MAXIMA FOR GRAPHS AND A NEW PROOF OF A THEOREM OF TURÁN

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1. Maximum of a square-free quadratic form on a simplex. The following question was suggested by a problem of J. E. MacDonald Jr. **(1)**:

Given a graph G with vertices $1, 2, \ldots, n$. Let S be the simplex in E^n given by $x_i \geqslant 0$, $\sum x_i = 1$. What is

$$\max_{x \in S} \sum_{(i,j) \in G} x_i x_j?$$

Here $(i, j) = (j, i)$ denotes an edge of G. We denote this maximum by $f(G)$. (The minimum is 0.) The above-mentioned problem is: Prove that $f(G) = \frac{1}{4}$ for

$$G = G_0 = \{(1, 2), (2, 3), \ldots, (n-1, n)\}, \qquad n \geqslant 2.$$

The general answer is as follows.

THEOREM 1. *Let k be the order of the maximal complete graph contained in G. Then*

$$f(G) = \frac{1}{2}\left(1 - \frac{1}{k}\right). \tag{1}$$

Proof. Let $1, \ldots, k$ be the vertices of a complete subgraph of G; then setting $x_1 = \ldots = x_k = 1/k$ and $x_{k+1} = \ldots = x_n = 0$, we get

$$f(G) \geqslant \binom{k}{2} \cdot \frac{1}{k^2} = \frac{1}{2}\left(1 - \frac{1}{k}\right). \tag{2}$$

To prove the opposite inequality we proceed by induction on n. For $n = 1$ we have $k = 1$ and $f(G) = 0$. Now assume the theorem true for graphs with fewer than n vertices. If $f(G) = F(x_1, \ldots, x_n)$ is attained on the boundary of S, then one of the x_i vanishes and $f(G) = f(G')$, where G' is obtained from G by deleting the corresponding vertex. Since the theorem holds for G' we have

$$f(G) = f(G') = \frac{1}{2}\left(1 - \frac{1}{k'}\right) \leqslant \frac{1}{2}\left(1 - \frac{1}{k}\right).$$

If $F(x)$ attains its maximum at an interior point of the simplex, we can say that $F(x)/s^2(x)$ (with $s(x) = x_1 + \ldots + x_n$) attains this maximum at an interior point of the positive orthant. In other words,

$$s^2 F_i = 2 s s_i F \qquad \text{or } F_i = 2F/s = 2F, \tag{3}$$

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for $i = 1, \ldots, n$, where the subscript denotes differentiation with respect to x_i. Now if G is not a complete graph, say $(1, 2) \notin G$, then

$$F(x_1 - c, x_2 + c, x_3, \ldots, x_n) = F(x) - c(F_1(x) - F_2(x)) = F(x)$$

for all c. In particular, for $c = x_1$,

$$F(0, x_1 + x_2, x_3, \ldots, x_n) = F(x),$$

so that the maximum is also attained for the subgraph G' obtained from G by deleting the vertex 1. Thus the contention of the theorem is again true by the induction hypothesis.

If G is a complete graph, then

$$F(x) = \tfrac{1}{2}[(x_1 + \ldots + x_n)^2 - x_1^2 - \ldots - x_n^2] = \tfrac{1}{2}(1 - ||x||^2)$$
$$\leqslant \frac{1}{2}\left(1 - \min_{|x_1|+\ldots+|x_n|=1} ||x||^2\right) = \frac{1}{2}\left(1 - \frac{1}{n}\right).$$

This completes the proof.

COROLLARY. *If l is the order of the maximal empty subgraph of G and*

$$g(G) = \min_S \left\{\frac{1}{2}(x_1^2 + \ldots + x_n^2) + \sum_{(i,j)\in G} x_i x_j\right\},$$

then $g(G) = 1/(2l)$.

Proof. If $\bar{G}$ is the complementary graph of G, then

$$f(\bar{G}) = \tfrac{1}{2} - g(\bar{G}) = \tfrac{1}{2}(1 - 1/l).$$

2. Homomorphic graphs.

Definition. A graph G_1 is *homomorphic* to a graph G if G_1 can be mapped onto G so that the edges of G are exactly the images of those of G_1. If, in addition, every pair mapped on an edge of G is an edge of G_1, then G_1 is *completely homomorphic* to G.

