Equitable Partitions, Coherent Algebras and Random Walks: Applications to the Correlation Structure of Landscapes

P.F. Stadler,
Institut f"ur Theoretische Chemie, Universität Wien, A-1090 Vienna &
Santa Fe Institute, Santa Fe, NM, USA

G. Tinhofer,
Zentrum Mathematik, Technische Universität München,
D-80290 Munich

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Abstract

A landcape is a fitness function $f : V \longrightarrow \mathbb{R}$ defined on the vertex set V of a configuration graph G. The pair (G, f) is a mathematical model for studying functions on a discrete set V where the neighborhood relation on the graph defines how one is able to move within this set and get access to the values of f. There are many situations where such a model is of high interest, in chemistry and elsewhere. Configuration spaces im molecular biology, spin glass models in physics, QSAR models in chemistry or pharmacology are landscapes in our sense, as well as the solution spaces of combinatorial optimization problems together with a solution heuristic like simulated annealing or some version of a genetic algorithm are a few examples.

Autocorrelation functions are strong mathematical tools for a profound study of landscapes. These functions are defined in terms of random walks on G and represented conveniently either using eigenvalues and eigenspaces of the configuration graphs G or via equitable partitions derived from its coherent algebra. In this paper we give a comprehensive introduction into the use of equitable partitions for investigating spectral properties of typical configuration graphs. The techniques demonstrated here are certainly useful in a wide range of applications in chemistry, not only in the study of landscapes. Further we present some basic notions from the theory of coherent algebras and show how they enable us to work out a rich panel of autocorrelation functions for a fixed fitness function f.

1 Introduction

1.1 When one is asked to express a "landscape" in mathematical terms, then it seems straightforward to start with a function $f : S^2 \longrightarrow \mathbb{R}$ that expresses the altitude of a location in terms of its geographical coordinates. In fact, this is how topographical maps are represented in a computer. Sewall Wright [80] used this picture to describe evolutionary adaptation as an uphill walk on a "fitness landscape", where altitude is replaced by reproductive success and the geographic coordinates are replaced by a representation of an organisms genetic composition.

Conceptually, there is a close connection between the (biological) *landscapes* and the *potential energy surfaces* (PES) that constitute one of the most important issues of theoretical chemistry [52, 32]. As a consequence of the validity of the Born-Oppenheimer approximation, the PES provides the potential energy as a function of the nuclear geometry of the system, $U(\vec{R})$. PES are therefore defined on a high-dimensional *continuous* space and they are assumed to be smooth (at least twice continuously differentiable).

An important difference, however, becomes immediately evident. While geographic or atomic coordinates are taken from a continuous space, genes are inherently discrete and finite objects. While the analysis of PES makes extensive use of differential topology, we need different tools to work with *discrete* landscapes. By replacing the sphere S^2 of geographic coordinates or the $3N$-dimensional Euclidean space of atomic coordinates for an N-atomic molecule by a discrete set, we give up all hope to use calculus on our landscapes. For instance, the critical points of a PES, characterized by $\nabla U(\vec{R}) = 0$, have no obvious discrete counter part. Local minima and maxima are easily defined given a proper adjacency relation or metric on the set of genes. The proper analogue of a "saddle point", however, remains elusive.

1.2 A landscape, hence, consists of a finite set V of *configurations*, which is usually very large, and a *fitness* function that "evaluates" the configurations. In order to speak about "geometric" notions such as a "hill" that has to be "climbed", we need a notion of closeness, accessibility, or distance among the members of V. In the simplest case we assume a neighborhood relation among the configurations. In biological terms, we say that two genes are neighbors of each other if and only if one can be converted into the other one by means of a single mutation event. Our set of configuration thus becomes a *configuration graph*, with vertex set V and an edge connecting "neighboring", that is mutually accessible, configurations.

1.3 Such a construction is by no means restricted to models in evolutionary biology. Hamiltonians of disordered systems, such as spin glasses [7, 51], and the cost functions of combinatorial optimization problems [26] have the same basic structure. Let us briefly consider a few examples:

Given a set of n spins σ_i with two orientations up $(+1)$ and down (-1), the most common form of spin glass Hamiltonian is

$$\mathcal{H}(\boldsymbol{\sigma}) = \sum_{i \cdot j} J_{ij} \sigma_i \sigma_j$$

where the sum runs over a set of "interacting" pairs of spins. Assuming that the spins are arranged on a lattice $i \cdot j$ refers to lattice neighbors, while in a long-range model, such as the Sherrington-Kirkpatrick model [62] the sum runs over all $i < j$. The dynamical behavior of spin glasses is commonly investigated based on the assumption that the "elementary move" is flipping a single spin, $\sigma_i \to -\sigma_i$. This arranges the spin configurations $\{\boldsymbol{\sigma}\}$ in a hypercube of dimension n, see **3.9.4**.

Lattice models of protein folding [15] and RNA folding [21] belong to the same class of models. The configuration sets in these cases, however, contain more complicated objects than strings in these cases. One has to deal with self-avoiding walks on certain lattices and a particular class of sub-cubic outerplanar graphs, respectively.

A combinatorial optimization problem, by definition, consists of a set V of configurations and cost function $f : V \to \mathbb{R}$. The configurations may be encoded as strings taken from a alphabet $\mathtt{A}$ as is commonly the case in applications of genetic algorithms [36], permutations as in the case of the Travelling Salesman Problem (see **3.9.5**), or trees as in genetic programming [44]. Similar constructions can be found in search theory [58]. A large class of optimization heuristics, including simulated annealing, works by iteratively testing "neighboring" configurations and accepting them under certain conditions. Hence, they are implicitly defining a landscape, as emphasized in [39, 40].

1.4 The relationships between the chemical or pharmacological activity of a molecule and its underlying structure is of utmost importance in drug design. In the language of this article, the molecular structures, represented by their structure formulas (graphs), take on the role of configurations, while to cost function measures the activity. In methods such as QSAR (Quantitative structure-activity relationships) [31, 45] so-called "descriptors" or "indices" (i.e., numerical parameters) are derived from a molecular graph, or via the detour of computing the detailed three-dimensional spatial and electronic structure of the molecule. The vector of these indices is then related to a particular physical, chemical, or biological property of interest by means of multivariate statistical data analysis.

In the language of this paper we may interpret QSAR as a landscape problem. The fitness function $f : V \longrightarrow \mathbb{R}$ assigns an activity $f(x)$ to each molecular structure graph $x \in V$ taken from a predefined class V of molecules. The computation of the descriptors and their translation into activity is all encapsulated in the fitness function f in this picture. A graph structure on V could be imposed by simple "edit operations" on the backbone, preferrably operations that correpond to reasonable chemical reactions.

1.5 One crucial difference, however, separates landscapes in chemistry, biology, and physics from those of operations research and computer science. The neighborhood relations are predefined by nature in the former cases as spin flips, point mutations, or chemical reactions. When designing search strategies or optimization heuristics, on the other hand, we have a free choice of the "move set". In fact the efficiency of an optimization heuristic depends crucially on selecting a suitable one.

The theory of algorithmic complexity [56] hence starts with the definition of V and f, asking e.g. whether an efficient (i.e., polynomial) algorithm exists to find $\min_{x\in V} f(x)$. In most physical applications, however, the complexity of the problem in this strict sense is irrelevant. Nature has already provided a search strategy (that is, a configuration graph) and we are stuck with it. In this contribution we will therefore mostly investigate properties of a landscape on a fixed configuration graph, although we will expand our investigation to certain classes of related weighted graphs in section 5.

1.6 The main challenge to *landscape theory* is to determine which features of the fitness landscape determine the evolvability of the systems on the landscape. It has been known since Eigen's [17] pioneering work on the molecular quasispecies that the dynamics of evolutionary adaptation (optimization) on a landscape depends crucially on detailed structure of the landscapes itself. Extensive computer simulations, see, e.g., [22, 23] have made it very clear that a complete understanding of the dynamics is impossible without a thorough investigation of the underlying landscape [18, 38].

Ruggedness has been identified as one of the most important characteristics of a landscape [76, 18, 65, 55, 42]. The ruggedness of a landscape is most easily quantified by measuring the correlation of fitness values in "neighboring" positions. Weinberger [76, 77] suggested the following procedure. Given a Markov process on V, we sample the fitness values $f(x^{(t)})$ along a trajectory of this process, interpret them as a "time series", and compute its autocorrelation function. Alternatively, [55] proposed to use local optima, and [41] suggested the length distribution of so-called adaptive walks. Some connections between these measures are discussed in [25]. It should be kept in mind, however, that a landscape is of course not determined completely by its correlation functions, see [1] for an instructive example. Correlation measures are good predictors for the "optimizability" of a landscape provided the landscape is typical in a sense which can be made precise in terms of maximum entropy type property called "isotropy" [71].

1.7 Methods from spectral graph theory have been used in [69, 70, 72, 67] to explore landscapes by ways of the structure of their correlation functions. Much of this work is based on expanding a landscape into a "Fourier series", with a "Fourier basis" that is implied in a natural way by the configuration graph (or a more general so-called P-structure in the case of recombination spaces [72, 67, 75]).

In this contribution we generalize previous results and put them into a unified perspective making consequent use of two related contructions from algebraic combinatorics: *equitable partitions* and *coherent algebras.*

This paper is organized as follows: In section 2 we define the notation and rehearse some basic properties of landscapes on graphs and their "random walk" correlation functions. Equitable partitions of matrices are employed in section 3 to simplify the task of computing the spectrum of large graphs with a high degree of regularities. The problem of finding usefully coarse equitable partitions is addressed in section 4. Coherent algebras are used in section 5 to extend the notion of so-called elementary landscapes to certain classes of random walks. We close with some concluding remarks in section 6.

2 Graphs and random walks on graphs

2.1 Let G be a graph with n vertices, vertex set $V = \{1, \ldots, n\}$ and edge set E. Unless explicitely stated otherwise our graphs are undirected and have neither loops nor multiple edges, i.e. E may be identified with an irreflexive and symmetric binary relation on V. If u und v are adjacent vertices in G we denote this by writing $u \sim v$. An undirected edge connecting u and v is denoted by $[u, v]$, or simply by uv.

For $v \in V$ the set $N(v) = \{u : u \sim v\}$ is called the set of neighbours of v, its cardinality $|N(v)|$ is called the degree of v and is denoted by d_v. A graph G is called *D-regular*, if all its vertices have equal degree D.

All graphs considered in this paper are connected.

The adjacency matrix of a graph G is denoted by $\mathbf{A}(G)$, or simply by $\mathbf{A}$, if G is fixed. It is a symmetric matrix with entries from $\{0, 1\}$. The ij-entrie of $\mathbf{A}$ is A_{ij} (or sometimes $(\mathbf{A})_{ij}$). Vectors are denoted by bold letters like $\mathbf{x}$, with components x_1, x_2, and so on. Let $\mathbf{e}$ be the $n-$dimensional vector of all 1's. The transpose of a matrix $\mathbf{A}$ (or a vector $\mathbf{x}$) is $\mathbf{A}^T$ (or $\mathbf{x}^T$).

2.2 Let a connected graph G and a real-valued function $f : V \longrightarrow \mathbb{R}$ be given. (G, f) is called a *landscape*, G the *configuration graph* and f a *cost* or *fitness function* on G. If f is constant we call (G, f) a *flat landscape*.

A landscape f determines an n-dimensional vector $\mathbf{f}$ with $f_v = f(v)$. Define

$$\bar{f} = \frac{1}{|V|} \sum_{i \in V} f(i), \quad \mathbf{f}^* = \bar{f}\mathbf{e}, \quad F = \{f(v) : v \in V\}$$

$$\sigma_f^2 = \frac{1}{|V|}(\mathbf{f} - \mathbf{f}^*)^T(\mathbf{f} - \mathbf{f}^*).$$

If f is considered as a random variable with uniform distribution over F then

$$\bar{f} = \mathrm{Exp}(f), \quad \sigma_f = \mathrm{Var}(f),$$

i.e. $\bar{f}$ is the expectation and σ_f^2 the variance of f.

A *Markov chain* on V is a sequence of random Variables $Z_0, Z_1, Z_2, \ldots$, with common range V, a stochastic matrix $\mathbf{T}$ of dimension $n \times n$ (the transition matrix) and a stochastic vector $\mathbf{p}$ such that

$$\mathrm{Prob}\{Z_0 = i\} = p_i, \ 1 \leq i \leq n,$$
$$\mathrm{Prob}\{Z_k = i\} = (\mathbf{p}^T\mathbf{T}^k)_i.$$

If $\mathbf{T}$ is such that $T_{uv} > 0$ implies $uv \in E$ then the Markov chain is called a *random walk* on the graph G. We may consider a random walk on G as a stochastic process where we start at a vertex v with probability p_v and move along the edges of G from vertex to vertex, the probability for reaching vertex u after k moves beeing $((\mathbf{p}^T\mathbf{T}^k)_u$. The *standard random walk* on a graph G is the random walk with transition matrix $\mathbf{T}$ defined with the aid of the adjacency matrix $\mathbf{A}$ by

$$T_{uv} = \frac{1}{d_u} A_{uv}.$$

If G is D-regular this reduces to $\mathbf{T} = D^{-1}\mathbf{A}$.

A Markov chain is called *stationary*, if $\mathbf{p}$ is such that

$$\mathbf{p}^T\mathbf{T} = \mathbf{p}^T.$$

In this case, $\mathbf{p}$ is called the *stationary distribution* of the chain. For random walks on connected graphs there is a unique stationary distribution, namely

$$\mathbf{p} = \frac{\mathbf{d}}{2|E|},$$

where $\mathbf{d}$ is the *degree vector* of G. In the case of a k-regular graph this reduces to the uniform distribution

$$\mathbf{p} = \frac{\mathbf{e}}{|V|}.$$

2.3 Consider the set F as a (in general huge) ensemble of datas and G as a system of rules specifying how one is able to move around in this ensemble. As it is most frequently the case in dealing with a huge amount of datas the final goal ist to get a "global" description of the function f "belonging" to F, i.e. one would like to know the details of the fitness function f. A more realistic goal is to gather some amount of information about f and infer statistical properties of the set of fitness functions that fit the given data. Such statistical properties are conveniently expressed by values of statistical parameters like the mean $\bar{f}$ and the variance σ_f^2. Another convenient way is to use a stationary random walk on G and investigate its autocorrelation function.

