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PERMUTATION INEQUALITIES

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Abstract. We formulate and solve some special cases of the following (in general NP-hard) extremal problem: "*Given a graph G (or a hypergraph H), label its vertices with given different n non-negative numbers $a_1 \geqslant a_2 \geqslant \ldots \geqslant a_n \geqslant 0$ in such a way that the sum of the products of labels in adjacent vertices $f = \sum a_i a_j$ will be maximal (or minimal)*". Solving this problem for some special families of graphs (e.g. paths, trees and stars) we obtain examples of "permutation inequalities" $f_{min} \leqslant f \leqslant f_{max}$.

1. Introduction: the problem and its context

CONTENT. We discuss the following very general extremal problem: "*Given a function $F : \mathbb{R}^n \to \mathbb{R}$ and a point $a = (a_1, a_2, \ldots, a_n) \in \mathbb{R}^n$, whose components form a decreasing sequence of non-negative numbers $a_1 \geqslant \ldots \geqslant a_n \geqslant 0$ find a permutation $\pi : \{1,2,\ldots,n\} \to \{1,2,\ldots,n\}$ for which the value of the "permutation function" $f_{F,A} := F(a_{\pi(1)}, a_{\pi(2)}, \ldots, a_{\pi(n)})$ is maximal (or minimal)*". We solve this general problem for some functions F of the class $\mathbb{L}$ of bilinear (or multilinear) functions with all nonzero coefficients equal to 1. For such functions our problem can be rephrased in terms of "maximal (or minimal) labelings" of graphs G (and hypergraphs H) with numbers $a_1, a_2, \ldots, a_n$.

AIM. The aim of this paper is to present three interrelated ideas:

1. The problem of finding maxima and minima (Problem 2) of *permutation functions* f (Definiton 1) leads to various *permutation inequalities* $f_{min} \leqslant f \leqslant f_{max}$ (Definiton 2).

2. Graphs G (and hypergraphs H) can be represented by bilinear (and multilinear) functions $F : R^n \to R$ having all nonzero coefficients equal to 1 (and vice versa); this builds on an old idea (1869) of Camille Jordan [7]. For a definition of a graph see Hartsfield, Ringel [6], for a definition of a hypergraph see BERGE [1]. In a hypergraph there are hyperedges instead of edges. A hyperedge connects more than two vertices. Every hypergraph can be interpreted as a bipartite graph with two sets of vertices, "black" and "white"; the black ones correspond to hyperedges and the white ones to vertices.

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3. Various families of graphs and hypergraphs "produce" various permutation inequalities, and these inequalities may be used in turn for the comparison of their structure!

STRUCTURE. The structure of the paper follows the pattern for exploring, investigating and discovering in mathematics, proposed by Berinde [2]: *Study a simple "source problem", formulate its solution in a form of an algorithm and then generalize it.*

PROBLEM BACKGROUND, BASIC NOTIONS. Hardy, Littlewood and Pólya [5] solved some special cases of the following extremal problem:

PROBLEM 1. Let $F : \mathbb{R}^n \to \mathbb{R}$ be a real valued function and let $a_1 \geqslant a_2, ..., \geqslant a_n \geqslant 0$ be a decreasing sequence of nonnegative numbers. Find a permutation $\pi : \{1,2,\dots,n\} \to \{1,2,\dots,n\}$ for which the value of $f = F(a_{\pi(1)}, a_{\pi(2)}, \dots, a_{\pi(n)})$ is maximal (or minimal).

DEFINITION 1. Let $F = F(x_1, x_2, \dots, x_n) : \mathbb{R}^n \to \mathbb{R}$ be a real-valued function, let $A = \{a_1, a_2, \dots, a_n\}$ be a decreasing sequence of nonnegative numbers and let $\pi : \mathbb{N}_n \to \mathbb{N}_n$ be any permutation of their indices. Let $f = F_{\pi,A}$ be a function, whose domain consists of all sequences $(a_{\pi(i)})$, called rearrangements of A. Then f is called a permutation function corresponding to F and A. Any permutation π_{max} or π_{min} for which f attains its maximal or minimal value (f_{max}, f_{min}) is called a maximal or minimal permutation, respectively.

