OPTIMISATION OF QUADRATIC FORMS ASSOCIATED WITH GRAPHS

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1. Introduction. Quadratic forms associated with graphs were introduced over a century ago by Jordan [4]. We are concerned with the optimisation of such quadratic forms, following Motzkin and Straus [5], and we use the setting of categories and functors to express the nice interplay between the algebra and the graph theory. Applications to interchange graphs are also obtained.

G denotes a simple graph with vertex set $V(G) = \{v_1, \ldots, v_n\}$, edge set $E(G)$ and complement $\bar{G}$. As usual, K_n denotes the complete n-graph and $K_{r_1,\ldots,r_k}$ a complete k-partite graph.

With G is associated a real quadratic form

$$F_G(x_1, \ldots, x_n) = (1/2)\mathbf{x}^t\mathbf{G}\mathbf{x}, \qquad \mathbf{x} = (x_1, \ldots, x_n) \in \mathbb{R}^n,$$

where $\mathbf{G}$ denotes the adjacency matrix of the graph G. Thus the coefficient of $x_i x_j$ in the quadratic form is 1 if the vertices v_i and v_j are adjacent, denoted $v_i \sim v_j$ (i.e. joined by an edge $[v_i, v_j] \in E(G)$), and 0 if not. We put in the coefficient 1/2 rather than use each edge twice.

The *standard simplex* $\sigma = \sigma^{n-1} \subset \mathbb{R}^n$ given by $\{(x_1, \ldots, x_n) \in \mathbb{R}^n : x_i \geqq 0, \sum_{i=1}^{n} x_i = 1\}$ has vertices indexed by those of the graph $G : (0, \ldots, 0, x_r = 1, 0, \ldots, 0) \leftrightarrow v_r$. Let $f(G) = \max_{\mathbf{x} \in \sigma} F_G(\mathbf{x})$. The *clique number* $\omega(G)$ of G is the order k of the largest complete subgraph $K_k \subset G$. We denote by $D(G)$ the subgraph $\bigcup_{j \in J} K_k^j$ of G, i.e. the union of all such maximal cliques of (fixed) order $k = \omega(G)$.

Evaluation of $f(G)$ was obtained by Motzkin and Straus [5]. Their Theorems 1 and 2 can be summarised as follows.

THEOREM 1.1.

(i) $f(G) = \dfrac{\omega(G)-1}{2\omega(G)}$,

(ii) $f(G)$ *is attained at an interior point of* σ *if and only if* G *is a complete multipartite graph.*

It follows that complete graphs are characterised by f.

COROLLARY 1.2. *If* G *has* n *vertices, then*

$$f(G) = \frac{n-1}{2n} \Leftrightarrow G = K_n.$$

We shall denote by $\mu(G)$ the region of the simplex where the maximum is attained, i.e.

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$\mu(G) = \{\mathbf{x} \in \sigma : F_G(\mathbf{x}) = f(G)\}$. Our main object is to investigate the structure of such regions, and their relationships to the graphs with which they are associated.

2. The optimising cell-complex. The case $\omega(G) = 1$ is disposed of separately.

PROPOSITION 2.1. $\omega(G) = 1 \Leftrightarrow E(G) = \varnothing \Leftrightarrow G = \bar{K}_n \Leftrightarrow f(G) = 0$ *and* $\mu(G) = \sigma^{n-1}$.

Henceforth in this section suppose $E(G) \neq \varnothing$ for all graphs.

We label the vertices of σ according to the indexing above, and let $i_1, i_2, \ldots, i_r$ denote the barycentre of the face of σ spanned by the vertices labelled $i_1, i_2, \ldots, i_r$. As preparation for the study of $\mu(G)$, we observe that it follows from Theorems 1.1 and 1.2 that only k-cliques of G of order $k = \omega(G)$ can contribute to $f(G)$; thus if $D(G)$ is isomorphic to $D(H)$, then $f(G) = f(H)$, and so $\mu(G) = \mu(H)$.

To be more precise, and to see in what way the k-cliques contribute to $\mu(G)$, we obtain a few lemmas showing the special role played by complete k-partite graphs. Firstly, in the case $k = 2$, we obtain a characterisation.