Let $Z_0, Z_1, Z_2, \ldots$ be a stationary Markov chain on V with transition matrix $\mathbf{T}$ and stationary distribution $\mathbf{p}$. Define $F_i = f(Z_i)$, $i \geq 0$. Then

$$\begin{aligned}
\mathrm{Exp}(F_i) &= \sum_{k=1} f(k) p_k, \\
\mathrm{Var}(F_i) &= \sum_{k=1}^{n} (f(k) - \mathrm{Exp}(F_i))^2 p_k, \\
\mathrm{Cov}(F_i, F_j) &= \sum_{k=1}^{n} \sum_{l=1}^{n} (f(k) - \mathrm{Exp}(F_i))(f(l) - \mathrm{Exp}(F_j)) p_k (\mathbf{T}^{j-i})_{kl}, \\
\mathrm{Cor}(F_i, F_j) &= \frac{\mathrm{Cov}(F_i, F_j)}{\sqrt{\mathrm{Var}(F_i)}\sqrt{\mathrm{Var}(F_j)}}
\end{aligned}$$

Here the expressions $\mathrm{Exp}(F_i)$ and $\mathrm{Var}(F_i)$ are independent of i, while the covariance $\mathrm{Cov}(F_i, F_j)$ depends on i and j only via the difference $k = j - i$. The same observation holds for the correlation $\mathrm{Cor}(F_i, F_j)$. Given f, the function $r_f(k) = \mathrm{Cor}(F_i, F_{i+k})$ is called the *autocorrelation* function of the Markov chain.

2.4 If G is D-regular, then for the standard random walk $\mathbf{T} = D^{-1}\mathbf{A}$, $\mathrm{Exp}(F_i) = \bar{f}$, $Var(F_i) = \sigma_f^2$. Further,

$$\mathrm{Cor}(F_i, F_{i+k}) = \frac{(\mathbf{f} - \mathbf{f}^*)^T \mathbf{A}^k (\mathbf{f} - \mathbf{f}^*)}{D^k |V|}.$$

The autocorrelation function is

$$r_f(k) = \left[\frac{\mathbf{f} - \mathbf{f}^*}{\sigma_f}\right]^T \left[\frac{\mathbf{A}}{D^k |V|}\right] \left[\frac{\mathbf{f} - \mathbf{f}^*}{\sigma_f}\right].$$

Hence, $r_f(k)$ is a quadratic form

$$r_f(k) = \frac{1}{|V|} \tilde{\mathbf{f}}^T \mathbf{T}^k \tilde{\mathbf{f}}$$

where

$$\tilde{\mathbf{f}} = \frac{\mathbf{f} - \mathbf{f}^*}{\sigma_f}, \quad \mathbf{T}^k = \frac{\mathbf{A}^k}{D^k}, \quad k \geq 0.$$

Since $\tilde{f}$ has mean $\overline{\tilde{f}} = 0$ and $\sigma_{\tilde{f}}^2 = 1$, we have

$$r_{\tilde{f}}(k) = r_f(k), \quad k \geq 0.$$

For this reason, in what follows we may assume w.l.o.g. that $\bar{f} = 0$ and $\sigma_f^2 = 1$. Under this assumption we have

$$r_f(k) = \frac{1}{|V|}\mathbf{f}^T\mathbf{T}^k\mathbf{f}.$$

The function r_f depends on the landscape only, i.e., on f and on the graph G. It is therefore a characteristic of this landscape. Its "shape" has been the topic of several investigations reported in the literature, see e.g. [24, 37, 42, 63, 70, 76]. An important result of these investigations is expressed by the following proposition.

Proposition 1. *Let (G, f) be a non-flat landscape on a connected, D-regular graph G with adjacency matrix $\mathbf{A}$. Then r_f is an exponential function if and only if $\mathbf{f}$ is an eigenvector of $\mathbf{A}$.*

Proof. A proof of this statement has been given in [70]. Since it needs only a few lines, we add it here for the convenience of the reader.

Since $\mathbf{A}$ is symmetric, there is a system on n orthonormal eigenvectors $\mathbf{x}^1, \mathbf{x}^2, \dots, \mathbf{x}^n$ for $\mathbf{A}$. Let $\lambda_1, \lambda_2, \dots, \lambda_n$ be the corresponding eigenvalues. Then

$$\mathbf{T}^k\mathbf{x}^i = (\frac{\lambda_i}{D})^k\mathbf{x}^i, \ \ 1 \le i \le n.$$

Write

$$\mathbf{f} = \sum_{i=1}^{n} \alpha_i \mathbf{x}^i,$$

with appropriate constants $\alpha_1, \dots, \alpha_n$. Inserting this into the formula for $r_f(k)$ gives

$$r_f(k) = \sum_{i=1}\sum_{j=1}^{n} \alpha_i\alpha_j(\frac{\lambda_j}{D})^k {\mathbf{x}^i}^T\mathbf{x}^j = \sum_{i=1} \alpha_i^2(\frac{\lambda_i}{D})^k.$$

Hence, $r_f(k)$ is exponential if and only if $\alpha_i \neq 0$ for exactly one index i. $\diamond$

2.5 If G is not D-regular define a matrix $\mathbf{D}$ by $D_{ij} = 0$ if $i \neq j$ and $D_{ii} = d_i$, $1 \le i \le n$. Then the transition matrix of a random walk on G is $\mathbf{T} = \mathbf{D}^{-1}\mathbf{A}$. Since for a non-regular graph the stationary distribution is

$$\mathbf{p} = \frac{\mathbf{d}}{2|E|},$$

in the definition for $r_f(k)$ no longer the arithmetic mean of the values of f appears. We have to redefine $\bar{f}$ by

$$\bar{f} = \sum_{i=1} f(i) \frac{d_i}{2|E|}.$$

Further, the variance of the stationary distribution is

$$\sigma_f^2 = \sum_{i=1} (f(i) - \bar{f})^2 \frac{d_i}{2|E|}.$$

Under analogous assumptions as before ($\bar{f} = 0$ and $\sigma_f^2 = 1$) the autocorrelation function reads now

$$r_f(k) = \mathbf{f}^T \mathbf{T}_k \mathbf{f}$$

where

$$\mathbf{T}_k = \frac{1}{2|E|} \mathbf{D} \mathbf{T}^k.$$

Again using the representation of $\mathbf{f}$ via the eigenvectors of $\mathbf{A}$ we find

$$r_f(k) = \frac{1}{2|E|} \sum_{j=1}^{n} \sum_{i=1}^{n} \alpha_i \alpha_j \lambda_i^k \mathbf{x}^j \mathbf{D}^{-k+1} \mathbf{x}^i.$$

Form this expression we see that Poposition 1 can be extended to non-regular graphs as follows: *A non-flat landscape has an autocorrelation function of the form*

$$r_f(k) = (\mathbf{f}^T \mathbf{D}^{-k+1} \mathbf{f}) \lambda_i^k$$

if and only if $\mathbf{f}$ *is an eigenvector of* $\mathbf{A}$ *for the eigenvalue* λ_i $(1 \leq i \leq n)$.

2.6 Note that in the non-regular case the transition matrix $\mathbf{T}$ of the standard random walk is not symmetric. In the case where this matrix is not diagonalizable, the $\mathbf{x}^1, \ldots, \mathbf{x}^n$ are not necessarily eigenvectors of $\mathbf{T}$. For this reason, when studying the properties of random walks on a graph, the matrix $\mathbf{L} = \mathbf{D} - \mathbf{A}$ is a another useful tool which for certain goals is more convenient than the adjacency matrix $\mathbf{A}$. The matrix $\mathbf{L}$ is symmetric and, therefore, we can represent any vector $\mathbf{f}$ as a linear combination of the eigenvectors of $\mathbf{L}$. However, if G is D-regular, then $\mathbf{L}$ and $\mathbf{A}$ have the same eigenvectors, and if λ is an eigenvalue of $\mathbf{A}$, then $D - \lambda$ is an eigenvalue of $\mathbf{L}$, and vice versa. For a non-regular graph G this is not true. The matrix $\mathbf{L}$ is often called the *admittance matrix* of G, and $-\mathbf{L}$ is called the *Laplacian* of G (for an explanation of this name see [11, 53, 54]). For the study of the autocorrelation function of a landscape, the Laplacian $-\mathbf{L}$ is in general not more advantageous than the adjacency matrix $\mathbf{A}$.

In many practical applications an idealized model is used where the configuration graph is regular (even in a stronger sense than D-regularity expresses). The non-regular case becomes important when one wants to investigate the effects of slight perturbations of the idealized model.

2.7 The autocorrelation functions of landscapes have been studied in numerous papers, see e.g. [24, 37, 42, 63, 70, 76]. Its shape can be determined using the eigenvalues and eigenspaces of the configuration graph. Therefore for this field of research the *spectral theory* of graphs is of considerable importance. Spectra and eigenspaces of graphs have been intensively investigated in the literature for several different reasons. Standard books on this topic are [6, 13, 14, 28]. In many cases, combinatorial considerations allow (at least partly) the determination of the eigenvalues of graphs, i.e. of their adjacency matrices, without applying numerical methods. Numerous combinatorial tools have been developed for this aim. In this paper we give an introduction into the use of one particular useful combinatorial tool for investigating the spectra of graphs, the so-called equitable partitions. Combined with a second powerful combinatorial tool, the coherent algebra of a graph, we will be able to formulated further interesting results about autocorrelation functions of landscapes.

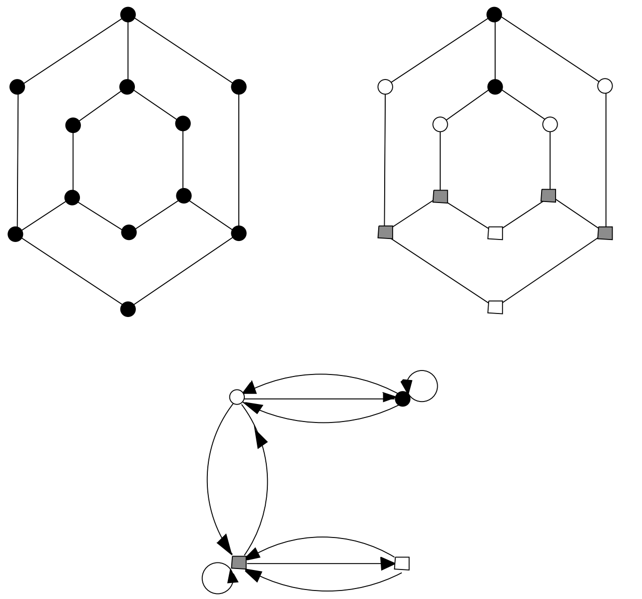

Figure 1

3 Equitable partitions

3.1 Let G be a graph and let $\pi = (V_1, \dots, V_s)$ be a partition of the vertex set V into s non-empty and pairwise disjoint cells V_i. The partition π is called *equitable* (with respect to G) if for each i and k the number of neighbors of a vertex $u \in V_i$ which belong to V_k, i.e. $|\{v : v \sim u\} \cap V_k|$, depends only on the cell indices i and k and not on the vertex u selected. We denote this number by R_{ik}.

An equitable partition is accompanied by a so-called *quotient graph* G/π. This is a directed multigraph having the cells V_i of π as vertices and R_{ik} arcs leading from V_i to V_k $(1 \leq i, k \leq s)$. The quotient graph is not necessarily symmetric, since in general $R_{ik} \neq R_{ki}$. It can be considered as a visualization of the matrix $\mathbf{R} = (R_{ik})$, which plays a crucial role in the study of the spectrum of G, as will be shown below.

To have an example, consider the graph in Figure 1. In a copy on its right side an equitable partition is indicated by using different symbols for the vertices in different cells. The third figure is the corresponding quotient graph.

Other examples one finds with the help of groups of automorphisms of a graph G. Let $\mathsf{Aut}[G]$ be the group of all automorphisms of G, H any subgroup of $\mathsf{Aut}[G]$. The orbits $O_1^H, \dots, O_s^H$ of V under the action of H is an equitable partition. In the example of Figure 1 the mentioned equitable partition is the partition into the orbits of the group of those automorphisms which fix the set of the two vertices marked by a full circle.

There are two trivial examples for equitable partitions: the *trivial partition* $\pi = \{V\}$, where $s = 1$ and $V_1 = V$, and the *discrete partition* $\pi = \{V_1, \dots, V_n\}$, where $s = n$ and $V_i = \{i\}$.

Equitable partitions and the notion of the quotient graph have been introduced by Sachs [60, 61]. The notation *equitable partition* was introduced in [64]. In [49] equitable partitions were studied to some extend in connection with their use in graph isomorphism algorithms. Today, these concepts are well-known and treated thoroughly in several monographies (see [10, 14, 28]).

3.2 For the aim of this paper we shall use a somewhat different approach to the notion of equitable partitions. We will define them not as partitions of the vertex set of a graph G , but as a partition of the rows and columns of an arbitrary matrix $\mathbf{A}$. A similar approch, however in a different context, can be found in [28].

Let again $V = \{1, 2, \dots, n\}$. For a partition $\pi = \{V_1, V_2, \dots, V_s\}$ of V into s cells let $\mathbf{g}^1, \mathbf{g}^2, \dots, \mathbf{g}^s$ be the characteristic vectors of the cells, i.e. $(\mathbf{g}^i)_k = 1$ if $k \in V_i$, and $(\mathbf{g}^i)_k = 0$ otherwise.

A partition π is called *row equitable* with respect to a matrix $\mathbf{A}$ if there exist real numbers R_{ik}, $1 \le i, k \le s$, such that

$$\mathbf{A}\mathbf{g}^i = \sum_{k=1}^{n} R_{ki}\mathbf{g}^k, \quad 1 \le i \le s.$$

It is called *column equitable* with respect to $\mathbf{A}$ if there exist real numbers C_{ik} such that

$$\mathbf{g}^{iT}\mathbf{A} = \sum_{k=1}^{n} C_{ik}\mathbf{g}^{kT}, \quad 1 \le i \le s.$$

For two cells V_i and V_k let $\mathbf{A}^{(i,k)}$ denote the submatrix of $\mathbf{A}$ (of dimension $|V_i| \times |V_k|$) consisting of all entries A_{st} with $s \in V_i$ and $t \in V_j$. In terms of these submatrices row equitable means that all rows of $\mathbf{A}^{(i,k)}$ sum up to the same value R_{ik}, i.e.

$$R_{ik} = \sum_{t \in V_k} A_{st},$$

independent of $s \in V_i$. Column equitable means that all columns of $\mathbf{A}^{(i,k)}$ sum up to the same value C_{ik}, i.e.

$$C_{ik} = \sum_{s \in V_i} A_{st},$$

independent of $t \in V_k$. By summing up the entries in $\mathbf{A}^{(i,k)}$ in two different ways, once row-wise and once column-wise, we get the equalities

$$|V_i| R_{ik} = C_{ik} |V_k|, \; 1 \leq i, k \leq s.$$

Clearly, if $\mathbf{A}$ is symmetric, then row equitable implies column equitable, and vice versa. In this case we call π simply *equitable*. If $\mathbf{A}$ is the adjacency matrix of a graph G, then π is equitable with respect to $\mathbf{A}$ if and only if π is equitable with respect to G.

