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

$$F_G(x_1, \ldots, x_n) = \frac{1}{2}x^tGx, \quad x = (x_1, \ldots, x_n) \in \mathbb{R}^n,$$

where $G$ 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 $\{(x_1, \ldots, x_n) \in \mathbb{R}^n : x_i \geq 0, \sum_{i=1}^n x_i = 1\}$ has vertices indexed by those of the graph $G$:

$$(0, \ldots, 0, x_r = 1, 0, \ldots, 0) \leftrightarrow v_r.$$

Let $f(G) = \max_{x \in \sigma} F_G(x)$. 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 $\bigcup_{K_k \subset G} K_k$ 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) $f(G) = \frac{\omega(G) - 1}{2\omega(G)}$.

(ii) $f(G)$ is attained at an interior point of $\sigma$ 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.
2. The optimising cell-complex. The case $\omega(G) = 1$ is disposed of separately.

**Proposition 2.1.** \( \omega(G) = 1 \Leftrightarrow E(G) = \emptyset \Leftrightarrow G = K_n \Leftrightarrow f(G) = 0 \) and \( \mu(G) = \sigma^{n-1} \).

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

We label the vertices of \( G \) according to the indexing above, and let \( i_1, i_2, \ldots, i_r \) denote the barycentre of the face of \( G \) 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 \( G \), which is zero. Thus \( F_G \) factorises if and only if \( G \) 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 \( \sigma^{n-1} \) 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 \( x_i \geq 0 \), \( \sum x_i = 1 \) 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 \( C_n \)) 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) \( \mu(C_4) \) 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. \( \mu(K_{r_1, \ldots, r_n}) \) is the mutual intersection of \( \sigma \) and a collection of \( k \) hyperplanes \( s_q = 1/k, \) for \( q = 1, \ldots, k, \) where \( s_q \) is the sum \( \sum x_i \) corresponding to the vertices in the \( q \)th "part" of \( K_{r_1, \ldots, r_n}. \)

Proof. We have \( \omega(K_{r_1, \ldots, r_n}) = k. \) An obvious grouping of terms gives \( F_G(x) = \sum_{p \neq q} s_p s_q. \) 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 \( \sum x_i = 1, \) \( q = 1, \ldots, k, \) and the result follows.

REMARK 2.5. The set \( \omega(K_{r_1, \ldots, r_n}) \) has the structure of a polyhedron whose vertices correspond to the \( k \)-cliques \( K_{r_i} \) of \( K_{r_1, \ldots, r_n}. \) It is clear from Lemma 2.4 that the polyhedron is the underlying space of a product of simplexes: \( \prod_{q=1}^{k} \sigma^{s_q-1}. \)

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 \( c_1 = \prod_{i=1}^n \sigma^{t_i}, \) \( c_2 = \prod_{i=1}^n \tau^{t_i} \) with \( \tau^{t_i} \) a (simplex-) face of \( \sigma^{t_i} \) 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 \( \prod_{i} \sigma^{s_i}, \) which is a face of both \( c_1 \) and \( c_2. \)

THEOREM 2.6. If \( \omega(G) = k \) \((>1), \) with \( D(G) = \bigcup_{j \in J} K_{r_i}^j, \) 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 \( i_1, \ldots, i_k \) of the face of \( \sigma \) whose vertices correspond to the vertices of some \( k \)-clique \( K_{r_i}^j \subset D(G); \)

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

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

\[
x^{j}_{i} = \begin{cases} 
1/k_i & \text{if } u_i \text{ is one of the } (k) \text{ vertices of } K_{r_i}^j \\
0, & \text{otherwise.}
\end{cases}
\]

Such \( x^j \) 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 \( D(G) = \bigcup_{j \in J} K_{r_i}^j. \)

For each "subunion" \( \bigcup_{j \in J} K_{r_i}^j \) which constitutes a complete \( k \)-partite graph, we can
apply Lemma 2.4 and obtain a contribution to $\mu(G)$ of a cell $\prod_{q=1}^{k} \sigma^{q-1}$. 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.** $\mu(K_n) = \sigma^0$; $\mu(P_n) = P_{n-1}$; $\mu(C_n) = C_n, n > 4$.

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 $K_2 \times C_m, n > 4$, 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 $K_k^1, \ldots, K_k^r$ of $k$-cliques with

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

**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 $K_2, \ldots, K_2$, 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 ($r \geq 5$), 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 $\mu$. The cell-complexes defined above form a category $\mathcal{C}$ in which a morphism is a map $\alpha : K \to L$ whose restriction to each cell is a product of simplicial maps:

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

Thus $\mathcal{C}$ 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 $\ast$ of graphs (see for example Harary [3, p. 21]) is very useful in studying the maximisation of the quadratic form $F^\omega$, since this operation $\ast$ is compatible with all of the above mappings $\omega, D$ and $\mu$.