Now we can reformulate Problem 1 as follows:

PROBLEM 2. For the given permutation function $f = f_{F,A}$ find its extreme values f_{max} and f_{min} and at least one maximal and minimal permutation π_{max} and π_{min}.

DEFINITION 2. Inequalities $f_{max} \geqslant f$ and $f_{min} \leqslant f$, obtained as solutions of Problem 2 for various permutation functions $f = f_A$, are called permutation inequalities.

REARRANGEMENT INEQUALITY. An example of such inequality (called also "the rearrangement inequality") with many important consequences (e.g. the arithmetic mean – geometric mean inequality, the Cauchy-Schwarz inequality, and Chebyshev's sum inequality [10]) is given in the following lemma (proved easily by an induction argument – see Prešić [9], p. 230, or Bruin [3]):

LEMMA 1. *Let* $0 \leqslant a_1 \leqslant a_2 \leqslant \dots \leqslant a_n$, $0 \leqslant b_1 \leqslant b_2 \leqslant \dots \leqslant b_n$. *Then*

$$a_1b_1 + a_2b_2 + \dots + a_nb_n = max(a_1b_{i_1} + a_2b_{i_2} + \dots + a_nb_{i_n}),$$

where S_n *is the set of all permutations* $\sigma = (i_1, i_2, ..., i_n)$ *of numbers* $(1, 2, \dots, n)$.

This result is intuitively clear: to get the maximum, large numbers must be multiplied with large numbers. Likewise, to get the minimum, large numbers a_i must be multiplied with small numbers b_j. "Minimal" problems are in general harder than "maximal".

The above rearrangement inequality can be given the following real-life interpretation: If n workers with ratings $a_1 \geqslant \ldots \geqslant a_n$ work in pairs with another n workers with ratings $b_1 \geqslant \ldots \geqslant b_n$, and if the contribution of each two co-workers to the common project is proportional to the product of their ratings, then the sum of the contributions of these $2n$ workers will be maximal if the pairs are: $(a_1,b_1),\ldots,(a_n,b_n)$.

EXAMPLE 1. Let $A = B = \{1,2,\ldots,n\}$. Then for $f = \sum a_i b_j$ we get $f_{max} = 1^2+2^2+\ldots+n^2 = n(n+1)(2n+1)/6$, while $f_{min} = 1\times n+2\times(n-1)+\ldots+n\times 1$.

EXAMPLE 2. Let $F:\mathbb{R}^6 \to \mathbb{R}$ be defined by the formula $F(x_1,x_2,x_3,x_4,x_5,x_6) = x_1x_2x_3+x_4x_5x_6$. Let A be any increasing sequence of nonnegative numbers $a_1 \leqslant a_2 \leqslant a_3 \leqslant a_4 \leqslant a_5 \leqslant a_6$ and let $f = f_{F,A}$ be the corresponding permutation function. It is easy to see that $f_{max} = a_1a_2a_3+a_4a_5a_6$ for any values a_i (at least two of the numbers a_1,a_2,a_3 are factors of the same monomial; if the third number is in another monomial, then a straightforward application of Lemma 1 for $n=2$ shows that the value of f may be increased), while the structure of the formula for f_{min} depends on the concrete values a_i.

2. Method

In this section we present a method for finding f_{max} (and f_{min}) of permutation functions $f = f_{F,A}$ (or at least good approximations to them).

PROPOSITION 1. *Let $f = f_{F,A}$ and let $\tau = \tau_{i,j}:\mathbb{N}_n \to \mathbb{N}_n$ denote the transposition interchanging indices i and j. Then $f(a_{\pi_{max}}) \geqslant f(a_{\tau\pi_{max}})$ and $f(a_{\pi_{min}}) \leqslant f(a_{\tau\pi_{min}})$.*

In the algorithm below let the notation $x \leftarrow y$ denote the replacement of x with y.

ALGORITHM 1. To find an increasing sequence of approximations to f_{max} do:
Step 1. Start with any permutation $\pi:\mathbb{N}_n \to \mathbb{N}_n$ of indices of (a_i).
Step 2. If you can find a $\tau = \tau_{i,j}$ such that $f(a_{\tau\pi(i)}) \geqslant f(a_{\tau\pi(j)})$ then let $\pi \leftarrow \tau\pi$.
Step 3. Repeat Step 2 as long as its condition is fulfilled.
To find a decreasing sequence of approximations to f_{min} replace Step 2 with:
Step 2'. If you can find a $\tau = \tau_{i,j}$ such that $f(a_{\tau\pi(i)}) \leqslant f(a_{\tau\pi(j)})$ then let $\pi \leftarrow \tau\pi$.