Let G_1 with vertices $1, \ldots, n$ be homomorphic to G with vertices $1^*, \ldots, m^*$. As before we define

$$F_1(x) = \sum_{(i,j)\in G_1} x_i x_j, \qquad F(y) = \sum_{(k^*, l^*)\in G} y_{i^*} y_{l^*}.$$

Then

$$F(\textstyle\sum_1 x_i, \ldots, \sum_m x_i) \geqslant F_1(x),$$

where $\sum_j$ is extended over all pre-images of j^*, and therefore $f(G) \geqslant f(G_1)$. Hence, we do not need induction to prove Theorem 1 for graphs homomorphic to a complete graph of order k (that is, k-colourable graphs) which contain a complete subgraph of order k. But even for such graphs there need not be a maximum of $F(x)$ in the interior of S. In fact, the following result obtains.

THEOREM 2. *The form $F(x)$ has a maximum in the interior of S if and only if G is completely homomorphic to a complete k-graph (that is, G is a maximal k-colourable graph).*

Proof. If G is completely homomorphic to the complete graph with vertices $1^*, \ldots, k^*$, then all x with $\sum_j x_i = 1/k$ ($x_i > 0$, $j = 1, \ldots, k$) give interior maxima. If, conversely, $F(x)$ has an interior maximum $F(x) = (1 - 1/k)/2$, then $n \geqslant k$. For $n = k$ the contention is trivial. Assume that $n > k$ and the contention is true for $n - 1$. Let $(1, 2) \notin G$; then as in the proof of Theorem 1, $F'(x)$ belonging to G' (G with 1 deleted) has an interior maximum. Hence G' is completely homomorphic to the complete graph with vertices $1^*, \ldots, k^*$. If 1 were connected with pre-images of each j^*, $j = 1, \ldots, k$, then G would contain a complete graph of order $k + 1$. Hence we may assume that 1 is not connected with any pre-image of 1^*. Let i be a pre-image of 1^*. Then by the induction hypothesis, the set H of all j with $(i, j) \in G$ is the set of all vertices of G that are not pre-images of 1^*. But

$$\sum_{(1,j)\in G} x_j = \sum_{(i,j)\in G} x_j$$

and all $x_j > 0$, so every vertex in H is connected to 1 in G. This completes the proof.

Any local maximum in the interior of S is also a (global) maximum. More generally the following theorem is valid.

THEOREM 3. *The point $x \in S$ yields a local maximum of $F(x)$ if and only if*

(1) *the restriction of G to those j for which $x_j > 0$ is completely homomorphic to a complete k-graph (with vertices, say, $1^*, \ldots, k^*$), and $\sum_i x_j = 1/k$ for $i = 1, \ldots, k$;*

(2) *no two vertices of G that are connected with all pre-images of the same $k - 1$ vertices among $1^*, \ldots, k^*$ are connected with each other;*

(3) *for every vertex i connected with at least one pre-image of each of $1^*, \ldots, k^*$, we have $\sum_{(i,j)\in G} x_j < 1 - 1/k$.*

Proof. Obviously, condition (1) is necessary because of Theorem 2 and the remark preceding Theorem 3. If (1) holds and if we compare $F(x)$ and $F(x + \epsilon)$, then already a consideration of the first-order variation gives (3) with $\leqslant 1 - 1/k$ instead of $< 1 - 1/k$. If these two conditions hold, then the first-order variation is $\leqslant 0$, and we need only non-positivity of the second-order variation for vanishing first-order variation. However, if

$$\sum_{(i,j)\in G} x_j = 1 - 1/k$$

in (3), then there exist two pre-images j_1 and j_2 of different elements of $(1^*, \ldots, k^*)$ that are not connected with i, and by setting $\epsilon_i > 0$, $\epsilon_{j_1} = \epsilon_{j_2} = -\epsilon_i/2$, all other $\epsilon_j = 0$, we obtain a positive second-order variation. Now if (2) does not hold, say for i_1, i_2, and i^*, then by (3) i_1 and i_2 are not connected with

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any pre-image i_3 of i^*; setting $\epsilon_{i_1} = \epsilon_{i_2} = -\epsilon_{i_3}/2 > 0$, all other $\epsilon_i = 0$, we again obtain a positive second-order variation. The sufficiency is now trivially assured.

