}(i) = \frac{\{\#\text{shortest paths through } i\}}{\{\#\text{all shortest paths}\}}. \tag{2.82}$$

Betweenness is, in some sense, a measure of the influence a node has over the spread of information through the graph. The betweenness centrality is essential in the analysis of many real world networks and social networks, in particular, but costly to compute. The Dijkstra algorithm and the Floyd-Warshall algorithm (Cormen et al. 2001), may be used in order to calculate betweenness.

2.12 Concluding Remarks and Further Reading

When a finite ordered set is endowed with an additional internal structure descried by a binary relation of adjacency, the collection of order pairs from this set is a graph. Each graph can be uniquely represented by its adjacency operator characterized by the adjacency matrix, with respect to the canonical basis of vectors in Hilebrt space. Spectral properties of the adjacency operator are related to walks and cycles of the correspondent graph.

There are many handbooks of graph theory, perhaps the most popular topic in discrete mathematics. Suggested readings are Harary (1969), Bollobas (1979), Chartrand (1985), Gould (1988), Biggs et al. (1996), Tutte (2001), Bona (2004), Diestel (2005), Harris et al. (2005) and Gross (2008). The textbooks (Bona 2004; Harris et al. 2005) are essentially appropriate for undergraduates. The classical surveys on the relationship between structural and spectral properties of graphs are Chung (1997) and Cvetkovic et al. (1997, 1980). An introduction to algebraic graph theory concerned with the interplay between algebra and graph theory can be found in Biggs (1993), Chan and Godsil (1997) and Godsil and Royle (2001).

Many interesting invariants of graphs can be computed from the Tutte polynomials (Tutte 1954). For a wealth of information on the applications of Tutte polynomial, see Brylawski and Oxley (1992) and Bollobas (1979). Problems involving some form of geometric minimum or maximum spanning tree are discussed in geometric network design theory (Eppstein 1999; Wu and Chao 2004).

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