From now on we focus on permutation functions $f_{F,A}$, where F is bilinear or multilinear.

DEFINITION 3. A function $F:\mathbb{R}^n \to \mathbb{R}$ of the form $= F(x_1,x_2,\ldots,x_n) = \sum_{i,j=1}^{n} c_{ij}x_ix_j$ is called a bilinear function. Likewise, a multilinear function $F:\mathbb{R}^n \to \mathbb{R}$ is of the form $F(x_1,x_2,\ldots,x_n) = \sum_{i,j,\ldots,k=1}^{n} c_{i,j,\ldots,k}x_ix_j\ldots x_k$. The family of all bilinear and multilinear functions whose nonzero coefficients c_{ij} or $c_{i,j,\ldots,k}$ are all equal to 1 we denote by $\mathbb{L}$.

THEOREM 1. *Let* $F : \mathbb{R}^n \to \mathbb{R}$ *be a bilinear or multilinear function and let* $\Delta_{i,j}F := F(x_{\tau_{i,j}(k)}) - F(x_k) = F(x_1,\ldots,x_j,\ldots,x_i,\ldots,x_n) - F(x_1,\ldots,x_i,\ldots,x_j,\ldots,x_n)$. *Then:*

i) If the variables x_i *and* x_j *are not adjacent (i.e. they do not correspond to adjacent vertices) then* $\Delta_{i,j}F = (x_j - x_i)(F_j - F_i)$;

ii) If the variables x_i *and* x_j *are adjacent (*$x_i \sim x_j$*), then* $\Delta_{i,j}F = (x_j - x_i)((F_j - F_{i,j}x_i) - (F_i - F_{i,j}x_j))$. *If* $F \in \mathbb{L}$ *and* F *bilinear then* $\Delta_{i,j}F = (x_j - x_i)((F_j - x_i) - (F_i - x_j))$.

Proof. i) $\Delta_{i,j}F$ depends only of those monomials M_k that contain exactly one of the variables x_i or x_j as a factor, hence: $\Delta_{i,j}F = (x_j(F_j - F_{i,j}x_i) + x_i(F_i - F_{i,j}x_j)) - (x_i(F_j - F_{i,j}x_i) + x_j(F_i - F_{i,j}x_j)) = (x_j - x_i)((F_j - F_{i,j}x_i) - (F_i - F_{i,j}x_j))$. If x_i and x_j are not adjacent, then $F_{i,j} = 0$ and we get i). If $F \in \mathbb{L}$ and F bilinear then all the nonzero $F_{i,j}$ are equal to 1. Note that this proof does not work for general polynomial functions! □

COROLLARY 1. Let $F : \mathbb{R}^n \to \mathbb{R}$ be a bilinear or multilinear function. If $\pi = \pi_{max}$ is the maximal permutation, then $a_{\pi(i)} \geqslant a_{\pi(j)}$ if and only if $F_i - F_{i,j}a_j \geqslant F_j - F_{i,j}a_i$. If $\pi = \pi_{min}$ is the minimal permutation, then $a_{\pi(i)} \geqslant a_{\pi(j)}$ if and only if $F_i - F_{i,j}a_j \leqslant F_j - F_{i,j}a_i$.

THEOREM 2. *Functions* $F \in \mathbb{L}$ *are in 1-1 correspondence with bipartite graphs (bilinear functions* $F = \sum x_i x_j$ *correspond to graphs, multilinear* $F = \sum x_i x_j \ldots x_k$ *to hypergraphs).*

Proof. For $F \in \mathbb{L}$ let $G = G_F$ be a bipartite graph, whose edges connect “white” vertices corresponding to variables x_i with “black” vertices corresponding to monomials $x_i x_j \ldots x_k$ of F. This G can be interpreted also as a hypergraph – each of the black vertices corresponds to a hyperedge.