Assume that π is equitable with respect to $\mathbf{A}$. The numbers R_{ij} and C_{ij} are called the *structur constants* of $(\mathbf{A}, \pi)$. The matrices

$$\mathbf{R} = (R_{ij})_{1 \leq i,j \leq s} \text{ and } \mathbf{C} = (C_{ij})_{1 \leq i,j \leq s}$$

are called the *structure matrices* of $(\mathbf{A}, \pi)$. Obviously, if $\mathbf{A}$ is symmetric, then $\mathbf{C} = \mathbf{R}^T$.

In the example of Figure 1, the structure matrices are

$$\mathbf{R} = \begin{pmatrix} 1 & 2 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 2 & 0 \end{pmatrix}, \qquad \mathbf{C} = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 2 & 0 & 1 & 0 \\ 0 & 1 & 1 & 2 \\ 0 & 0 & 1 & 0 \end{pmatrix} = \mathbf{R}^T.$$

Remark. Define $\mathbb{R}(\pi) = span(\mathbf{g}^1, \ldots, \mathbf{g}^s)$ (the subspace of the n-dimensional real space $\mathbb{R}^n$ spanned by the characteristic vectors $\mathbf{g}^1, \ldots, \mathbf{g}^s$ of π). Note that π is equitable with respect to $\mathbf{A}$ if and only if $\mathbb{R}(\pi)$ is a left and right invariant subspace of $\mathbb{R}^n$ with respect to the action of $\mathbf{A}$ on $\mathbb{R}^n$.

3.3 The usefulness of equitable partitions is expressed in the following proposition. By $\mathrm{spec}(\mathbf{A})$ we denote the set of different eigenvalues, by $\chi_{\mathbf{A}}(x)$ the characteristic polynomial of $\mathbf{A}$.

Proposition 2. *Let* $\mathbf{R}$ *and* $\mathbf{C}$ *be the structure matrices of* $(\mathbf{A}, \pi)$*. Then*

(1) $\mathrm{spec}(\mathbf{R}) = \mathrm{spec}(\mathbf{C}) \subseteq \mathrm{spec}(\mathbf{A})$.

(2) $\mathbf{Ax} = \lambda x$, $\mathbf{g}^{iT}\mathbf{x} \neq 0$ *for at least one* i, $1 \leq i \leq s$, *implies* $\lambda \in \mathrm{spec}(\mathbf{C})$.

(3) $\chi_{\mathbf{R}}(x) = \chi_{\mathbf{C}}(x)$*; if* $\mathbf{A}$ *is diagonalizable, then* $\mathbf{R}$ *and* $\mathbf{C}$ *are also diagonalizable and* $\chi_{\mathbf{R}}(x)$ *is a factor of* $\chi_{\mathbf{A}}(x)$.

Proof. Assume that $\mathbf{Ru} = \lambda\mathbf{u}$, $\mathbf{Cw} = \mu\mathbf{w}$, for some $\mathbf{u} \neq 0, \mathbf{w} \neq 0$. Define a vector $\mathbf{x} = \sum_{i=1}^{s} u_i \mathbf{g}^i$. Then

$$\mathbf{Ax} = \sum_{i=1}^{s} u_i \mathbf{A}\mathbf{g}^i = \sum_{k=1}^{s}\sum_{i=1}^{s} u_i R_{ki}\mathbf{g}^k = \lambda \sum_{k=1}^{s} u_k \mathbf{g}^k = \lambda\mathbf{x}.$$

Since $|V_i| \cdot R_{ik} = C_{ik} \cdot |V_k|$, we get

$$\sum_{k=1}^{s} R_{ik}u_k = \lambda u_i \Longrightarrow \sum_{k=1}^{s} C_{ik}u_k|V_k| = \lambda u_i|V_i|,$$

$$\sum_{k=1}^{s} C_{ik}w_k = \mu w_i \Longrightarrow \sum_{k=1}^{s} R_{ik}\frac{w_k}{|V_k|} = \mu\frac{w_i}{|V_i|}.$$

This proves (1) and the first part of (3).

To prove (2) assume $\mathbf{Ax} = \lambda\mathbf{x}$, $\mathbf{x} \neq 0$. It follows

$$\mathbf{g}^{iT}\mathbf{Ax} = \sum_{k=1}^{s} C_{ik}\mathbf{g}^{kT}\mathbf{x} = \lambda\mathbf{g}^{iT}\mathbf{x}.$$

Hence, $\mathbf{C}$ has eigenvalue λ with eigenvector $\mathbf{u}$, where $u_i = \mathbf{g}^{iT}\mathbf{x}$, $1 \leq i \leq s$.

Recall that a matrix is diagonalizable if and only if its minimal polynom has only simple roots. Thus, in this case (1) implies that also the minimal polynomials of $\mathbf{R}$ and of $\mathbf{C}$ have simple roots only, and these matrices are also diagonalizable. The proof of (1) shows that a set of linearly independent eigenvectors of $\mathbf{R}$ determines a set of equally many linearly independent eigenvectors of $\mathbf{A}$. This completes the proof of (3). $\diamond$

Remark. It follows from part (2) of the proposition that, if λ is an eigenvalue of $\mathbf{A}$ the eigenspace of which is not orthogonal to $span\{\mathbf{g}^1, \ldots, \mathbf{g}^s\}$, then $\lambda \in \operatorname{spec}(\mathbf{C})$. Note that (3) holds for any symmetric matric $\mathbf{A}$.

According to [14] the *main part* of the spectrum of a matrix $\mathbf{A}$ is the set of those eigenvalues of $\mathbf{A}$ which have an eigenvector not orthogonal to $\mathbf{e}$. Since a vector which is not orthogonal to $\mathbf{e}$ cannot be orthogonal to all vectors $\mathbf{g}^1, \ldots, \mathbf{g}^s$ it follows from Proposition 2(2) that the main part of $\operatorname{spec}(\mathbf{A})$ is contained in $\operatorname{spec}(\mathbf{R})$.

Remark. Condition (2) in Proposition 2 can be used to guide the search for graphs that have equitable partitions with a 1-point cell V_i and $\operatorname{spec}(\mathbf{R}) \neq \operatorname{spec}(\mathbf{A})$. Suppose $V_i = \{v\}$ and let λ be an eigenvalue of $\mathbf{A}$. Then $\lambda \in \operatorname{spec}(\mathbf{R})$ whenever there is an eigenvector $\mathbf{x}$ of λ such that $x_v \neq 0$. Hence, we have to look for eigenvectors that vanish on certain vertices of a graph. Oftentimes, such eigenvectors occur in graphs with "small" symmetry groups.

Example. For the adjacency matrix $\mathbf{A}$ of the path graph 2–1–3 we get

$$\begin{aligned}
\lambda_1 &= 0, \;\; \mathbf{x}^1 = (0, -1, 1), \\
\lambda_2 &= -\sqrt{2}, \;\; \mathbf{x}^2 = (-\sqrt{2}, -1, 1), \\
\lambda_3 &= \sqrt{2}, \;\; \mathbf{x}^3 = (\sqrt{2}, -1, 1).
\end{aligned}$$

The partition $\pi_1 = \{\,\{1\}, \{2, 3\}\,\}$ is equitable since it is an orbit partition. We find $\operatorname{spec}(\mathbf{R}) = \{-\sqrt{2}, \sqrt{2}\} \subset \operatorname{spec}(\mathbf{A})$.

Proposition 3. *Let $\pi^{(k)} = \{V_1^{(k)}, \ldots, V_{s_k}^{(k)}\}$, $1 \leq k \leq \nu$, be a sequence of equitable partitions satisfying the condition that for every $k \in V$ there is a κ with $\{k\} \in \pi^{(\kappa)}$. Then*

$$\bigcup_{k=1}^{\nu} \operatorname{spec}(\mathbf{C}^{(k)}) = \bigcup_{k=1}^{\nu} \operatorname{spec}(\mathbf{R}^{(k)}) \subseteq \operatorname{spec}(\mathbf{A}) \subseteq \bigcup_{k=1}^{\nu} \operatorname{spec}(\mathbf{R}^{(k)}),$$

where $\mathbf{R}^{(k)}$ and $\mathbf{C}^{(k)}$ are the structure matrices of $\pi^{(k)}$.

Proof. The first inequality follows from the first statement of Proposition 2. To prove the second inequality assume that $\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$, $\mathbf{x} \neq 0$. There is a k, such that $x_k \neq 0$. Then $\mathbf{x}$ is not orthogonal to $\mathbb{R}(\pi^k)$. Hence, the claim follows from the remark following Proposition 2. $\diamond$

Remark: Proposition 3 may be viewed as a generalization of a result in [8]. There, a graph is called *highly regular* if for every vertex $v \in V$ there is a partition

$$\pi_v = \left\{V_1^v = \{v\}, V_2^v, \ldots, V_s^v\right\}$$

such that each vertex $u \in V_i^v$ is adjacent to exactly R_{ij} vertices in V_j^v. By definition, each π_v is equitable in this case and $\mathbf{R} = \mathbf{R}^{(v)}$ is the same for all $v \in V$. Thm. 6(ii), p. 159, of [8] states that the adjacency matrix $\mathbf{A}$ of a highly regular graph and the structure matrix $\mathbf{R}$ have the same minimal polynomial, i.e., $\mathrm{spec}(\mathbf{A}) = \mathrm{spec}(\mathbf{R})$. Highly regular graphs with structure matrix $\mathbf{R}$ are of course D-regular with $D = \sum_j R_{1j}$.

3.4 Let π be equitable with respect to $\mathbf{A}$ and consider the orthogonal space $\mathbb{R}^\perp(\pi)$ of $\mathbb{R}(\pi)$. It consists of all vectors $\mathbf{x}$ satisfying $\mathbf{x}^T\mathbf{g}^i = 0$, $1 \le i \le s$, and has dimension $n - s$. Assume that $\hat{\mathbf{g}}^1 \ldots, \hat{\mathbf{g}}^{n-s}$ is a linear basis for $\mathbb{R}^\perp(\pi)$.

If $\mathbf{x} \in \mathbb{R}^\perp(\pi)$ implies $\mathbf{Ax} \in \mathbb{R}^\perp(\pi)$, then we say that $\mathbb{R}^\perp(\pi)$ is a *right modul* (invariant linear space) for $\mathbf{A}$. In this case

$$\mathbf{A}\hat{\mathbf{g}}^i = \sum_{k=1}^{n-s} \hat{R}_{ki}\hat{\mathbf{g}}^k$$

with appropriate constants $\hat{R}_{ki}$.

If $\mathbf{x} \in \mathbb{R}^\perp(\pi)$ implies $\mathbf{A}^T\mathbf{x} \in \mathbb{R}^\perp(\pi)$, then we say that $\mathbb{R}^\perp(\pi)$ is a *left modul* for $\mathbf{A}$. In this case

$$\hat{\mathbf{g}}^{iT}\mathbf{A} = \sum_{k=1}^{n-s} \hat{C}_{ik}\hat{\mathbf{g}}^{kT}$$

again with appropriate constants $\hat{C}_{ik}$.

If $\mathbb{R}^\perp(\pi)$ is both a left and a right modul for $\mathbf{A}$, then the matrices $\hat{\mathbf{R}}$ and $\hat{\mathbf{C}}$ have the same properties as the matrices $\mathbf{R}$ and $\mathbf{C}$, i.e. Proposition 2 and Proposition 3 are valid likewise with $\hat{\mathbf{R}}$ instead of $\mathbf{R}$ and $\hat{\mathbf{C}}$ instead of $\mathbf{C}$. Morover, the following statement is valid.

Proposition 4. *Let π be an equitable partition for a matrix $\mathbf{A}$ for which $\mathbb{R}^\perp(\pi)$ is a left and right modul, then*

$$\mathrm{spec}(\mathbf{A}) = \mathrm{spec}(\mathbf{C}) \cup \mathrm{spec}(\hat{\mathbf{C}}).$$

Proof. Basic facts from Linear Algebra. $\diamond$

Note that for a symmetric matrix $\mathbf{A}$ and each of its equitable partitions π the hypothesis of this proposition is fulfilled.

3.5 Before we study some examples in order to demonstrate the usefulness of the above notions we add still a very helpful lemma.

Suppose that $\mathbf{P}$ is a permutation matrix corresponding to some permutation $\gamma : V \longrightarrow V$ and suppose that $\mathbf{PA} = \mathbf{AP}$. In the case when $\mathbf{A}$ is the adjacency matrix of a graph G this means that γ is an automorphism of G (and $\mathbf{P}$ is a permutational representation of it). Let $\pi = \{V_1, \ldots, V_s\}$ a partition of V and define its image under γ by $\pi^\gamma = \{V_1^\gamma, \ldots, V_s^\gamma\}$, where $V_i^\gamma = \{v^\gamma : v \in V_i\}$ and v^γ is the image of v under γ.

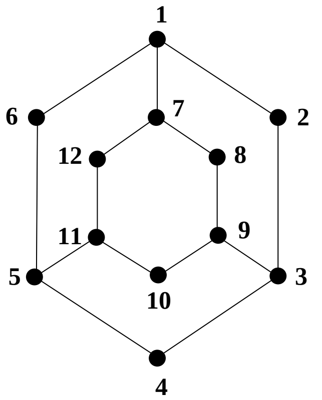

Figure 2

Lemma 1. *If π is equitable with respect to A, then π^γ is equitable for every permutation γ such that the corresponding permutation matrix $\mathbf{P}$ commutes with $\mathbf{A}$. Further, the permutation $\hat{\gamma}$ of the cells of π defined by*

$$\hat{\gamma}(V_i) = V_i^\gamma, \ 1 \leq i \leq s,$$

has a permutational representation $\mathbf{Q}$ satisfying

$$\mathbf{Q}^T\mathbf{R}\mathbf{Q} = \mathbf{R}, \ \ \mathbf{Q}^T\mathbf{C}\mathbf{Q} = \mathbf{C}.$$

This means, the structure matrices remain unchanged when we replace π by π^γ.

Proof. ¿From

$$\mathbf{A}\mathbf{g}^i = \sum_{k=1}^{s} R_{ik}\mathbf{g}^k$$

it follows

$$\mathbf{P}^T\mathbf{A}\mathbf{P}\mathbf{P}^T\mathbf{g}^i = \sum_{k=1}^{s} R_{ik}\mathbf{P}^T\mathbf{g}^k.$$

Since $\mathbf{P}^T\mathbf{A}\mathbf{P} = \mathbf{A}$, we get

$$\mathbf{A}\mathbf{P}^T\mathbf{g}^i = \sum_{k=1}^{s} R_{ik}\mathbf{P}^T\mathbf{g}^k.$$

Since $\mathbf{P}\mathbf{g}^i$ is the characteristic vector of V_i^γ, we see that π^γ is row equitable if π has this property. In the same way it is shown that π^γ is column equitable, if π is so. $\diamond$

3.6 In the following examples, if we deal with a symmetric matrix $\mathbf{A}$ and its equitable partitions, we work with the structure matrix $\mathbf{R}$. We mention the second structure matrix $\mathbf{C}$ only, if $\mathbf{C} \neq \mathbf{R}^T$.