3. Non-square-free forms. The above discussion can be extended to the case

$$F(x_1, \ldots, x_n) = \sum_{(i,j)\in G} q(x_i, x_j)$$

where $q(x, y)$ is a general binary quadratic form. Since the summation is symmetric, we may assume that $q(x, y) = q(y, x)$ so that $q(x, y) = a(x^2+y^2) + bxy$. The case $a = 0$ has been discussed already; so we may assume that $|a| = 1$, and since a change of sign only interchanges maxima and minima, we may restrict attention to $q(x, y) = x^2 + y^2 + bxy$.

THEOREM 4. *Let v_i denote the valence of the vertex i and let $v(G) = \max_G v_i$.*

If $v(G) > b/2$, then $f(G) = \max_S F(x) = v(G)$ and this maximum is attained only by setting $x_i = 1$ where $v_i = v(G)$ and $x_j = 0$ for $j \neq i$.

If $v(G) = b/2$, then $f(G) = v(G)$ and the maximum is attained by setting $x_j = 0$ except for the vertices of a complete subgraph all of whose vertices have valence $v(G)$.

If $v(G) < b/2$, then $f(G) = b/2 - c/2$, where $1/c = \max_{G'} \sum_{G'} (b - 2v_i)^{-1}$ as G' ranges over the complete subgraphs of G. This maximum is attained by setting $x_i = c/(b - 2v_i)$ for $i \in G'$ and $x_j = 0$ for $j \notin G'$. Whenever $F(x)$ has a local maximum the subgraph G' whose vertices are the points with $x_i > 0$ is complete.

Note that, as $b \to \infty$, the value $f(G)/b$ tends to that obtained in Theorem 1. However, in contrast to Theorems 2 and 3, the maximum is only attained for x so that the points i with $x_i > 0$ form a complete graph.

Proof. Let $f(G) = F(x_1, \ldots, x_n)$ and let G' be the subgraph whose vertices are the points i with $x_i > 0$. As in the proof of Theorem 1, we have

$$F_i = 2v_i x_i + b \sum_{(i,j)\in G'} x_j = 2f(G) \qquad \text{for all } i \in G'. \tag{4}$$

If G' were not complete, it would contain vertices i, j with $(i, j) \notin G'$. Then, replacing x_i by $x_i + \epsilon$ and x_j by $x_j - \epsilon$ would increase F by $(v_i + v_j)\epsilon^2$ contrary to the assumption that F was a (local) maximum. Thus

$$\sum_{(i,j)\in G'} x_j = 1 - x_i,$$

and (4) becomes

$$(2v_i - b)x_i = 2f(G) - b. \tag{5}$$

If $v(G) > b/2$, then $f(G) \geqslant v(G) > b/2$ and (5) implies $v_i > b/2$ for each $i \in G'$. If G' contained two vertices i, j, then replacing x_i by $x_i + \epsilon$ and x_j by

$x_j - \epsilon$ would increase F by $(v_i + v_j - b)\epsilon^2 > 0$, a contradiction. Thus G' consists of a single vertex in this case.

If $v(G) = b/2$, then $f(G) \geqslant b/2$, and therefore again $v_i \geqslant b/2$ for each $i \in G'$, which means $v_i = b/2$ for each $i \in G'$. The choice of x_i is then arbitrary and leads to $f(G) = b/2 = v(G)$.

If $v(G) < b/2$, set $2f(G) - b = -c$. Then according to (5) we have $x_i = c/(b - 2v_i)$ so that $\sum x_i = c \sum (b - 2v_i)^{-1} = 1$ or $c = (\sum (b-2v_i)^{-1})^{-1}$ and $f(G) = b/2 - c/2$. This completes the proof.

For the general quadratic form $q(x, y)$ the evaluation of $\min_S F(x) = \phi(G)$ is also non-trivial. Partial results are contained in the following theorem.