LEMMA 2.2. *F_G factorises (as distinct real linear factors) if and only if G is complete bipartite.*

Proof. The *rank* (resp. *index*) of a quadratic form is the number of non-zero (resp. negative) elements in an equivalent diagonal form. A real quadratic form factorises as distinct real linear factors if and only if it has rank 2 and index 1, equivalently if and only if the corresponding matrix has one positive and one negative eigenvalue.

The sum of the eigenvalues of a simple graph G is equal to the trace of $\mathbf{G}$, which is zero. Thus F_G factorises if and only if $\mathbf{G}$ has eigenvalues $\{\pm\lambda, 0[n-2 \text{ times}]\}$. It is well known (see for example [**6**, §5]) that this is true if and only if G is a complete bipartite graph.

It is now easy to show for a complete bipartite graph $G = K_{r,n-r}$ that the maximising region is the mutual intersection of σ^{n-1} and two hyperplanes.

LEMMA 2.3.

$$\mu(K_{r,n-r}) = \{(x_1, \ldots, x_n) \in \sigma^{n-1} : \sum_{i=1}^{r} x_i = 1/2, \sum_{i=r+1}^{n} x_i = 1/2\}.$$

Proof. Taking the vertex-sets of the two " parts " to be $\{v_1, \ldots, v_r\}$, $\{v_{r+1}, \ldots, v_n\}$, F_G factorises as $(x_1 + \ldots + x_r)(x_{r+1} + \ldots + x_n)$. Maximising this product subject to $x_i \geqq 0$, $\sum x_i = 1$ is clearly obtained by $\sum_{i=1}^{r} x_i = 1/2 = \sum_{i=r+1}^{n} x_i$, (giving $f(G) = 1/4$ in Theorem 1.1).

EXAMPLES. This result provides some simple examples of $\mu(G)$. Let P_n (resp $\mathscr{C}_n$) denote the *path-graph* (resp. *circuit*) with n vertices (labelled in order). Then

(i) $\mu(P_3)$ is a 1-simplex, whose end-points are the barycentres 1.2 and 2.3 of the standard 2-simplex with vertices 1, 2 and 3;

(ii) $\mu(\mathscr{C}_4)$ is a solid square;

(iii) the star-graph $K_{1,n}$ has $\mu(K_{1,n})$ as a (solid) $(n-1)$-simplex.

Lemma 2.3 generalises to complete k-partite graphs as follows.

LEMMA 2.4. *$\mu(K_{r_1,\dots,r_k})$ is the mutual intersection of σ and a collection of k hyperplanes $s_q = 1/k$, $q = 1, \dots, k$, where s_q is the sum $\sum x_i$ corresponding to the vertices in the qth "part" of $K_{r_1,\dots,r_q,\dots,r_k}$.*

Proof. We have $\omega(K_{r_1,\dots,r_k}) = k$. An obvious grouping of terms gives $F_G(\mathbf{x}) = \sum_{p \neq q} s_p s_q$. This expression is the quadratic form of the complete graph K_k, and so Corollary 1.2 gives the maximum $f(G) = (k-1)/(2k)$, which is attained when $s_q = 1/k$ (which ensures that $\sum_i x_i = 1$), $q = 1, \dots, k$, and the result follows.

REMARK 2.5. The set $\mu(K_{r_1,\dots,r_k})$ has the structure of a polyhedron whose vertices correspond to the k-cliques K_k^j of $K_{r_1,\dots,r_k}$. It is clear from Lemma 2.4 that the polyhedron is the underlying space of a product of simplexes: $\prod_{q=1}^{k} \sigma^{r_q-1}$.

The next theorem shows that for an arbitrary graph G, the set $\mu(G)$ is a polyhedron with a natural facial structure as a product of simplicial complexes. We shall refer to the polyhedra with this facial structure as *cell-complexes*, defined as follows:

A *cell c* is a finite product of (closed euclidean) simplexes. The cell c_2 is a face of the cell c_1, denoted $c_2 < c_1$, if $c_1 = \prod_{i=1}^{n} \sigma^{r_i}$, $c_2 = \prod_{i=1}^{n} \tau^{s_i}$ with τ^{s_i} a (simplex-) face of σ^{r_i} for each i.
A *cell-complex K* is a set of cells such that

(i) $c_1 \in K$, $c_2 < c_1 \Rightarrow c_2 \in K$,
(ii) for all c_1, $c_2 \in K$, $c_1 \cap c_2$ is a well-defined cell $\prod_i \sigma^{k_i}$, which is a face of both c_1 and c_2.