Consider the graph in Figure 2 which is the same as in Figure 1 with the exception that now the vertices are numbered. Its adjacency matrix is

$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}.$$

Let us denote the equitable partition indicated in Figure 1 by π_1 and its structure matrix $\mathbf{R}$ given in subsection **3.2** by $\mathbf{R}^{(1)}$. Using the numbering in Figure 2 we have

$$\pi_1 = \{1,7\}, \{2,6,8,12\}, \{3,5,9,11\}, \{4,10\}.$$

The matrix $\mathbf{A}$ has more equitable partitions. We list here three of them. For reasons becoming clear somewhat later on, we denote them by π_4, π_5 and π_6:

$$\begin{aligned} \pi_4 &= \{1\}, \{4\}, \{7\}, \{10\}, \{2,6\}, \{3,5\}, \{8,12\}, \{9,11\}; \\ \pi_5 &= \{3\}, \{6\}, \{9\}, \{12\}, \{4,2\}, \{5,1\}, \{10,8\}, \{11,7\}; \\ \pi_6 &= \{5\}, \{2\}, \{11\}, \{8\}, \{6,4\}, \{1,3\}\{12,10\}, \{7,9\}. \end{aligned}$$

Here π_4 was found using an algorithm described in a later subsection. π_5 and π_6 we get from π_4 with the help of automorphisms (Lemma 1).

The three partitions π_4, π_5 and π_6 fulfill the condition of Proposition 3. Let $\mathbf{R}^{(4)}, \mathbf{R}^{(5)}$ and $\mathbf{R}^{(6)}$ be the corresponding structure matrices. We have

$$\mathbf{R}^{(4)} = \begin{pmatrix} 0 & 0 & 1 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \end{pmatrix} = \mathbf{R}^{(5)} = \mathbf{R}^{(6)}.$$

Hence, $\operatorname{spec}(\mathbf{A}) = \operatorname{spec}(\mathbf{R}^{(4)})$, where some of the eigenvalues have larger multiplicity in $\mathbf{A}$ than in $\mathbf{R}^{(4)}$.

3.7 In the foregoing example we have reduced the computation of the spectrum of a 12×12 matrix to the computation of the spectrum of a 8×8 matrix. However, a further reduction is possible.

Let us compare the equitable partition π_4 with the partition π_1. Evidently, the cells of π_1 are unions of cells of π_4, namely

$$\{1,7\} = \{1\} \cup \{7\},\ \{2,6,8,12\} = \{2,6\} \cup \{8,12\},$$

$$\{3,5,9,11\} = \{3,5\} \cup \{9,11\},\ \{4,10\} = \{4\} \cup \{10\}.$$

This observation motivates us to recall here the well known relations *finer*, respectively *coarser*, between two partitions. A partition $\pi = \{V_1, \dots, V_s\}$ is called *finer* than a partition $\pi' = \{V'_1, \dots, V'_{s'}\}$ (in symbols $\pi \prec \pi'$), if $\pi \neq \pi'$ and every cell V_i of π is completely contained in some cell V'_j of π', or in other words, if every cell of π' is a union of cells of π. In this case π' is also called *coarser* than π (denoted by $\pi' \succ \pi$).

If $\pi \prec \pi'$ or $\pi = \pi'$, then we say π is *at least as fine as* π' and denote this by $\pi \preceq \pi'$.

A possible further reduction of the problem size in our example is based on the following statement.

Proposition 5. *Let π and π' be two equitable partitions for* $\mathbf{A}$ *with structure matrices* $\mathbf{R}$ *and* $\mathbf{C}$*, respectively* $\mathbf{R}'$ *and* $\mathbf{C}'$*. Assume that π is finer than π' and that $\omega = \{W_1, \ldots, W_{s'}\}$ is a partition of $\{1, 2, \ldots, s\}$ such that*

$$V'_j = \sum_{i \in W_j} V_i, \ 1 \leq j \leq s'.$$

Then ω is row equitable with respect to $\mathbf{R}$ *with structure matrix* $\mathbf{R}'$*, and column equitable with respect to* $\mathbf{C}$ *with structure matrix* $\mathbf{C}'$*.*

Proof. Let $\mathbf{g}^i$, $1 \leq i \leq s$, and $\mathbf{h}^j$, $1 \leq j \leq s'$, be the characteristic vectors of the partitions π and π', respectively. We have

$$\mathbf{h}^j = \sum_{i \in W_j} \mathbf{g}^i.$$

¿From

$$\mathbf{A}\mathbf{h}^j = \sum_{l=1}^{s'} R'_{lj} \mathbf{h}^l$$

it follows

$$\sum_{i \in W_j} \mathbf{A}\mathbf{g}^i = \sum_{l=1}^{s'} R'_{lj} \sum_{i \in W_l} \mathbf{g}^i.$$

On the other hand

$$\sum_{i \in W_j} \mathbf{A}\mathbf{g}^i = \sum_{i \in W_j} \sum_{k=1}^{s} R_{ki} \mathbf{g}^k = \sum_{k \in W_j} \sum_{i=1}^{s} R_{ik} \mathbf{g}^i.$$

Comparing the coefficients of $\mathbf{g}^i$ in these two expressions gives

$$i \in W_l \Longrightarrow R'_{lj} = \sum_{k \in W_j} R_{ik}.$$

This proves that ω is row equitable with respect to $\mathbf{R}$ and with structure matrix $\mathbf{R}'$.

The second part of the proposition is proved by analogous arguments. $\diamond$

Let us continue with the example above. We mention three more equitable partitions of $\mathbf{A}$, namely

$$\begin{aligned}
\pi_0 &= \{1, 3, 5, 7, 9, 11\}, \{2, 4, 6, 8, 10, 12\}, \\
\pi_2 &= \{1, 3, 5\}, \{2, 4, 6\}, \{7, 9, 11\}, \{8, 10, 12\}, \\
\pi_3 &= \{1, 7\}, \{2, 8\}, \{3, 9\}, \{4, 10\}, \{5, 11\}, \{6, 12\}.
\end{aligned}$$

Their structure matrices are

$$\mathbf{R}^{(0)} = \begin{pmatrix} 1 & 2 \\ 2 & 0 \end{pmatrix}, \quad \mathbf{R}^{(2)} = \begin{pmatrix} 0 & 2 & 1 & 0 \\ 2 & 0 & 0 & 0 \\ 1 & 0 & 0 & 2 \\ 0 & 0 & 2 & 0 \end{pmatrix}, \quad \mathbf{R}^{(3)} = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}.$$

We have

$$\chi_{\mathbf{R}^{(0)}} = x^2 - x - 4.$$

Note that $\pi_1 \prec \pi_0$ and $\pi_2 \prec \pi_o$. Hence, by Proposition 5, $\chi_{\mathbf{R}^{(0)}}$ divides $\chi_{\mathbf{R}^{(1)}}$ and $\chi_{\mathbf{R}^{(2)}}$, and we find

$$\begin{aligned} \chi_{\mathbf{R}^{(1)}} &= x^4 - 2x^3 - 4x^2 + 5x + 4 = (x^2 - x - 4)(x^2 - x - 1), \\ \chi_{\mathbf{R}^{(2)}} &= x^4 - 9x^2 + 16 = (x^2 - x - 4)(x^2 + x - 4). \end{aligned}$$

Since we have many equitable partitions at hand, there are numerous ways to finish this example and find the spectrum of $\mathbf{A}$. We choose one which uses Proposition 4.

Since $\pi_4 \prec \pi_1$, the partition π_1 determines an equitable partition ω for $\mathbf{R}^{(4)}$ (see Proposition 5). Suppose that $\mathbf{R}^{(4)}$ is indexed using the primed numbers $1', 2', \ldots, 8'$, then ω reads

$$\omega = \{1', 3'\},\ \{5', 7'\},\ \{6', 8'\},\ \{2', 4'\}.$$

It is easy to check that

$$\hat{\mathbf{g}}^1 = \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \hat{\mathbf{g}}^2 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ -1 \\ 0 \end{pmatrix}, \quad \hat{\mathbf{g}}^3 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ -1 \end{pmatrix}, \quad \hat{\mathbf{g}}^4 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

is a linear base for $\mathbb{R}^{\perp}(\omega)$ with

$$\begin{array}{rcl} \mathbf{R}^{(4)}\hat{\mathbf{g}}^1 & = & -\hat{\mathbf{g}}^1 + \hat{\mathbf{g}}^2, \\ \mathbf{R}^{(4)}\hat{\mathbf{g}}^2 & = & 2\hat{\mathbf{g}}^1 + \hat{\mathbf{g}}^3, \\ \mathbf{R}^{(4)}\hat{\mathbf{g}}^3 & = & \hat{\mathbf{g}}^2 - \hat{\mathbf{g}}^3 + 2\hat{\mathbf{g}}^4, \\ \mathbf{R}^{(4)}\hat{\mathbf{g}}^4 & = & 2\hat{\mathbf{g}}^3 \end{array}$$

This gives

$$\hat{\mathbf{R}}^{(1)} = \begin{pmatrix} -1 & 1 & 0 & 0 \\ 2 & 0 & 1 & 0 \\ 0 & 1 & -1 & 2 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

The characteristic polynomial of this matrix is

$$\chi_{\hat{\mathbf{R}}^{(1)}} = x^4 + 2x^3 - 4x^2 - 5x + 4.$$

Since we have already three quadratic factors of $\chi_{\mathbf{R}^{(4)}}$, two in $\chi_{\mathbf{R}^{(1)}}$ and one additional in $\chi_{\mathbf{R}^{(2)}}$ the polynomial $\chi_{\hat{\mathbf{R}}^{(1)}}$ must be divisible by one of these quadratic factors. Checking this fact we get

$$\chi_{\hat{\mathbf{R}}^{(1)}} = (x^2 + x - 4)(x^2 + x - 1).$$

Thus, finally

$$\chi_{\mathbf{R}^{(1)}} = (x^2 - x - 4)(x^2 + x - 4)(x^2 - x - 1)(x^2 + x - 1).$$

¿From this expression we can easily compute the spectrum of $\mathbf{A}$.

Note that in the course of the determination of this factorized form of $\chi_{\mathbf{R}^{(1)}}$ the largest size of a matrix the characteristic polynomial of which we have determined was 4×4, while the adjacency matrix $\mathbf{A}$ is of size 12×12.

3.8 In the example with the graph in Figure 1 all considered equitable partitions are orbit partitions, that means, their cells are the orbits with respect to some subgroup of the automorphism group. The coarsest equitable partition which we found, namely π_0, is the orbit partition of the full automorphism group. This is not the general case. In general, an equitable partition must not be an orbit partition. The simplest counter-example is the trivial partition $\{V\}$ of a regular graph G the automorphism group of which is not transitive, i.e. which has at least two different orbits under its group of automorphisms. A further example is given in **4.4**.

3.9 The problem of how to find equitable partitions of a graph will be addressed in the next section. We finish this section by mentioning some special classes of graphs for which finding a system of equitable partitions satisfying the hypothesis of Proposition 3 is particularly easy.

1. Distance-Regular Graphs. The *distance* $\delta(u,v)$ of two vertices u und v in a connected graph G is the minimum number of edges in a path of G connecting these vertices. The maximum distance between any two vertices is called the *diameter* of G and denoted by Δ. For $v \in V$ define the *distance partition* $\mathcal{S}(v) = \{S_0(v), S_1(v), \ldots, S_{\Delta(v)}(v)\}$ of V with respect to v by

$$S_i(v) = \{u \in V \,:\, \delta(u,v) = i\},\ 0 \leq i \leq \Delta(v),\ \Delta(v) = \max\{\delta(u,v) \,:\, u \in V\}.$$

A graph G is called *distance regular* if $\Delta(v) = \Delta$, independently of v, and if there are numbers $a_i, b_i, c_i,\ 0 \leq i \leq \Delta$, (the *intersection numbers*) such that in every distance partition (no matter with respect to which v) every vertex in S_i has exactly a_i neighbours in S_i, b_i neighbours in S_{i+1} and c_i neighbours in S_{i-1} (with $S_1 = S_{\Delta+1} = \emptyset$ this condition is well stated for all $i \in [0,d]$). It says exactly that all distance partitions $\mathcal{S}(v)$ are equitable with identical structure matrices

$$\mathbf{R} = \begin{pmatrix} 0 & b_1 & & & & \\ c_1 & a_1 & b_1 & & & \\ & c_2 & a_2 & b_2 & & \\ & \cdots & \cdots & \cdots & \cdots & \\ & & c_{d-1} & a_{d-1} & b_{d-1} & \\ & & & c_d & a_d & \end{pmatrix}.$$

Here, $\mathbf{R}$ is called the *intersection matrix.*

Since this matrix is independent of v, Proposition 3 implies that the different eigenvalues of $\mathbf{A}$ are exactly the different eigenvalues of $\mathbf{R}$.

Note that any equitable partition wich contains the cell $\{v\}$ is finer that the distance partition $\mathcal{S}(v)$. This shows that for a distance-regular graph the system $\mathcal{S}(v),\ v \in V$ is the "coarsest" system of partitions satisfying the hypothesis of Proposition 3.

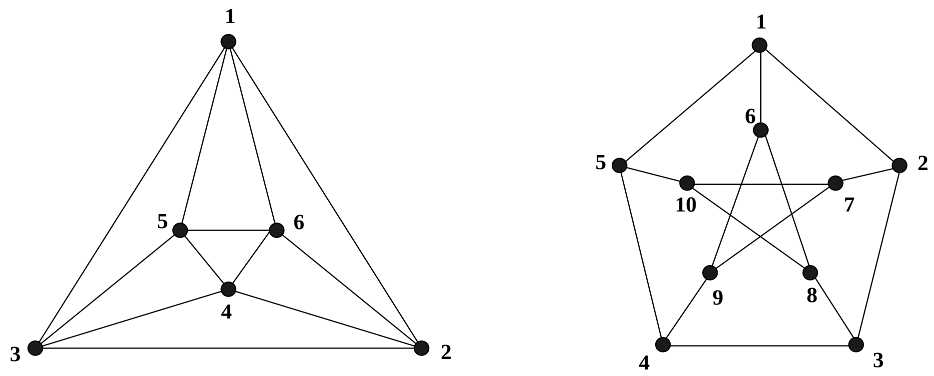

Figure 3: Oktahedron and Petersen Graph

To have an example consider the first graph in Figure 3. It is the regular oktahedron. Let $\mathbf{A}$ be its adjacency matrix. There are three different distance partitions, namely

$$\begin{aligned}\mathcal{S}(1) = \mathcal{S}(4) &= \{1\}, \{2,3,5,6\}, \{4\},\\ \mathcal{S}(2) = \mathcal{S}(5) &= \{2\}, \{1,3,4,5\}, \{5\},\\ \mathcal{S}(3) = \mathcal{S}(6) &= \{3\}, \{1,2,4,5\}, \{6\}.\end{aligned}$$

There common structure matrices are

$$\mathbf{R} = \mathbf{C}^T = \begin{pmatrix} 0 & 4 & 0 \\ 1 & 2 & 1 \\ 0 & 4 & 0 \end{pmatrix}.$$

Hence, this graph is distance-regular. Therefore, $\mathrm{spec}(\mathbf{A}) = \mathrm{spec}(\mathbf{R})$. Now, since

$$\chi_{\mathbf{R}}(x) = x^3 - 2x^2 - 8x = x(x-4)(x+2),$$

we get $\mathrm{spec}(\mathbf{A}) = \{-2, 0, 4\}$.