THEOREM 5. (i) $\phi(G) < 0$ *if* $b < -2$, $v(G) > 0$; $\phi(G) = 0$ *if* $b < -2$, $v(G) = 0$, *or* $b = -2$, *or* $b > -2$, $\min_G v_i = 0$; $\phi(G) > 0$ *if* $b > -2$, $\min_G v_i > 0$. (ii) *If G has no isolated vertex and if*

$$b > \max_{(i,j)\in G} (v_i + v_j),$$

then

$$\phi(G) = \left(\max_{G'} \sum_{G'} \frac{1}{v_i}\right)^{-1} \tag{6}$$

where G' is any empty subgraph of G. This minimum is attained by setting $x_i = 2\phi(G)/v_i$ for $i \in G'$ and $x_j = 0$ for $j \notin G'$. Whenever $F(x)$ has a local minimum in this case, the subgraph G' whose vertices are the points i with $x_i > 0$ is empty.

Proof. The first statement is easily verified. Assume now that

$$b > \max_{(i,j)\in G} (v_i + v_j)$$

and $\phi(G) = F(x_1, \ldots, x_n)$. Let G' be the subgraph whose vertices are the points i with $x_i > 0$. If G' is non-empty, then there are two vertices i, j with $(i, j) \in G'$. Now $F_i(x) = F_j(x)$ and therefore replacing x_i by $x_i + \epsilon$ and x_j by $x_j - \epsilon$ changes F by $(v_i + v_j - b)\epsilon^2 < 0$, contrary to the hypothesis of (local) minimality of F. Thus G' is empty and $F(x) = \sum v_i x_i^2$, so that $F_i = 2v_i x_i = 2\phi(G)$ for $i \in G'$. In other words, either $v_i = 0$ for all $i \in G'$, or $x_i = \phi(G)/v_i$ and $\phi(G) \sum_{G'} 1/v_i = 1$. This completes the proof.

4. Proof of a theorem of Turán and generalizations. Turán **(2)** proved the following result.

THEOREM 6. *A graph with n vertices which contains no complete subgraph of order k has no more than*

$$e(n, k) = m^2\binom{k-1}{2} + m(k-2)r + \binom{r}{2}, \tag{7}$$

$$n = (k-1)m + r,\ 0 \leqslant r < k - 1$$

edges. This maximum is attained only for a graph in which the vertices are divided into $k-1$ classes of which r contain $m+1$ vertices and the remainder contain m vertices with two vertices connected if and only if they belong to different classes.

We derive this theorem from Theorems 1 and 2.

If we set $x_i = 1/n$, $i = 1, \ldots, n$, then according to Theorem 1

$$\frac{1}{2}\left(1 - \frac{1}{k-1}\right) \geqslant f(G) \geqslant F(x) = \frac{e}{n^2}\,;$$

thus

$$e \leqslant \frac{n^2}{2}\left(1 - \frac{1}{k-1}\right), \tag{8}$$

which proves (7) for the case $r = 0$. In order to prove the remainder of the theorem for the case $r = 0$, we observe that in this case the point $x_i = 1/n$ represents an interior maximum, so that by Theorem 2 the graph G is completely homomorphic to a complete $(k-1)$-graph, C. Since $F_i = 2F$, each vertex is joined to

$$2nF = n(1 - 1/(k-1)) = (m-1)(k-1)$$

vertices, and the number of vertices in each pre-image of a vertex of C is m.

We now proceed by induction on r. Assume the contention true for $r - 1$. According to (8), the average valence does not exceed $n - n/(k-1)$, so for $r > 0$ there must be a vertex with no more than

$$n - m - 1 = m(k-2) + r - 1$$

edges. By the induction hypothesis, (7) holds for the graph G' obtained by deleting such a vertex, and hence

$$\begin{aligned} e &\leqslant m^2\binom{k-1}{2} + m(k-2)(r-1) + \binom{r-1}{2} + m(k-2) + r - 1 \\ &= m^2\binom{k-1}{2} + m(k-2)r + \binom{r}{2} = e(n,k). \end{aligned}$$

Thus equality is possible in (7) only if it holds for G' and, by the induction hypothesis, this means that the vertices of G' are divided into $k-1$ classes with $m+1$ or m elements each so that two vertices are connected if and only if they belong to different classes. Now, if the additional vertex were connected to elements in each class, then G would contain a complete k-graph. We can therefore adjoin it to one of the classes of G'. If that class already contained $m+1$ elements, then the number of edges at the vertex could be no greater than $m(k-2) + r - 2$. This completes the proof.