THEOREM 2.6. *If $\omega(G) = k$ (>1), with $D(G) = \bigcup_{j \in J} K_k^j$, then $\mu(G) \subset \sigma^{n-1}$ has the structure of a cell-complex defined as follows:*

(i) *v is a vertex of the cell-complex if and only if v is the barycentre $i_1 \dots i_k$ of the face of σ whose vertices correspond to the vertices of some k-clique $K_k^j \subset D(G)$;*

(ii) *the vertices $\{v^j\}_{j \in J'}$ span a cell $\prod_{i=1}^{k} \sigma^{r_i-1}$ if and only if the corresponding subgraph $\bigcup_{j \in J'} K_k^j$ is a complete k-partite subgraph $K_{r_1,\dots,r_k}$ in G.*

Proof. (i) For each complete subgraph $K_k^j \subset G$, the required maximum $(k-1)/(2k)$ (as in Theorem 1.1) is attained at the vector $\mathbf{x}^j$ with coordinates

$$x_i^j = \begin{cases} 1/k, & \text{if } v_i \text{ is one of the } (k) \text{ vertices of } K_k^j \\ 0, & \text{otherwise.} \end{cases}$$

Such $\mathbf{x}^j$ is one of the required barycentres, and (i) follows.

(ii) Since (by Corollary 1.2) only k-cliques of G can contribute to the required maximum $F(G) = (k-1)/(2k)$, we can confine attention to $D(G) = \bigcup_{j \in J} K_k^j$.

For each "subunion" $\bigcup_{j \in J'} K_k^j$ which constitutes a complete k-partite graph, we can apply Lemma 2.4 and obtain a contribution to $\mu(G)$ of a cell $\prod_{q=1}^{k} \sigma^{r_q - 1}$. It follows from Theorem 1.1 that the maximum $f(G)$ can be attained in no other way.

The required incidence conditions of these cells follows from the respective incidences of the corresponding complete k-partite subgraphs of G, and the result follows.

EXAMPLES. $\mu(K_n) = \sigma^0$; $\mu(P_n) = P_{n-1}$; $\mu(\mathscr{C}_n) = \mathscr{C}_n$, $n > 4$.
If G is a Möbius ladder graph [**2**] with at least 8 vertices, then $\mu(G)$ is a Möbius band. If G is a prism $K_2 \times \mathscr{C}_n$, $n > 4$, then $\mu(G)$ is a cylinder.

We can characterise graphs G with $\mu(G)$ contractible as follows.

PROPOSITION 2.7. *If $\omega(G) = k$, then $\mu(G)$ is contractible if and only if G contains no sequence $K_k^1, \ldots, K_k^r$, $r \geqq 5$ of k-cliques with*

$$K_k^s \cap K_k^t = K_{k-1} \Leftrightarrow |s-t| = 1 \bmod r.$$

Proof. If G does contain r such maximal cliques then we obtain r corresponding vertices $v_1, \ldots, v_r$ in $\mu(G)$. Each adjacent pair of these maximal cliques constitutes a complete k-partite graph $K_{2,1,\ldots,1}$, and so, by Theorem 2.6, the corresponding pair of vertices in $\mu(G)$ span a 1-simplex. Thus $\{v_1, \ldots, v_r\}$ is the vertex-set of an r-circuit ($r \geqq 5$), which cannot be contracted in the polyhedron.

Conversely if $\mu(G)$ contains such an r-circuit, then it must have been derived from a " cyclic sequence " of r maximal cliques.

COROLLARY 2.8. *If the graph G is a tree, then the polyhedron $\mu(G)$ is contractible.*

Thus the construction $\mu(G)$ mirrors some of the geometry of the graph G. This can be made more precise as follows.

3. The functor μ. The cell-complexes defined above form a category $\mathfrak{C}$ in which a morphism is a map $\alpha : K \to L$ whose restriction to each cell is a product of simplicial maps:

$$\left(\alpha \middle| \prod_{i=1}^{n} \sigma^{r_i}\right)\left(\prod_{i=1}^{n} \sigma^{r_i}\right) = \prod_{i=1}^{n} \sigma^{s_i}.$$

Thus $\mathfrak{C}$ is a " combinatorial category " in that it is of primary importance which vertices span simplexes; however a morphism does determine a continuous map of the underlying polyhedra, simply by extending linearly.