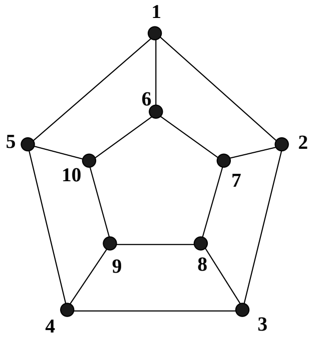

Figure 4

A distance-regular graph has a transitive automorphism group, such graphs are called *vertex transitiv*. However, the converse statement is not true. A vertex transitive graph is not necessarily distance-regular. Consider the graph in Figure 4 which is obviously vertex transitiv. It is the regular pentagonal prism (a chemical graph, the corresponding hydrocarbon has been synthesized). Its distance partition for vertex 1 is

$$\mathcal{S}(1) = \{1\}, \{2, 5, 6\}, \{3, 4, 7, 10\}, \{8, 9\}$$

which is not equitable.

2. Strongly Regular Graphs. A graph Γ is called *strongly regular* if there are natural numbers k, a and c such that Γ is k-regular, and any two vertices u and v have exactly a joint neighbours, if they are adjacent, and exactly c joint neighbours, if they are non-adjacent.

Strongly regular graphs are exactly the distance-regular graphs with diameter $\Delta = 2$. Select an arbitrary vertex $v \in V$ and consider the partition $V_1 = \{v\}, V_2 = N(v), V_3 = V - N(v) - \{v\}$, which is equitable. From the definition of a stronlgy regular graph it follows that a vertex $u \in V_2$ has a neighbours in V_2, and hence, $k-1-a$ neighbours in V_3, while a vertex $w \in V_3$ has c neighbours in V_2, and hence, $k-c$ neighbours in V_3. Thus, the structure matrix $\mathbf{R}$ of the equitable partition is

$$\mathbf{R} = \begin{pmatrix} 0 & k & 0 \\ 1 & a & k-1-a \\ 0 & c & k-c \end{pmatrix}.$$

The characteristic polynomial of $\mathbf{R}$ is

$$\chi_{\mathbf{R}}(x) = x^3 - (a+k-c)x^2 + [k(a-c) + c - k]x + k(k-c).$$

Since a k-regular graph has eigenvalue $\mu_1 = k$, $\chi_{\mathbf{R}}(z)$ is divisible by $x - k$ and we get

$$\chi_{\mathbf{R}}(x) = (x-k)(x^2 - (a-c)x + c - k).$$

Using this result, since the structure matrix $\mathbf{R}$ is independent of the vertex v, we find that a strongly regular graph with parameters n, k, a, c has exactly three different eigenvalues, namely k and the two roots of $(x^2 - (a-c)x + c - k)$, which are

$$\mu_{2,3} = \frac{a - c \pm \sqrt{(a-c)^2 + 4(k-c)}}{2}.$$

To have a concrete example consider the second graph in Figure 3. This is the often cited Petersen graph which has numerous interesting properties.

Take $v = 1$. The corresponding equitable partition is

$$\{1\},\ \{2,5,6\},\ \{3,4,7,8,9,10\}.$$

This gives

$$\mathbf{R} = \begin{pmatrix} 0 & 3 & 0 \\ 1 & 0 & 2 \\ 0 & 1 & 2 \end{pmatrix}.$$

With $a = 0$ and $c = 1$ the above considerations gives the three different eigenvalues $\mu_1 = 3$, $\mu_2 = 1$, $\mu_3 = -2$.

3. Hamming Graphs. This class of graphs is another special case of distance-regular graphs. A *Hamming graph* $H(\nu, \alpha)$ is defined on the base of a finite alphabet $\mathtt{A}$. Assume that $\mathtt{A}$ contains α different symbols and let $\mathtt{A}^*$ be the set of all possible sequences of symbols of length ν, also called *words* of length ν. For example, if $\nu = 2$ and $\mathtt{A} = \{0,1,2\}$ then $\mathtt{A}^* = \{00,01,02,10,11,12,20,21,22\}$. The set $\mathtt{A}^*$ is the vertex set of $H(\nu, \alpha)$. Edges are introduced by the following rule: Two words are adjacent if and only if they differ in exactly one position. Hence, in the case $\nu = 2$ and $\alpha = 3$ just mentioned this rule requires the edges

$$[00,01], [00,02], [00,10], [00,20], [01,02], [01,11], [01,21], \ldots$$

and so on. Note that the kind of the symbols is obviously irrelevant for the definition of $H(\nu, \alpha)$, only their number is relevant. Therefore we always may assume that the alphabet for $H(\nu, \alpha)$ is $\{0, 1, \ldots, \alpha - 1\}$.

Hamming graphs arise in a natural way in molcular biology, since genes are sequences taken from the alphabet $\mathtt{A}=\{A, C, G, T\}$. Extensive studies of landscapes derived from models of RNA secondary structures are discussed in [24, 63, 66], and the references therein.

The eigenvalues and eigenvectors of Hamming graphs are well known, see e.g. [16]. It also well known that the Hamming graphs are distance transitive and hence distance regular.

"Generalized" Hamming graphs, which have a different alphabet at each position of the sequence, play a role in population genetics. Here, each sequence position corresponds to an entire gene, and different "letters" represent the different allels, see

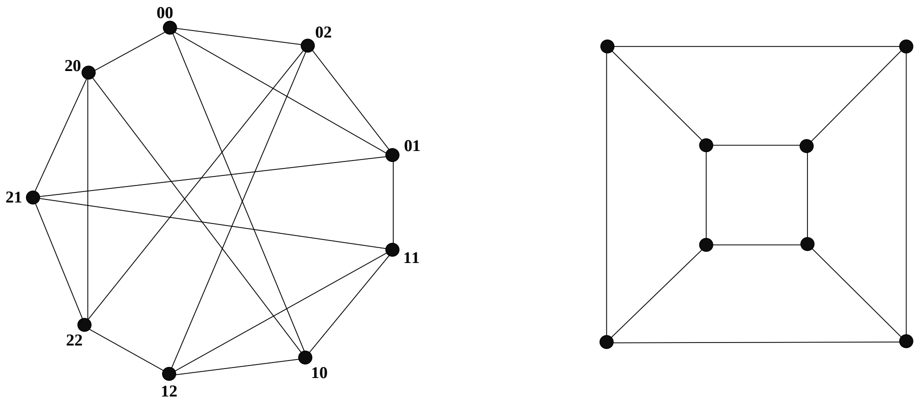

Figure 5: $H(2,3)$ and $H(3,2)$.

e.g. [67] for a discussion in the context of landscapes. These graphs are not distance regular any more. However, generalized Hamming graphs are products of complete graphs, which allows the explicit computation of eigenvalues and eigenvectors, see e.g. [13]. Furthermore, they are Cayley graphs derived from suitable commutative groups.

4. Hypercubes. Hamming graphs $H(n,2)$ are called *hypercubes*. $H(1,2)$ consists of a single edge, $H(2,2)$ is a unit square, $H(3,2)$ is the unit cube (in the second part of Figure 5 drawn as planar graph). Hypercubes are by far the most used configuration graphs. In fact, most combinatorial optimization problems and even continuous optimization problems are deliberately encoded in terms of binary strings with fixed length in order to run standard optimization heuristics, in particular genetic algorithms.

The eigenvalues of $H(n,2)$ are $\mu_p = n - 2p$ with multiplicity $\binom{n}{p}$, the eigenvectors are known as Walsh-functions and play an important role in the analysis of genetic algoritms [29, 67, 74].

5. Cayley Graphs of S_n. Let G be a permutation group acting on a finite set X and let $\imath$ denote the identity in G. Furthermore, let $\Omega \subset \mathsf{G}$ be a set of generators of G such that (i) $\imath \notin \Omega$ and (ii) $x \in \Omega \implies x^{-1} \in \Omega$. A graph $G = G(\mathsf{G}, \Omega)$ with vertex set $V = \mathsf{G}$ and edges $\{x,y\} \in E$ if and only if $xy^{-1} \in \Omega$ is called a *Cayley graph* of the group G. Cayley graphs form a special class of vertex transitive graphs. The most important configuration graphs, including the Hamming graphs discussed above, are Cayley graphs of suitable groups.

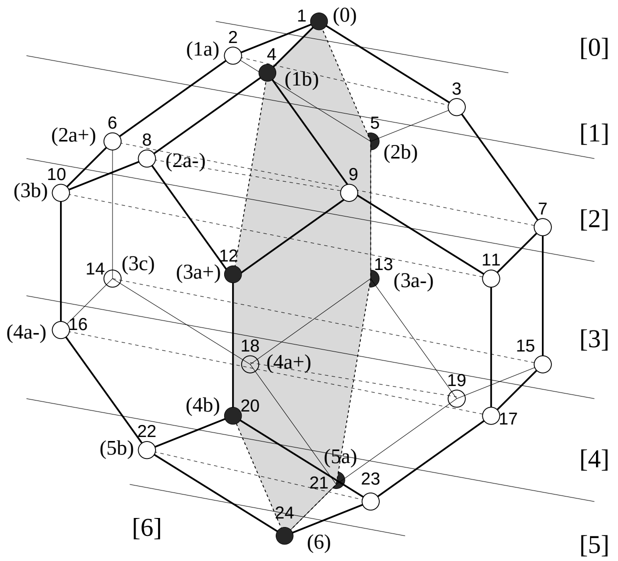

Figure 6: The permutohedron $G(\mathsf{S}_4, \mathcal{K})$.

Distance classes are indicated by square brackets, the orbits of the stabilizer subgroup $\mathsf{Aut}[G(\mathsf{S}_4, \mathcal{K})]_0 = \{\imath, \eta\}$ are labeled with symbols in round parentheses. Vertices shown in black are fixed by this group, while vertices shown in white belong to orbits of lenght two. Dashed lines connect vertices belonging to the same orbit. Reflexion on the shaded plane is a symmetry of the permutohedron corresponding to the involution η.

A typical combinatorial optimization problem on a set of permutations is the *Quadratic Assignment Problem* (QAP). We are given n facilities and n locations. There is a flow f_{ij} between facility i and facility j, a distance or cost rate per unit flow d_{ij} between locations i and j, and a cost c_{ij} for setting up facility i at location j. The total cost of a particular assignment $\pi \in \mathsf{S}_n$ is then

$$f(\pi) = \sum_{i=1}^{n} \sum_{j=1}^{n} f_{ij} d_{\pi(i)\pi(j)} + \sum_{i=1}^{n} c_{i,pi(i)}$$

For a survey see [57]. The *Traveling Salesman Problem* (TSP), in which X is a set of cities that have to be visited exactly once by a salesman, who at the end of his tour has to return to the starting point, can be seen as a special case of QAP. One has to set $f_{ij} = \delta_{j,i+1}$ (indices taken modulo n), and $c_{ij} = 0$.

Oftentimes sets of generators of S_n are chosen as move sets for optimization heuristics such as simulated annealing. Most commonly, tranpositions, or so-called reversals are used. The landscape of the TSP with these two move sets is considered in [68].

Canonical transpositions, $\mathcal{K} = \{(i, i+1), 0 \leq i < n\}$, are a reasonable choice if one wants to get relatively small vertex degrees in the configuration graph.

The Cayley graphs $G(\mathsf{S}_n, \mathcal{K})$ exhibit a wealth of regularities, but are in many respects much more complicated than Hamming graphs, in particular their coherent algebras (see **5.5**) are homogeneous but not commutative for $n \geq 4$. $G(\mathsf{S}_2, \mathcal{K}) = P_2$, the path of length 2, and $G(\mathsf{S}_3, \mathcal{K}) = C_6$, the cycle of length 6. The graph $G(\mathsf{S}_4, \mathcal{K})$ is known as the permutohedron, Figure 6.

4 How to find equitable partitions

4.1 In this subsection equitable means row equitable. With obvious changes in the formulation all results remain valid also for column equitable partitions.

Suppose we are given a matrix $\mathbf{A}$ and some initial partition π of V. Is there an equitable partition which is at least as fine as π? Since we are interested in coarse equitable partitions mainly (the structure matrix should be small), we should specify this question to: What is the coarsest equitable partition, if any, which is at least as fine as π.

Suppose that π is not equitable and that ω is an equitable partition which is finer than π. Take any two cells $U, W \in \pi$. Let $\mathbf{g}_U$ and $\mathbf{g}_W$ be the characteristic vectors of U and W. Then W is a union of some cells of ω, to be concrete, say $W = W' \cup W'' \cup \dots$, with $W', W'', \dots \in \omega$. Now, if $u, u' \in U$ belong to the same cell of ω, then

$$(\mathbf{A}g_{W'})_u = (\mathbf{A}g_{W'})_{u'}, \ \ (\mathbf{A}g_{W''})_u = (\mathbf{A}g_{W'})_{u''}, \dots$$

and therefore

$$(\mathbf{A}g_W)_u = (\mathbf{A}g_W)_{u'}.$$

With other words, if $(\mathbf{A}g_W)_u \neq (\mathbf{A}g_W)_{u'}$, then u, u' must belong to different cells of ω. Thus let us assume that $\{a_1, \dots, a_t\}$ is the set of different values of the term $(\mathbf{A}g_W)_u$ when u varies over U. Define

$$U_i = \{u \in U \, : \, (\mathbf{A}g_W)_u = a_i\}, \ 1 \leq i \leq t,$$

and replace in π the cell U by the new cells $U_1, \dots, U_t$ to get a new partition π' which is finer than π (if $t > 1$). Any equitable partition which is finer than π must either equal π' or be finer than π'. Thus, when looking for the coarsest equitable partition which is finer than π we may replace π by π'.

Computing π' from π is called a *refinement step*. As long as π is not equitable, the new partition π' is strictly finer than π. We may repeat this step now choosing two cells U' and W' of π'. In this way we get a sequence of continuously strictly finer partitions which are all coarser than ω. This sequence must finish after a finite number of steps, since the number of partitions of a finite set is finite. It ends when no further refinement step is possible, i.e. when the current partition is equitable.