**Proposition 3.1.** For any graphs $G_i$,

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

(ii) $D \left( \bigast_{i=1}^{m} G_i \right) = \bigast_{i=1}^{m} D(G_i)$.
(iii) if \( p(G) \) denotes the set of complete \( \omega(G) \)-partite subgraphs in \( G \), then
\[
 p \left( \bigstar_{i=1}^{m} G_i \right) = \left\{ \bigstar_{i=1}^{m} q_i : q_i \in p(G_i) \right\},
\]
(iv) \( \mu \left( \bigstar_{i=1}^{m} G_i \right) = \prod_{i=1}^{m} (\mu(G_i)) \).

Proof. \( K_r \star K_s = K_{r+s} \). 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 \( \bigstar_{i=1}^{m} G_i \). The proposition follows easily.

**Corollary 3.2.**
\[
\mu(K_{r_1}, \ldots, r_n) = \prod_{i=1}^{k} (\sigma^{r_i-1}).
\]

For example \( \mu \) of the octahedron \( K_{2,2,2} \) is a cube.

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

We may now express the functorial property of this construction \( \mu \). 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 \( K_{r_1}, \ldots, r_n \) is any complete \( k \)-partite subgraph of \( G \), then its image under \( g \) is a complete \( k \)-partite subgraph \( K_{r_1}, \ldots, r_n \) of \( H \).

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

**Theorem 3.5.** For each natural number \( k \), \( \mu \) gives a covariant functor \( \mu : \text{Graph}_k \to \mathcal{C} \).

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 \( \text{Graph}_k \), then by Lemma 3.4(ii), 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 \( \mu \) 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 \( \mathcal{C} \), and finally that if also \( h : H \to J \) in \( \text{Graph}_k \), then \( \mu(h \cdot g) = \mu(h) \cdot \mu(g) : \mu(G) \to \mu(J) \) in \( \mathcal{C} \).

**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 \( \mu(g') \cdot \mu(g) = \mu(g' \cdot g) = \mu(1_G) = 1_{\mu(G)} \). It follows that \( \mu(g') \) is the inverse of \( \mu(g) \) in \( \mathcal{C} \).

4. Minimisation of the quadratic form of a graph. We mention, for completeness, the minimising of our quadratic form \( x'Gx \) on the simplex \( \sigma \). In analogy to the above, we define
\[
\bar{f}(G) = \min_{x \in \sigma} F_G(x) \quad \text{and} \quad \bar{\mu}(G) = \{ x \in \sigma : F_G(x) = \bar{f}(G) \}.
\]
This time the results are simple.

**Proposition 4.1.**
1. For any graph \( G \), \( \bar{f}(G) = 0 \).
2. \( \bar{\mu}(G) \) consists of those faces of \( \sigma \) whose vertices correspond to an edgeless subgraph \( K_m \) of \( G \).
3. \( \bar{\mu}(G) \) is a simplicial complex, whose 1-skeleton is a graph isomorphic to the complement graph \( \bar{G} \).

**Proof.** (i) \( F_G(x) = 0 \) for every vertex \( x \in \sigma \), since all coordinates \( x_i \) except one are zero;
(ii) \( F_G(x) = 0 \) if and only if every term \( x_i x_j \) is zero. This corresponds to points \( x \) 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 \( \text{Aut} \, G \cong \text{Aut} \, G \), 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 \( m \)-th 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 complete \( m \)-partite graph \( K_{n_1,...,n_k} \) 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. \( \bar{I}(G) = I_{\omega(G)-1}(G) \). For any graph \( G \), we can easily relate its associated graph \( \bar{I}(G) \) to the cell-complex \( \bar{\mu}(G) \).

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

**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 \( \bar{I}(G) \). 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 \( K_{n_1,...,n_k} \). 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 \( \bar{I}(G) \).
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 $I(G)$ now follow immediately. In particular, Proposition 3.1(iv) above implies that $I$ 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 (~) 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.

$$I\left( \bigstar_{i=1}^{m} G_i \right) = \bigotimes_{i=1}^{m} I(G_i).$$

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.

$$I(K_{r_1}, \ldots, r_k) = \bigotimes_{i=1}^{k} K_{r_i}.$$

REFERENCES