The m-ary operation of *join* $*$ of graphs (see for example Harary [**3**, p. 21]) is very useful in studying the maximisation of the quadratic form F_G, since this operation $*$ is compatible with all of the above mappings ω, D and μ.

PROPOSITION 3.1. *For any graphs G_i,*

(i) $\omega\left(\mathop{*}_{i=1}^{m} G_i\right) = \sum_{i=1}^{m} \omega(G_i)$,

(ii) $D\left(\mathop{*}_{i=1}^{m} G_i\right) = \mathop{*}_{i=1}^{m} D(G_i)$,

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(iii) *if $p(G)$ denotes the set of complete $\omega(G)$-partite subgraphs in G, then*

$$p\left(\mathop{*}_{i=1}^{m} G_i\right) = \left\{\mathop{*}_{i=1}^{m} q_i : q_i \in p(G_i)\right\},$$

(iv) $\mu\left(\mathop{*}_{i=1}^{m} G_i\right) = \prod_{i=1}^{m} (\mu(G_i))$.

Proof. $K_r * K_s = K_{r+s}$. Clearly the join of a set of graphs is a clique if and only if each of those graphs is a clique. Furthermore, the joins of the maximal cliques of graphs $G_1, \ldots, G_m$ are precisely the maximal cliques of the join $\mathop{*}_{i=1}^{m} G_i$. The proposition follows easily.

Corollary 3.2.

$$\mu(K_{r_1, \ldots, r_k}) = \prod_{i=1}^{k} (\sigma^{r_i - 1}).$$

For example μ of the octahedron $K_{2,2,2}$ is a cube.

Corollary 3.3. *$\mu(G * K_r) = \mu(G)$ for any graph G and for any complete graph K_r.*

We may now express the functorial property of this construction μ. By a *morphism* $g : G \to H$ of graphs is meant a map $g : V(G) \to V(H)$ which preserves adjacency, i.e. if $[v_i, v_j] \in E(G)$, then $[g(v_i), g(v_j)] \in E(H)$. Thus an edge cannot be collapsed to a vertex.

The following lemma is obvious but very useful.

Lemma 3.4. *Let $g : G \to H$ be a morphism of graphs. Then*

(i) *if K_k is any k-clique in G, then $g(K_k)$ is a k-clique in H;*
(ii) *if $K_{r_1, \ldots, r_k}$ is any complete k-partite subgraph of G, then its image under g is a complete k-partite subgraph $K_{s_1, \ldots, s_k}$ of H.*

Applying the lemma to the case $k = \omega(G)$, it becomes natural to consider the category $\mathcal{G}raph_k$ of (finite) graphs with clique number $\omega(G) = k$, and their morphisms.

Theorem 3.5. *For each natural number k, μ gives a covariant functor $\mu : \mathcal{G}raph_k \to \mathfrak{C}$.*

Proof. Again the $k = 1$ case is trivial. For $k > 1$, we assign the cell-complex $\mu(G)$ to G, as in Theorem 2.6. If $g : G \to H$ is a morphism of the category $\mathcal{G}raph_k$, then by Lemma 3.4(i), we obtain a well-defined induced map $\mu(g)$ from the vertices of $\mu(G)$ to those of $\mu(H)$. Furthermore, Lemma 3.4(ii) ensures that $\mu(g)$ sends cells to cells in the appropriate way.

To verify that μ is a functor, we observe that if 1_G denotes the identity morphism on the graph G, then $\mu(1_G)$ is equal to the identity morphism on $\mu(G)$ in $\mathfrak{C}$, and finally that if also $h : H \to J$ in $\mathcal{G}raph_k$, then $\mu(h \, . \, g) = \mu(h) \, . \, \mu(g) : \mu(G) \to \mu(J)$ in $\mathfrak{C}$.

Corollary 3.6. *If g is an automorphism of the graph G, then $\mu(g)$ is an automorphism of the cell-complex $\mu(G)$.*

Proof. Let $g' : G \to G$ be the inverse morphism of g. By Theorem 3.5 we have $\mu(g').\mu(g) = \mu(g'.g) = \mu(1_G) = 1_{\mu(G)}$. It follows that $\mu(g')$ is the inverse of $\mu(g)$ in $\mathfrak{C}$.