Of course, an analogous procedure will compute the coarsest column equitable partition which is finer than π. Just replace $\mathbf{A}g_W^T$ by $\mathbf{g}_W^T\mathbf{A}$ in the refinement step above. If $\mathbf{A}$ is not symmetric, then we have to compare $(\mathbf{A}g_W)_u$ to $(\mathbf{A}g_W)_{u'}$ and $(\mathbf{g}_W^T\mathbf{A})_u$ to $(\mathbf{g}_W^T\mathbf{A})_{u'}$ to decide whether u and u' can belong to the same cell of the coarsest equitable partition finer than π.

These considerations are summarized and restated in the following proposition.

Proposition 6.
(a) For every partition π of the index set V of a matrix $\mathbf{A}$ there is a uniquely determined (row or column) equitable partition ω which is at least as fine as π. In particular, there is a uniquely determined absolutely coarsest (row or column) equitable partition for $\mathbf{A}$.
(b) For every matrix $\mathbf{A}$ there is a system of coarsest (row or column) equitable partitions which satisfies the hypothesis of Proposition 3.

Proof. The second statement of part (a) follows with the initial partition $\pi = \{V\}$. Part (b) follows with the initial partitions $\pi_v = \big\{\{v\}, \{V \setminus \{v\}\}, \big\}\ v \in V$. $\diamond$

The absolutely coarsest equitable partition is also called *total degree partition* (see [73]).

4.2 If $\mathbf{A}$ is the adjacency matrix of a graph, then $(\mathbf{A}g_W)_u$ means the number of neighbors of the vertex u which belong to W, and a refinement step can be explained in terms of numbers of neighbors. It is also possible to combine several refinement steps into a single one by using all values $(\mathbf{A}g_W)_u$, $W \in \pi$ simultaneously. Let us explain this with the graph in Figure 7, the so-called *cunean*.

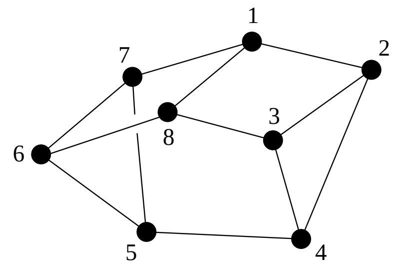

Figure 7: Cunean

The cunean is 3-regular, hence, the absolutely coarsest equitable partition is the trivial partition $\{V\}$.
Let us start with

$$\pi = \{1\}, \{2, 3, 4, 5, 6, 7, 8\}.$$

Take $U = \{2, 3, 4, 5, 6, 7, 8\}, W = \{1\}$ and $W' = U$. For $u \in U$ the term $(\mathbf{A}g_W)_u$ is the number of neighbours of u in $\{1\}$ (which is 0 or 1) while $(\mathbf{A}g_{W'})_u$ is the number of neighbours of u in W'. We associate to each $u \in U$ a list $L(u) = ((\mathbf{A}g_W)_u, (\mathbf{A}g_{W'})_u)$ of these two numbers, obtaining

$$L(2) = (1, 2);\ L(3) = (0, 3);\ L(4) = (0, 3);\ L(5) = (0, 3);$$
$$L(6) = (0, 3);\ L(7) = (1, 2);\ L(8) = (1, 2).$$

We have found two different lists. According to this result U splits into $\{2, 7\}$ and $\{3, 4, 5, 6\}$. The new partition is now

$$\pi' = \{1\}, \{2, 7, 8\}, \{3, 4, 5, 6\}.$$

The first refinement step is finished.

For the next step take $U = \{3, 4, 5, 6\}$. Since π' contains three cells we have now to construct a list of three entries for each $u \in U$, the number of neighbors of u in the three different cells. We get

$$L(3) = (0, 2, 1);\ L(4) = (0, 1, 2);\ L(5) = (0, 1, 2);\ L(6) = (0, 2, 1).$$

According to this result U splits into two parts $\{3, 6\}$ and $\{4, 5\}$. The new partition is now

$$\pi'' = \{1\}, \{2, 7, 8\}, \{3, 6\}, \{4, 5\}.$$

The second refinement step is finished.

For the next step take $U = \{2, 7, 8\}$. Since π'' has four cells, the lists $L(u), u \in U$ will have four entries. We get

$$L(2) = (1, 0, 1, 1);\ L(7) = (1, 0, 1, 1);\ L(8) = (1, 0, 2, 0).$$

Hence, U splits into two cells $\{2, 7\}$ and $\{8\}$.

The next few steps (one for every cell) don't strictly refine any more. They are nevertheless necessary in order to prove that the current partition is equitable. Therefore, the coarsest equitable partition of the cunean in which $\{1\}$ is a cell is

$$\pi_1 = \{1\}, \{2,7\}, \{3,6\}, \{4,5\}, \{8\}.$$

4.3 The refinement procedure for transforming a given partition into an equitable one which we have presented in **4.1** and demonstrated in **4.2** can easily be formalized and implemented as a computer programm. Numerous variants of this method are incorporated into graph isomorphism algorithms, see for example [50]. A detailed discussion of such variants can be found in [73].

Tricky computer programs are able to compute the coarsest equitable partition which is finer as a given one for matrices up to some million rows (graphs of some million vertices), the upper bound depends on the available computer power. The programm `qweil`, freely accessible under the address [], works on a PC with graphs of some hundred thousend vertices.

4.4 The partitions π_4, π_5 and π_6 in the example of **3.6** can been found by applying the above described refinement method. Starting with $\{1,3,5\}, V\backslash\{1,3,5\}$ we would get π_2, starting with $\{1,7\}, V \setminus \{1,7\}$ leads to π_3.

In the case of the cunean Proposition 3 does not yield a full reduction of the problem size. If we start with one of the vertices $v \in \{2,3,6,7\}$, the resulting coarsest equitable partition containing $\{v\}$ is the discrete partition the structure matrices of which are $\mathbf{C} = \mathbf{R} = \mathbf{A}$. If this happens, then the second part of Proposition 3, namely

$$\operatorname{spec}(\mathbf{A}) \subseteq \bigcup_{k=1}^{\nu} \operatorname{spec}(\mathbf{R}^{(k)}),$$

becomes trivial. Here only the first part

$$\bigcup_{k=1}^{\nu} \operatorname{spec}(\mathbf{R}^{(k)}) \subseteq \operatorname{spec}(\mathbf{A})$$

reduces the task of finding the eigenvalues auf $\mathbf{A}$ to the task of finding the eigenvalues of several smaller matrices, however, in general not the whole spectrum is covered by the spectra of those matrices $\mathbf{R}^{(k)}$ which are strictly smaller than $\mathbf{A}$.

In situations where the system of coarsest partitions satisfying the hypothesis of Proposition 3 contains the matrix $\mathbf{A}$ itself one can look for coarse equitable partitions which contain a given predetermined cell $Z \subset V$. This leads us to the question: Given a matrix $\mathbf{A}$ (or a graph G) and a subset Z of V, is there an equitable partition π wich contains the cell Z? The answer is not always positiv. Z must fullfill certain necessary conditions.

Proposition 7. *For any matrix* $\mathbf{A}$ *and any subset* Z *of* V *there is a coarsest row equitable partition containing the cell* Z *only if the row sums*

$$\sum_{j \in Z} A_{ij} \text{ and } \sum_{j \in V} A_{ij}$$

are independent of $i \in Z$. *There is a coarsest column equitable partition containing* Z *only if the column sums*

$$\sum_{i \in Z} A_{ij} \text{ and } \sum_{i \in V} A_{ij}$$

are independent of $j \in Z$. *In the positive case the coarsest equitable partition is unique.*

Proof. The conditions are obviously necessary. To show the uniqueness, apply the refinement method of **4.1** to the initial partition $Z, V \setminus Z$. Perform refinement steps as described in **4.1** always choosing a current cell $U \neq Z$. If no more refinement is possible in this way, then choose $U = Z$. If Z has to be split into several subcells, then no equitable partition containing the cell Z exists. Otherwise, the current partition is equitable. $\diamond$

Consider once more the cunean in Figure 6. Let us try to find an equitable partition which contains the cell $Z = \{2, 3\}$. We start with the partition

$$\pi = \{2, 3\}, \{1, 4, 5, 6, 7, 8\}.$$

In the first step we take $U = \{1, 4, 5, 6, 7, 8\}$ and $W = \{2, 3\}$ and construct the lists

$$L(1) = L(8) = (1, 2);\ L(4) = (2, 1);\ L(5) = L(6) = L(7) = (0, 3).$$

Thus, the new partition is

$$\pi' = \{2, 3\}, \{1, 8\}, \{4\}, \{5, 6, 7\}.$$

In the next step we take $U = \{1, 8\}$ getting no refinement. Taking $U = \{5, 6, 7\}$ results in

$$\pi'' = \{2, 3\}, \{1, 6\}, \{6, 7\}, \{4\}, \{5\}.$$

The next steps do not strictly refine any more. In the last step we take $U = \{2, 3\}$. Since also then now no refinement is made, the current partition is equitable. Denote it by π_2.

Note that for the cunean graph

$$\pi_0 = \{1, 4, 5, 8\}, \{2, 3, 6, 7\}$$

is also equitable. Since there is no automorphism of this graph which maps 1 onto 4, the set $\{1, 4, 5, 8\}$ is not an orbit of a group of automorphisms. Therefore, this partition is not an orbit partition. The orbit partition with respect to the full automorphism group of the cunean is

$$\pi_3 = \{1, 8\}, \{2, 3, 6, 7\}, \{4, 5\}.$$

Now we find

$$\chi_{\mathbf{R}^{(0)}} = x^2 - 2x - 3 = (x - 3)(x + 1)$$

and

$$\chi_{\mathbf{R}^{(3)}} = (x - 1)^3 - 4(x - 1) = (x - 3)(x + 1)(x - 1).$$

Since $\pi_1 \prec \pi_3$, we can find $\chi_{\mathbf{R}^{(1)}}$ by applying Proposition 4 to $\mathbf{R}^{(1)}$ and π_3. This gives

$$\chi_{\mathbf{R}^{(1)}} = (x - 3)(x + 1)(x - 1)(x^2 + 2x - 1).$$

Now, once more applying Proposition 4, this time to $\mathbf{A}$ and π_1 yields

$$\chi_{\mathbf{A}} = (x - 3)(x + 1)(x - 1)(x^2 + 2x - 1)(x^3 + x^2 - 3x + 1).$$

Since the cubic factor equals $(x - 1)(x^2 + 2x - 1)$ we see that this last step did not add anything to the spectrum of $\mathbf{A}$, and we have finally

$$\mathrm{spec}(\mathbf{A}) = \mathrm{spec}(\mathbf{R}^{(1)}) = \{3, 1, -1 + \sqrt{2}, -1, -1 - \sqrt{2}\}$$

where $-1, -1 + \sqrt{2}$ and $-1 - \sqrt{2}$ have multiplicity 2 each.

The examples presented here and in Section 3 are chosen in order to demonstrate as simply as possible the use of equitable partitions for finding the spectrum of a matrix. Its is clear that for matrices of this small size no unusual mathematical tools are necessary. Instead of treating the 12 adjacency matrix $\mathbf{A}$ of the example in Figure 1 "by hand" we could use one of the software packages like `mathematica` or `maple` which would provide us algorithms for computing the characteristic polynomials and the eigenvalues of matrices of even much larger size. Today there are reliable numerical methods for finding the spectra of matrices which can treat matrices up to some hundred thousend rows. With configuration graphs, however, we have to treat matrices the size of which is still enormously larger. It is here, where equitable partition can show their true power by reducing the problem size to a tractable one.

4.5 Let π be any partition of V and $\mathbb{R}(\pi)$ the linear space defined in **3.2**. The set $\mathcal{A}(\pi)$ of matrices for which π is (row or column) equitable is a matrix algebra. Indeed, let $\mathbf{A}$ and $\mathbf{A}'$ be contained in $\mathcal{A}(\pi)$, let α and α' be two arbitrary real numbers, and let $\mathbf{R}$ and $\mathbf{C}$, respectively, $\mathbf{R}'$ and $\mathbf{C}'$, be the corresponding structure matrices. A simple computation shows that $\alpha\mathbf{A} + \alpha'\mathbf{A}' \in \mathcal{A}(\pi)$ with structure matrices $\alpha\mathbf{R} + \alpha'\mathbf{R}'$ and $\alpha\mathbf{C} + \alpha'\mathbf{C}'$. Further, $\mathbf{A}\mathbf{A}' \in \mathcal{A}(\pi)$ with structure matrices $\mathbf{R}\mathbf{R}'$ and $\mathbf{C}\mathbf{C}'$.

In particular, if π is equitable for $\mathbf{A}$, then it is also equitable for every power $\mathbf{A}^l$ with structure matrices $\mathbf{R}^l$ and $\mathbf{C}^l$. If $p(x)$ is an arbitrary polynomial, then π is equitable for $p(\mathbf{A})$ with structure matrices $p(\mathbf{R})$ and $p(\mathbf{C})$.

5 Coherent algebras

5.1 A matrix algebra is a linear space of matrices which is closed with respect to matrix multiplication. The full matrix algebra of $n \times n$-matrices which contains all matrices the rows and columns of which are indexed with elements from V is denoted by Mat_V. In general, one is interested in subalgebras of Mat_V specified by certain conditions which the elements should fulfill.

Let $\mathbf{I}$ be the unit matrix of Mat_V and $\mathbf{J} = \mathbf{e}\mathbf{e}^T$ the matrix with all entries equal to 1. For two matrices $\mathbf{A}$ and $\mathbf{A}'$ define the *componentwise product* $\mathbf{A} \circ \mathbf{A}'$ by

$$(\mathbf{A} \circ \mathbf{A}')_{ij} = A_{ij}A'_{ij}.$$

A subalgebra $\mathcal{A}$ of Mat_V is called a *coherent algebra* (on V) if it contains $\mathbf{I}$ and $\mathbf{J}$, and if it is closed with respect to the componentwise product and with respect to transposition. Coherent algebras have been introduced and studied first in [78], [79], and independently in [33], [34]. Since that, a rich theory has been built up around them in the literature. Today, the notion coherent algebra and the equivalent notion *coherent configuration* (see [34]) are placed among the main tools of algebraic combinatorics.

5.2 A friendly introduction to coherent algebras is given in [43], while [20] is a collection of papers covering the most important aspects of their theory. We list here some important features of this type of algebras which are needed in the remaining part of our paper, for proofs see [33].

1. Every coherent algebra possesses a unique linear basis $\mathbf{A}_1, \dots, \mathbf{A}_s$ consisting of $0,1$-matrices $\mathbf{A}_i$, called the *the standard basis*, such that

   $$(a) \quad \mathbf{I} = \sum_{i=1}^{t} \mathbf{A}_i$$

   for some $t,\ 1 \le t < s$, and

   $$(b) \quad \mathbf{J} = \sum_{i=1}^{s} \mathbf{A}_i.$$

   The second condition says that $\mathbf{A}_i \circ \mathbf{A}_j = 0$ for $i \neq j$.