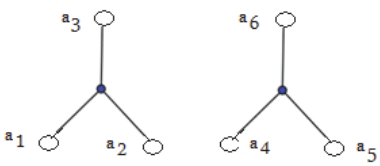


Figure 1: *A labeled bipartite graph (hypergraph) corresponding to Example 2 (left) and a labeled graph corresponding to Lemma 1 (right).*

If F is bilinear then all the hyperedges of G are in fact edges, the black vertices can be omitted (see Figure 1) and G can be interpreted as a graph. □

For the functions $f = f_{F,A}$ obtained from functions $F \in \mathbb{L}$ our problem (Problem 2) and our transposition method (Theorem 1, Corollary 1) can be reformulated in terms of “energy” and “potential” of “labeled graphs and hypergraphs” (Definitions 4, 5, 6):

DEFINITION 4. Let $G = G_F$ be a graph (or a hypergraph) corresponding to a bilinear (or multilinear) function F and let $\pi : \mathbb{N}_n \to \mathbb{N}_n$ be a permutation of the indices i of the set $A = (a_i)$ of nonnegative numbers. A function $\pi^* : V(G) \to A$, assigning to each vertex v_i of G a number $\pi^*(v_i) = a_{\pi(i)}$ is called a labeling of G with the labels from the set A.

DEFINITION 5. The energy $E_{A,\pi}(G)$ of a graph $G_{A,\pi}$, whose vertices are labeled with numbers $a_i \in A$, is the sum $\sum_{v_i \sim v_j} \pi^*(v_i)\pi^*(v_j)$ of products of labels in adjacent vertices of G. The maximal and minimal energy of G is denoted $E_{A,max}(G)$ and $E_{A,min}(G)$. Similarly, the energy $E_{A,\pi}(H)$ of a labeled hypergraph $H_{A,\pi}$ is the sum $\sum_{v_i \sim v_j} \pi^*(v_i)\pi^*(v_j)\ldots\pi^*(v_k)$ of products of labels in adjacent vertices of G.

DEFINITION 6. Let $H_{A,\pi}$ corresponds to a multilinear function $F : \mathbb{R}^n \to \mathbb{R}^n$.

The energy of each black vertex u_m corresponding to a monomial $M_m = x_i x_j \ldots x_k$ of F is the product $E_m = E_{m,A,\pi} := \pi^*(v_i)\pi^*(v_j)\ldots\pi^*(v_k)$ of labels in vertices $v_i, v_j, \ldots, v_k$.

The potential $P_i := \sum_{v_i \sim M_m} \frac{E_m}{\pi^*(v_i)}$ of the vertex v_i is the sum of all the energies of monomials in which x_i is a factor, divided by the label of v_i.

The relative potential $P_{i,j} = \sum_{v_i \sim M_m, v_j \sim M_m} E_m/\pi^*(v_i)$ is the sum of the energies of all the monomials containing both x_i and x_j, divided by the label of v_i.

Note that in general $P_{i,j} \neq P_{j,i}$. Now we can reformulate Problem 2 for $f \in \mathbb{L}$:

PROBLEM 3. For a given graph G (or hypergraph H) and a given set of labels A find $E_{A,max}$ and $E_{A,min}$ and the corresponding maximal and minimal labelings π^*_{max} and π^*_{min}.

Now we can give a necessary condition for maximal and minimal labelings.

PROPOSITION 2. *Let $\tau_{i,j} : \mathbb{N}_n \to \mathbb{N}_n$ denote the permutation of indices of the set of labels A interchanging only the indices i and j of vertices v_i and v_j. For every such $\tau_{i,j}$ we have $E(a_{\pi_{max}}) \geqslant E(a_{\tau\pi_{max}})$ and $E(a_{\pi_{min}}) \leqslant E(a_{\tau\pi_{min}})$.*

Proof. This follows from Proposition 1 for the special case of functions $F \in \mathbb{L}$. □

THEOREM 3. *Let v_i and v_j be any two vertices of a labeled hypergraph $H_{A,\pi}$. Then:*

i) $\Delta_{i,j}E = (\pi^*(v_j) - \pi^*(v_i)((P_j - P_{i,j}\pi^*(v_i)) - ((P_i - P_{j,i}\pi^*(v_j))$.

ii) if $\pi^* = \pi_{max}$ then $\pi^*(v_i) \geqslant \pi^*(v_j)$ if and only if $P_j - P_{i,j}\pi^*(v_i) \geqslant P_i - P_{j,i}\pi^*(v_j)$.

iii) if $\pi^* = \pi_{min}$ then $\pi^*(v_i) \geqslant \pi^*(v_j)$ if and only if $P_j - P_{i,j}\pi^*(v_i) \leqslant P_i - P_{j,i}\pi^*(v_j)$.