4. Minimisation of the quadratic form of a graph. We mention, for completeness, the minimising of our quadratic form $\mathbf{x'Gx}$ on the simplex σ. In analogy to the above, we define

$$\bar{f}(G) = \min_{\mathbf{x}\in\sigma} F_G(\mathbf{x}) \quad \text{and} \quad \bar{\mu}(G) = \{\mathbf{x}\in\sigma : F_G(\mathbf{x}) = \bar{f}(G)\}.$$

This time the results are simple.

PROPOSITION 4.1.

(i) *For any graph* $G, \bar{f}(G) = 0$.

(ii) $\bar{\mu}(G)$ *consists of those faces of* σ *whose vertices correspond to an edgeless subgraph* $\bar{K}_m$ *of* G.

(iii) $\bar{\mu}(G)$ *is a simplicial complex, whose* 1*-skeleton is a graph isomorphic to the complement graph* $\bar{G}$.

Proof. (i) $F_G(\mathbf{x}) = 0$ for every vertex $\mathbf{x}\in\sigma$, since all coordinates x_i except one are zero;
(ii) $F_G(\mathbf{x}) = 0$ if and only if every term $x_i x_j$ is zero. This corresponds to points $\mathbf{x}$ of any simplex-face whose vertices correspond to those of an edgeless subgraph of G;
(iii) follows immediately.

COROLLARY 4.2. *The automorphism group of* G *is isomorphic to the* (*simplicial*) *automorphism group of* $\bar{\mu}(G)$.

Proof. We have an isomorphism $\operatorname{Aut}\bar{G} \cong \operatorname{Aut} G$, since a permutation of $V(G)$ preserves non-adjacency of vertices if and only if it preserves adjacency of vertices. The result follows.

5. Interchange Graphs. The mth *interchange graph* $I_m(G)$ of the graph G is the graph whose vertices are indexed by the $(m+1)$-cliques of G, two vertices being adjacent if the corresponding $(m+1)$-cliques intersect in an m-clique.

In a recent paper **[1]**, C. R. Cook considers the $(m-1)$th interchange graph of the regular complete m-partite graph $K_{n,\dots,n}$ and obtains characterisations of graphs of this form.

More generally, it is natural to consider the " maximal " interchange graph of any graph G, i.e. $\tilde{I}(G) = I_{\omega(G)-1}(G)$. For any graph G, we can easily relate its associated graph $\tilde{I}(G)$ to the cell-complex $\mu(G)$.

THEOREM 5.1. *For any graph* G, *the* 1*-dimensional skeleton of* $\mu(G)$ *is a graph isomorphic to* $\tilde{I}(G)$.

Proof. The vertices of $\mu(G)$ (and hence of its 1-skeleton), correspond to k-cliques in G, $k = \omega(G)$, and hence to vertices of $\tilde{I}(G)$. From Theorem 2.6(ii), two vertices of $\mu(G)$ are adjacent if and only if the corresponding subgraph $K_k^1 \cup K_k^2$ of G is complete k-partite, i.e. equal to $K_{2,1,\dots,1}$. But this is precisely the condition that $K_k^1 \cup K_k^2 \cong K_{k-1}$, which is necessary and sufficient for adjacency of the two vertices in $\tilde{I}(G)$.

COROLLARY 5.2. *If G has edges but no triangles (i.e. $\omega(G) = 2$), then the line graph of G is the 1-skeleton of $\mu(G)$.*

Some structural properties of $\tilde{I}(G)$ now follow immediately. In particular, Proposition 3.1(iv) above implies that $\tilde{I}$ transforms joins of graphs to (cartesian) products of graphs. Recall that this *product* $G_1 \times G_2$ has vertex-set $V(G_1) \times V(G_2)$, with adjacency ($\sim$) given by $(v_1, v_2) \sim (v_1', v_2')$ whenever $[v_1 = v_1'$ and $v_2 \sim v_2']$ or $[v_1 \sim v_1'$ and $v_2 = v_2']$.

PROPOSITION 5.3.

$$\tilde{I}\left(\mathop{*}_{i=1}^{m} G_i\right) = \mathop{\times}_{i=1}^{m} \tilde{I}(G_i).$$

Proof. Proposition 3.1(iv) gives the result because the product graph is the 1-skeleton of the corresponding product-complex.

Note that this result is valid for case $\omega(G_i) = 1$, which is of importance as it gives:

COROLLARY 5.4.

$$\tilde{I}(K_{r_1, \ldots, r_k}) = \mathop{\times}_{i=1}^{k} K_{r_i}.$$

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