2. For every basis matrix $\mathbf{A}_i$ there is a basis matrix $\mathbf{A}_{i'}$ such that $\mathbf{A}_{i'} = \mathbf{A}_i^T$. Note that in general $i' \neq i$, the matrices $\mathbf{A}_i$ with $i > t$ are not necessarily symmetric.

3. The product of two basis matrices is a linear form
$$\mathbf{A}_i\mathbf{A}_j = \sum_{k=1}^{r} p_{ij}^k \mathbf{A}_k$$
with integral coefficients p_{ij}^k which are called the *structure constants* of the algebra.

4. According to 1(a) the sets $C_i = \{v \in V : (\mathbf{A}_i)_{vv} = 1\}$, $1 \leq i \leq t$, form a partition π_{cell} of V, the so-called *cell partition*. This partition is equitable with respect to every basis matrix $\mathbf{A}_i$. The cells C_i are called the *cells* of the coherent algebra.

5. The basis matrices $\mathbf{A}_i$ can be considered as adjacency matrices of (in general directed) graphs $G_i = (V, E_i)$, the *basis graphs*. Their arc sets are $E_i = \{(u, v) : (\mathbf{A}_i)_{uv} = 1\}$. The sets E_i, $1 \leq i \leq s$, are called the basis sets of the algebra. They form a partition of $V \times V$ which is called a *coherent configuration*.

6. For each basis set E_i there are cells $C_j, C_k \in \pi_{cell}$ such that $E_i \subseteq C_j \times C_k$. Further, in this case,
$$|\{v : (u, v) \in E_i\}| = \begin{cases} D_i^+ & \text{for } u \in C_j \\ 0 & \text{otherwise.} \end{cases}$$
and likewise,
$$|\{v : (v, u) \in E_i\}| = \begin{cases} D_i^- & \text{for } u \in C_k \\ 0 & \text{otherwise.} \end{cases}$$
where
$$D_i^+ = \frac{|E_i|}{|C_j|} \text{ and } D_i^- = \frac{|E_i|}{|C_k|}.$$

7. A coherent algebra for which $t = 1$ (or with other words, in which $\mathbf{I}$ is a basis matrix) is called *homogenous*. In a homogenous coherent algebra $C_1 = V$, the cell partition is trivial.

5.3. Our interest in coherent algebras is explained by the following facts.

Proposition 8. *Let $\mathcal{A}$ be a coherent algebra on V, let $\mathbf{A}_1, \ldots, \mathbf{A}_s$ be its standard basis and $E_1, \ldots, E_s$ its basis sets. For arbitrary $v \in V$ define the partition*

$$\pi_v = \{X_{i_1}(v), X_{i_2}(v) \ldots, X_{i_{s(v)}}\}$$

where the $X_{i_j}(v)$ are the non-empty sets among

$$X_i(v) = \{u \in V \, : \, (u,v) \in E_i\}, \; 1 \leq i \leq s.$$

Then each π_v is row equitable with respect to all basis matrices $\mathbf{A}_i$ and, hence, with respect to all matrices $\mathbf{A} \in \mathcal{A}$. The system π_v, $v \in V$, fulfills the hypothesis of Proposition 3.

Proof. Let $v \in V$ be fixed. The characteristic vector $\mathbf{g}^j$ of $X_j(v)$ is the column $((\mathbf{A}_j)_{1,v}, \ldots, (\mathbf{A}_j)_{n,v})^T$ of the basis matrix $\mathbf{A}_j$ with index v. Thus,

$$(\mathbf{A_i g}^j)_u = (\mathbf{A_i A}_j)_{u,v}.$$

Since

$$\mathbf{A}_i \mathbf{A}_j = \sum_{k=1}^{s} p_{ij}^k \mathbf{A}_k$$

we get

$$(\mathbf{A_i g}^j)_u = \sum_{k=1}^{s} p_{ij}^k (\mathbf{A}_k)_{u,v} = \sum_{k=1}^{s} p_{ij}^k (\mathbf{g}^k)_u$$

This gives

$$(\mathbf{A_i g}^j) = \sum_{k=1}^{s} p_{ij}^k \mathbf{g}^k$$

and proves that π_v is row equitable with respect to each basis matrix $\mathbf{A}_i$. Since every $\mathbf{A} \in \mathcal{A}$ is a linear combination of the $\mathbf{A}_i$'s, it follows that π_v is row equitable with respect to every matrix in $\mathcal{A}$.

The partition π_v contains the cell $\{v\}$. Therefore, $\{\pi_v \;\, v \in V\}$ fulfills the hypothesis of Proposition 3. $\diamond$

Remark: If we change the definition of the $X_i(v)$'s to

$$X_i(v) = \{u \, : \, (v,u) \in E_i\}, \; 1 \leq i \leq s,$$

then π_v is column equitable with respect to every matrix in $\mathcal{A}$.

5.4 The last proposition gives us a system of equitable partitions with the property that the spectra of their structure matrices $\mathbf{R}$ cover the spectrum of every matrix in $\mathcal{A}$. This is a strong and very useful property. However, the main source of our interest in coherent algebras is expressed by the following considerations.

Let again $\mathcal{A}$ be a coherent algebra on V with standard basis $\mathbf{A}_1, \ldots, \mathbf{A}_s$ and basis sets $E_1, \ldots, E_s$. Let $f : V \longrightarrow \mathbb{R}$ be function on V and define an *autocorrelation function* of f with respect to $\mathcal{A}$ by

$$\rho_f(i) = \frac{1}{|E_i|} \sum_{(u,v)\in E_i} f(u)f(v) = \frac{1}{|E_i|}\mathbf{f}^T A_i \mathbf{f}.$$

For $1 \leq i \leq s$ let i' be the index such that $\mathbf{A}_{i'} = \mathbf{A}_i^T$. Obviously, for all i we have $\rho_f(i') = \rho_f(i)$.

Proposition 9. *(a) Suppose that $\mathcal{A}$ contains the adjacency matrix $\mathbf{A}$ of a graph G. The random walk autocorrelation function r_f of a random walk on G is uniquely expressible in terms of the partitions π_v, $v \in V$ and the autocorrelation function ρ_f with respect to $\mathcal{A}$.*
(b) If $\mathcal{A}$ is homogenous, then the structure matrices $\mathbf{R}_v$ of π_v are all equal to some matrix $\mathbf{R}$. In this case r_f is exponential if and only if ρ_f is an eigenvector of $\mathbf{R}$.

Proof. (a) First we show that $\mathbf{A} \in \mathcal{A}$ implies $\mathbf{D}^{-1} \in \mathcal{A}$.

Suppose that the different vertex degrees in G are $\delta_1, \ldots, \delta_\sigma$ and define $U_i = \{v \in V : d_v = \delta_i\}$, $1 \leq i \leq \sigma$. These sets are the cells of the *degree partition* π of V with respect to G. Let ω be the absolutely coarsest equitable partition with respect to $\mathbf{A}$ and ω_0 the cell partition of $\mathcal{A}$. Since ω_0 is equitable with respect to $\mathbf{A}$, this partition is at least as fine as ω, and ω in turn is at least as fine as π. Hence, $\omega_0 \preceq \pi$.

For $U \subseteq V$ let $\mathbf{I}_U$ be the diagonal matrix with diagonal entries $(\mathbf{I}_U)_{uu} = 1$, if $u \in U$, and $(\mathbf{I}_U)_{uu} = 0$, if $u \notin U$. Note that for a cell C of $\mathcal{A}$, the matrix $\mathbf{I}_C$ is one of the basis matrices $\mathbf{A}_i$ with index $i < t$. The fact $\omega_0 \preceq \pi$ is now equivalent to the statement that each matrix $\mathbf{I}_{U_i}$ is a sum of certain basis matrices A_i, all with indices $i < t$. This proves that each matrix $\mathbf{I}_{U_i}$ belongs to $\mathcal{A}$. But

$$\mathbf{D}^{-1} = \sum_{i=1}^{\sigma} \frac{1}{\delta_i} I_{U_i}.$$

Hence, also $\mathbf{D}^{-1} \in \mathcal{A}$.

Consider now the autocorrelation function of a random walk on G. We have

$$r_f(k) = \mathbf{f}^T \mathbf{T}_k \mathbf{f}$$

with

$$\mathbf{T}_k = \frac{1}{2|E|}\mathbf{D}^{-k+1}\mathbf{A}^k.$$

Since $\mathbf{T}_k \in \mathcal{A}$ we may write

$$\mathbf{T}_k = \frac{1}{2|E|}\sum_{i=1}^{s} H_{ki}\mathbf{A}_i$$

with appropriate constants H_{ki}. This yields

$$r_f(k) = \frac{1}{2|E|}\sum_{i=1}^{s} H_{ki}\mathbf{f}^T\mathbf{A}_i\mathbf{f} = \frac{1}{2|E|}\sum_{i=1}^{s} H_{ki}|E_i|\rho_f(i).$$

Now, choose $v \in V$ and consider the partition π_v introduced in Proposition 8, let

$$\mathbf{g}^{i_1}, \dots, \mathbf{g}^{i_{s(v)}}$$

be the characteristic vectors of its cells and $\mathbf{R}_v$ its structure matrix. W. l. o. g we may assume that $X_{i_1}(v) = \{v\}$. Define $\Lambda(v) = \{i_1, \dots, i_{s(v)}\}$. Since π_v is row equitable, all vertices in a cell $X_l(v)$ have the same degree in G, denote it by η_l. Then

$$\mathbf{D}^{-k+1}\mathbf{g}^l = \frac{1}{\eta_l^{k-1}}\mathbf{g}^l,\ l \in \Lambda(v).$$

With this notation the structure matrix for π_v with respect to $\mathbf{T}_k$ is

$$(\mathbf{R}(\mathbf{T}_k))_{lj} = \frac{1}{2|E|}\frac{(\mathbf{R}_v^k)_{lj}}{\eta_l^{k-1}},\ l, j \in \Lambda(v).$$

For $1 \leq i \leq s$ let $\alpha(i)$ and $\beta(i)$ such that $E_i \subset C_{\alpha(i)} \times C_{\beta(i)}$. Then for $j \in \Lambda(v)$

$$(\mathbf{A}_i\mathbf{g}^j)_v = (\mathbf{A}_i\mathbf{A}_j)_{vv} = \sum_{l=1}^{n}(A_{i'})_{lv}(A_j)_{lv} = \begin{cases} 0 & \text{if } i' \neq j \text{ or } v \notin C_{\alpha(i)} \\ D_j^- & \text{otherwise.} \end{cases}$$

Further, since the assumption $v \in C_{\alpha(j')}$ implies $\alpha(j') = i_1$ and $\eta_{i_1} = d_v$, the equality

$$(\mathbf{T}_k\mathbf{g}^j)_v = \frac{1}{2|E|}\sum_{l=1}^{s}\frac{(\mathbf{R}_v^k)_{lj}}{d_l^{k-1}}(\mathbf{g}^l)_v = \frac{1}{2|E|}\sum_{i=1}^{s} H_{ki}(\mathbf{A}_i\mathbf{g}^j)_v$$

reduces to

$$\frac{(\mathbf{R}_v^k)_{i_1,j}}{d_v^{k-1}} = H_{kj'} D_j^- .$$

Changing indices j' to i gives

$$H_{ki} = \frac{1}{D_{i'}^-} \frac{(\mathbf{R}_v^k)_{i_1,i'}}{d_v^{k-1}}.$$

where $v \in C_{\alpha(i)}$. Note that $|E_i| = |E_{i'}| = |C_{\alpha(i)}| D_{i'}^-$. Inserting all this in the expression for r_f gives

$$r_f(k) = \frac{1}{2|E|} \sum_{i=1}^{s} |C_{\alpha(i)}| \frac{(\mathbf{R}_{v_i}^k)_{i_1,i'}}{d_{v_i}^{k-1}} \rho_f(i)$$

where in each summand v_i is an arbitrary vertex in $C_{\alpha(i)}$. This proves (a).

(b) If $\mathcal{A}$ is homogeneous then G must be D-regular (for some appropriate degree D). In this case $2|E| = |V|D$, $d_v = D, |C_{\alpha(i)}| = |V|$ and we may assume $i_1 = 1$. Thus, using the equality $\rho_f(i') = \rho_f(i)$, the expression for r_f reduces to

$$r_f(k) = \sum_{i=1}^{s} \frac{(\mathbf{R}^k)_{1,i}}{D^k} \rho_f(i).$$

Let $\boldsymbol{\rho}_f$ be the s-dimensional vector the components of which are $\rho_f(1), \ldots, \rho_f(s)$. Then the last equality reads

$$r_f(k) = \frac{1}{D^k} (\mathbf{R}^k \boldsymbol{\rho}_f)_1.$$

Let $\mathbf{y}^1, \ldots, \mathbf{y}^s$ a system of s orthonormal eigenvectors of $\mathbf{R}$ (which exists, see Proposition 2). Let $\mu_1, \ldots, \mu_s$ be the corresponding eigenvalues. Writing

$$\boldsymbol{\rho}_f = \sum_{i=1}^{s} \sigma_i \mathbf{y}^i$$

gives finally

$$r_f(k) = \sum_{i=1}^{s} \sigma_i \frac{\mu_i^k}{D^k} (\mathbf{y}^i)_1.$$

This completes the proof. $\diamond$

5.5 The investigation of the autocorrelation function r_f via its representation with the help of a coherent algebra $\mathcal{A}$ and its autocorrelation function ρ_f is the more convenient the "smaller" $\mathcal{A}$, which means the smaller the number s of basis matrices $\mathbf{A}_i$. Coherent algebras can be compared in terms of their basis matrices (or basis sets). An algebra $\mathcal{A}'$ is a coherent subalgebra of a coherent algebra $\mathcal{A}$, if every basis matrix $\mathbf{A}'_i$ of $\mathcal{A}'$ is a sum

$$\mathbf{A}'_i = \sum_{j \in \Lambda_i} \mathbf{A}_j,\ \Lambda_i \subset \{1, 2, \dots, s\}$$

of basis matrices of $\mathcal{A}$.

Given a graph G and its adjacency matrix $\mathbf{A}$ we need a coherent algebra $\mathcal{A}$ which contains $\mathbf{A}$. For each matrix A there is a "smallest" coherent algebra which contains $\mathbf{A}$ (and which is a coherent subalgebra of all coherent algebras containing $\mathbf{A}$). We called it the *coherent algebra generated by* $\mathbf{A}$ and denote it by $[\mathbf{A}]$.