If instead of Theorem 2 we use Theorems 4 and 5, we can obtain generalizations which combine information about the number of edges with information about valences. For example, using Theorem 5, we have

THEOREM 7. *Let G be a graph with n vertices, e edges, maximal valence v, and minimal valence w. If G contains no empty subgraph of order k, then*

$$(1 + v)e \geqslant \frac{n^2}{2}\frac{w}{k-1}. \tag{9}$$

Or, equivalently, if G contains no complete subgraph of order k, then

$$e \leqslant \binom{n}{2} - \frac{n^2}{2} \quad \frac{n - v - 1}{(k-1)(n-w)}. \tag{10}$$

Proof. Set

$$q(x, y) = x^2 + y^2 + (2v + 2\epsilon)xy, \qquad \epsilon > 0,$$

and let $w > 0$ so that Thorem 5 applies to yield

$$F\left(\frac{1}{n}, \ldots, \frac{1}{n}\right) > \phi(G) = (\max_{G'} \sum_{G'} v_i^{-1})^{-1}$$
$$\geqslant ((k-1)/w)^{-1} = w/(k-1).$$

On the other hand $F(1/n, \ldots, 1/n) = (2 + 2v + 2\epsilon)e/n^2$, so that

$$(1 + v + \epsilon)e > \frac{n^2}{2} \quad \frac{w}{k-1}.$$

Since this inequality holds for every $\epsilon > 0$, we get (9). Inequality (10) is obtained by considering the complementary graph $\bar{G}$ for which

$$\bar{n} = n, \quad \bar{e} = \binom{n}{2} - e, \quad \bar{v} = n - 1 - \bar{w}, \quad \text{and} \quad \bar{w} = n - 1 - v.$$

5. Theorems of Rademacher type. It is easy to see from Theorem 6 that a graph G with n vertices and $e(n, k) + 1$ edges contains more than one complete k-graph. For either the deletion of some edge reduces G to the graph described in Theorem 6, in which case G contains at least

$$(m + 1)^{r-1} m^{k-1-r} \quad (\text{if } r > 0)$$

or m^{k-2} (if $r = 0$) complete subgraphs of order k, or the deletion of any edge from G yields a graph which already contains a complete k-graph. In other words, the intersection of the complete k-subgraphs of G is empty, so that G contains at least two such subgraphs. However, we can state this more precisely:

THEOREM 8. *A graph G with n vertices which contains exactly one complete k-subgraph has no more than*

$$e'(n, k) = e(n-1, k) + k - 1 \tag{11}$$

edges. This bound is sharp.

Proof. Let $1, \ldots, k$ be the vertices of the complete k-subgraph. Then there are $\binom{k}{2}$ edges (i, j) with $1 \leqslant i, j \leqslant k$, and no vertex $l > k$ is joined to more than $k - 2$ of the vertices $1, \ldots, k$. Thus there are no more than $(k-2)(n-k)$ edges (i, l) with $1 \leqslant i \leqslant k < l \leqslant n$. Hence

$$e'(n, k) \leqslant \binom{k}{2} + (k-2)(n-k) + e(n-k, k) = e(n-1, k) + k - 1.$$

To see that this bound is sharp, we consider a graph G' with $n - 1$ vertices of the type described in Theorem 6 and adjoin one vertex which is joined to exactly one vertex in each of the $k - 1$ classes of G'.

It would not be difficult to give similar bounds under the assumption that the graph contains no more than some fixed number of complete k-subgraphs.

In view of Theorem 2 we can state the following result.

THEOREM 9. *If the function $F(x_1, \ldots, x_n)$ attains its maximum $(1 - 1/k)/2$ at an interior point of the simplex S, then G contains at least $(k - 1)(n - k/2)$ edges and at least $n - k + 1$ complete k-graphs.*

Proof. According to Theorem 2 the graph G is completely homomorphic to a complete k-graph. Let the elements of the k-graph have $n_1, n_2, \ldots, n_k$ pre-images. Then $n_1 + \ldots + n_k = n$ and the number of edges is

$$e = \sum n_i n_j \geqslant (k-1)(n - k/2),$$

where the minimum is attained by setting $n_1 = \ldots = n_{k-1} = 1$ and $n_k = n - k + 1$. The number of complete k-subgraphs is

$$\prod n_i \geqslant n - k + 1,$$

where the minimum is again attained for the above choice of n_i.

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