Given $\mathbf{A}$, the coherent algebra $[\mathbf{A}]$ can be computed using the so-called *Weisfeiler-Leman* algorithm (see [79]). There are also several other algorithms known for doing this task (for a discussion of this topic see [3], [2]). Today the most efficient one is an algorithm of Bastert, see [5][1].

5.6 Of particular interest are homogeneous coherent algebras, which are generated by very regular graphs such as vertex transitive graphs (which have a group of automorphisms that acts transitively on the vertex set), like Cayley graphs or the distance regular graphs discussed in **3.9**.

Example: To have an example consider once more the permutohedron, $G(\mathsf{S}_4, \mathcal{K})$, introduced at the end of **3.9**. We give here only some hints how to find the coherent algebra generated by the adjacency matrix of this graph.

We observe two types of edges: type a forms the sides of quadrangles, while type b forms the remaining sides of the hexagons which connect the six quadrangles, hence for instance the vertices 3 and 4 cannot belong to the same orbit of $\mathsf{Aut}[G(\mathsf{S}_4, \mathcal{K})]_0$. The adjacency matrix of the permutohedron graph is the sum of the characteristic matrices of these two orbits $\mathbf{A} = \mathbf{B}^{(1a)} + \mathbf{B}^{(1b)}$. In order to simplify the notation we set $\boldsymbol{\alpha} = \mathbf{B}^{(1a)}$ and $\boldsymbol{\beta} = \mathbf{B}^{(1b)}$. By direct computation one verifies

$$\boldsymbol{\beta}^2 = E \qquad \boldsymbol{\alpha}^3 = 4\boldsymbol{\alpha} \qquad (\boldsymbol{\alpha}\boldsymbol{\beta})^2 = \frac{1}{2}\boldsymbol{\alpha}^2\boldsymbol{\beta}\boldsymbol{\alpha} \qquad (\boldsymbol{\beta}\boldsymbol{\alpha})^2 = \frac{1}{2}\boldsymbol{\alpha}\boldsymbol{\beta}\boldsymbol{\alpha}^2$$

[1]Freely available at `http://******`

¿From here it is a tedious by straightforward computation to obtain the standard basis of $[\mathbf{A}]$ in the following form:

$$
\begin{array}{lcllcl}
\mathbf{A}^{(0)} & = & \mathbf{I} & & & \\
\mathbf{A}^{(1a)} & = & \boldsymbol{\alpha} & \mathbf{A}^{(1b)} & = & \boldsymbol{\beta} \\
\mathbf{A}^{(2a)-} & = & \boldsymbol{\alpha}\,\boldsymbol{\beta} & \mathbf{A}^{(2a)+} & = & \boldsymbol{\beta}\,\boldsymbol{\alpha} \\
\mathbf{A}^{(2b)} & = & \frac{1}{2}\boldsymbol{\alpha}^2 - \mathbf{I} & & & \\
\mathbf{A}^{(3a)-} & = & \frac{1}{2}\boldsymbol{\alpha}^2\boldsymbol{\beta} - \boldsymbol{\beta} & \mathbf{A}^{(3a)+} & = & \frac{1}{2}\boldsymbol{\beta}\boldsymbol{\alpha}^2 - \boldsymbol{\beta} \\
\mathbf{A}^{(3b)} & = & \boldsymbol{\beta}\boldsymbol{\alpha}\boldsymbol{\beta} & \mathbf{A}^{(3c)} & = & \boldsymbol{\alpha}\boldsymbol{\beta}\boldsymbol{\alpha} - \boldsymbol{\beta}\boldsymbol{\alpha}\boldsymbol{\beta} \\
\mathbf{A}^{(4a)-} & = & (\boldsymbol{\alpha}\boldsymbol{\beta})^2 - \boldsymbol{\beta}\boldsymbol{\alpha} & \mathbf{A}^{(4a)+} & = & (\boldsymbol{\beta}\boldsymbol{\alpha})^2 - \boldsymbol{\alpha}\boldsymbol{\beta} \\
\mathbf{A}^{(4b)} & = & \frac{1}{2}\boldsymbol{\beta}\boldsymbol{\alpha}^2\boldsymbol{\beta} - \mathbf{I} & & & \\
\mathbf{A}^{(5a)} & = & \frac{1}{4}\boldsymbol{\alpha}^2\boldsymbol{\beta}\boldsymbol{\alpha}^2 - \frac{1}{2}(\boldsymbol{\alpha}^2\boldsymbol{\beta} + \boldsymbol{\beta}\boldsymbol{\alpha}^2) + \boldsymbol{\beta} & \mathbf{A}^{(5b)} & = & \boldsymbol{\beta}\boldsymbol{\alpha}\boldsymbol{\beta}\boldsymbol{\alpha}\boldsymbol{\beta} - \boldsymbol{\alpha} \\
\mathbf{A}^{(6)} & = & \frac{1}{2}(\boldsymbol{\beta}\boldsymbol{\alpha})^3 - \frac{1}{2}\boldsymbol{\beta}\boldsymbol{\alpha}^2\boldsymbol{\beta} - \frac{1}{2}\boldsymbol{\alpha}^2 + \mathbf{I} & & &
\end{array}
$$

The matrices $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$, or more precisely their spectra and eigenvectors, contain the complete information about $[\mathbf{A}]$.

5.7 If $[\mathbf{A}]$ is homogeneous, then none of the classes $X_j(v)$ in Proposition 8 is empty. The structure matrix $\mathbf{R}_v$ can be obtained in this case as

$$(\mathbf{R}_v)_{ij} = \sum_{k:E_k \subseteq E} p_{ij}^k$$

where $E_k \subseteq E$ means that the pairs in E_k are edges of the graph, see [70] (Lemma 10). Clearly this is independent of v, i.e., the underlying graph is highly regular in the sense of Bollobás (see **3.3**), and anyone of the equitable partitions in proposition 8 contains the full spectral information on $\mathbf{A}$.

A homogenous coherent algebra is also called an *association scheme.* A *commutative algebra* is one with the property that $\mathbf{A}\mathbf{A}' = \mathbf{A}'\mathbf{A}$ for an two of its matrices $\mathbf{A}$ and $\mathbf{A}'$. Commutative coherent algebras are homogenous, and are therefore commutative association schemes. A coherent algebra which contains symmetric matrices only is necessarily commutative (and, hence, homogenous). Such an algebra is called a *symmetric association scheme.* A standard monography on association schemes is [4].

Symmetric association schemes $\mathcal{A}$ have the property that there exists an orthogonal matrix $\mathbf{X}$ such that $\mathbf{X}^{-1}\mathbf{A}\mathbf{X}$ is a diagonal matrix for every matrix $\mathbf{A} \in \mathcal{A}$ (i.e. the matrices in $\mathcal{A}$ are simultaneously diagonalizable). It follows that the set of columns

$\mathbf{x}^1, \dots \mathbf{x}^n$ of $\mathbf{X}$ is a set of n orthonormal eigenvectors for every matrix $\mathbf{A} \in \mathcal{A}$. Moreover, each eigenvector of a matrix $\mathbf{A} \in \mathcal{A}$ is also an eigenvector of all other matrices in $\mathcal{A}$.

If $[\mathbf{A}]$ is symmetric for some matrix $\mathbf{A}$, then this matrix must be regular, i.e. $\mathbf{Ae} = D\mathbf{e}$ for some constant D, for otherwise the globally coarsest equitable partition with respect to $\mathbf{A}$ would not be the trivial partition. However, the cell partition of $[\mathbf{A}]$ is trivial. Assume $\mathbf{B} \in [\mathbf{A}]$. This implies $[\mathbf{B}] \subseteq [\mathbf{A}]$. Hence, $[\mathbf{B}]$ is symmetric, and therefore, also $\mathbf{B}$ is regular. Thus, a symmetric association scheme $[\mathbf{A}]$ consists of regular matrices only.

Assume now that G is a graph with adjacency matrix $\mathbf{A}$ such that $[\mathbf{A}]$ is a symmetric association scheme. For each matrix $\mathbf{B} \in [\mathbf{A}]$ define an associated graph $G(\mathbf{B})$ by

$$G(\mathbf{B}) = (V, E(\mathbf{B})\,), \text{ where } E(\mathbf{B}) = \{uv \,:\, B_{uv} \neq 0\}.$$

Clearly, $G(\mathbf{A}) = G$.

For each $\mathbf{B} \in [\mathbf{A}]$ let $\mathbf{Be} = D_B\mathbf{e}$. Then $D_B^{-1}\mathbf{B}$ is doubly stochastic and defines a (non-standard) random walk on $G(\mathbf{B})$ with correlation function $r_{\mathbf{B},f}$ which we define by

$$r_{\mathbf{B},f}(k) = \frac{1}{|V|D_B^k}\mathbf{f}^T\mathbf{B}^k\mathbf{f},\ k \geq 1.$$

In this way, starting with the landscape (G, f) we get a rich system of landscapes

$$(G_{\mathbf{T}}, f), \mathbf{T} \in \mathcal{X}([\mathbf{A}])$$

with the same cost function f. Here $\mathcal{X}([\mathbf{A}])$ is the set of all doubly stochastic matrices in $[\mathbf{A}]$. Using this notation we implicitely include the type of random walk that we want to consider as a part of the definition of a landscape. Each $(G_{\mathbf{T}}, f)$ is a structural model of the set of data $F = \{f(1), \dots, f(n)\}$. We may use the properties of this model in order to describe "the structure" of F. In particular, we may use the autocorrelation functions $r_{\mathbf{T},f}$ for this description.

5.8 It has been proposed in the literature (see [70]) to call a landscape f *elementary*, if f is an eigenvector of the Laplacian of the configuration graph G. A surprising number of well known examples, including spin glasses and many combinatorial optimization problems such as the TSP, graph bipartitioning and graph matching, and certain satisfyability problems are of this type, see [12, 30, 70, 25].

We propose here in accordance with [67] to call a landscape $(G_{\mathbf{T}}, f)$ *elementary w.r.t. the transition operator* $\mathbf{T}$, if f is an eigenvector of the random walk transition matrix $\mathbf{T}$ with eigenvalue $\lambda \neq 1$ (the case $\lambda = 1$ appears when f is a flat landscape.)

The above considerations lead us to the following statement.

Proposition 10. *Let* $\mathbf{A}$ *be the adjacency matrix of a* D*-regular graph such that* $[\mathbf{A}]$ *is symmetric. If* $(G_{D^{-1}\mathbf{A}}, f)$ *is elementary (w.r.t.* $D^{-1}\mathbf{A}$*), then every landscape* $(G_{\mathbf{T}}, f)$ *is elementary (w.r.t.* $\mathbf{T}$*), where* $\mathbf{T}$ *is any matrix in* $\mathcal{X}([\mathbf{A}])$*. In the positive case, each random walk autocorrelation function* $r_{\mathbf{T},f}$*,* $\mathbf{T} \in \mathcal{X}([\mathbf{A}])$*, is exponential.*

Proof. The proof is by application of Proposition 9(b) and the observation that if f is an eigenvector of $\mathbf{A}$, then it is an eigenvector for every $\mathbf{T} \in \mathcal{X}([\mathbf{A}])$. $\diamond$

5.9 Numerous practically important landscapes are such that the adjacency matrix of the configuration graph generates a symmetric association scheme. This is true in particular for all landscapes on distance-regular graphs (see **3.9**).

Let G be a distant-regular graph with adjacency matrix $\mathbf{A}$ and define $E_i = \{uv : d(u,v) = i\}$, $1 \leq i \leq \Delta$. Let $\mathbf{A}_i$ be the adjacency matrix of E_i. Then $\{\mathbf{A}_1, \ldots, \mathbf{A}_\Delta\}$ is the standard basis of $[\mathbf{A}]$ (see [4] or [9], for example). Thus, a distance-regular graph generates a symmetric association scheme.

The association schemes generated by Hamming graphs $H(\nu, \alpha)$ are called *Hamming schemes*. As discussed in the introduction, Hamming graphs are of particular interest as configuration graphs. In our opinion, Proposition 10 opens a new approach for further studies of landscapes on Hamming graphs and other graphs which generate a symmetric association scheme. Proposition 10 can be easily extended to the case of commutative but not necessarily symmetric association schemes. However, for this extension it is necessary to consider coherent algebras over the field of complex numbers.

6 Concluding remarks

6.1 The ruggedness of a landscape on a given configuration graph, as expressed by correlation measures, is conveniently represented in terms of spectral properties of the underlying configuration graph. In the most important cases these graphs are very regular. The Hamming graphs which are distance regular and the Cayley graph of the symmetric group, both considered in subsection **3.9**, may serve as examples.

In this contribution we have explored to what extent these regularities can be used to simplify the task of computing the spectrum of a configuration graph. We have seen that two related concepts, namely equitable partitions and coherent algebras play a key role in this context. Since, these concepts maybe very useful also in different contexts of chemical, physical or biological problems, we have introduced and discussed them on a rather broad level.

6.2 Generalizing the discussion in **2.5** and **5.7** we may express the correlation function of a landscape $(G_{D^{-1}\mathbf{A}}, f)$ on a D-regular graph G in the form

$$r_f(k) = \sum_{p>0} B_p(\lambda_p/D)^k$$

where λ_p denotes the distinct eigenvalues of G, $\lambda_0 = D$, and $\{B_p\}$ is the so-called *amplitude spectrum* of the landscape [37]. The interpretation of the amplitude spectrum is, in many cases, straight forward and sometimes highlights the physics that underlies the fitness function, as in the case of RNA folding landscapes.

6.3 The spectral properties of Cayley graphs are determined by their irreducible representations. For some cases, including the Hamming graphs and Cayley graphs of the symmetric group it is possible to determine the amplitude spectra by means of Fast Fourier Transform techniques for the underlying group [46, 48, 59].

6.4 Model landscapes in physics and computer science oftentimes include a random element in the sense that a set of parameters is chosen at random, usually i.i.d., from a given distribution. In this setting it makes sense to investigate the covariance matrix of "random landscapes"

$$\mathbf{C} = \mathbb{E}[f(x)f(y)] - \mathbb{E}[f(x)]\mathbb{E}[f(y)]$$

where $\mathbb{E}[\,.\,]$ denotes the expectated value w.r.t. the distribution of random parameters. The structure of $\mathbf{C}$, and its relation to a maximum entropy condition and to the eigenvectors of the underlying graph, is discussed in [25, 71]. The relationships of the coherent algebras [$\mathbf{A}$] and [C] might well encapsulated important, as yet unexplored information about such model landscapes.

6.5 So far, almost exclusively landscapes on graphs have been considered. More complex search operators, most notably recombination or cross-over operators, however do not lead to graphs. The spectral approach to analyzing the landscape structure can be extented to this class of operators by considering Markov chains [75, 67] or based on certain hypergraphs [72]. In the case of string recombination one obtains association schemes that are at least closely related to Hamming schemes. More difficult types of recombination, such as "tour recombination" in the TSP or recombination of trees so far have not been considered from the algebraic point of view.

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