If v_i and v_j are not adjacent, then $P_{i,j} = P_{j,i} = 0$ and we get simpler conditions

i') $\Delta_{i,j}E = (\pi^*(v_j) - \pi^*(v_i)(P_j - P_i)$.

ii') if π^* is a maximal labeling then $\pi^*(v_i) \geqslant \pi^*(v_j)$ if and only if $P_j \geqslant P_i$.

iii') if π^* is a minimal labeling then $\pi^*(v_i) \geqslant \pi^*(v_j)$ if and only if $P_j \leqslant P_i$.

Proof. This is just a reformulation of Theorem 1 in terms of energy of hypergraphs. $\square$

THEOREM 4. *Let $G_{A,\pi}$ be a labeled graph corresponding to $F = \sum_{v_i \sim v_j} x_i x_j$. Then:*
i) The potential of a vertex v_i can be expressed as: $P_{i,A,\pi} = \frac{\partial F}{\partial x_i}(a_{\pi(1)}, \ldots, a_{\pi(n)})$,
ii) $E_{A,\pi}(G) = (1/2)\sum_{i=1}^{n} a_{\pi(i)} P_{i,A,\pi} = (1/2)\sum_{i=1}^{n} a_{\pi(i)} F_i(a_{\pi(1)}, \ldots, a_{\pi(n)})$.

Proof. i) The partial derivative $\frac{\partial F}{\partial x_i}$ of the bilinear $F = \sum_{v_i \sim v_j} x_i x_j$ is $\frac{\partial F}{\partial x_i} = \sum_{v_i \sim v_j} x_j$.
ii) In the sum $\sum_{i=1}^{n} a_{\pi(i)} P_{i,A,\pi}$ the energy $x_i x_j$ of each edge is counted twice. $\square$

The next theorem (Theorem 5) expresses the difference of energies $\triangle_{i,j} E$ in a labeled graph after and before any transposition $\tau_{i,j}$ in terms of potentials of vertices v_i and v_j.

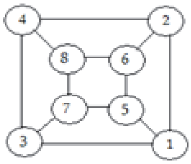
THEOREM 5. *For any labeled graph $G_{A,\pi}$ we have:*
i.a) $\triangle_{i,j} E = (\pi^*(v_i) - \pi^*(v_j)(P_{i,A,\pi} - P_{j,A,\pi})$ if v_i and v_j are not adjacent.
i.b) $\triangle_{i,j} E = (\pi^*(v_i) - \pi^*(v_j)((P_{i,A,\pi} - \pi^*(v_j)) - (P_{j,A,\pi} - (\pi^*(v_i))$, if $v_i \sim v_j$.
Let $\pi^*(v_i) \geqslant \pi^*(v_j)$. If the vertices v_i and v_j are not adjacent, then:
ii.a) if $P_{i,A,\pi} \leqslant P_{j,A,\pi}$ then $E_{A,\pi\tau_{i,j}(G)} \geqslant E_{A,\pi\tau_{i,j}}(G)$,
ii.b) if $P_{i,A,\pi} \geqslant P_{j,A,\pi}$ then $E_{A,\pi\tau_{i,j}(G)} \leqslant E_{A,\pi\tau_{i,j}})(G)$.
If the vertices v_i and v_j are adjacent, then:
iii.a) if $P_{i,A,\pi} - \pi(j) \leqslant P_{j,A,\pi} - \pi(v_j)$ then $E_{A,\pi(\tau_{i,j}(G)} \geqslant E_{A,\pi\tau_{i,j}})(G)$,
iii.b) if $P_{i,A,\pi} - \pi(j) \geqslant P_{j,A,\pi} - \pi(v_i)$ then $E_{A,\pi(\tau_{i,j}(G)} \leqslant E_{A,\pi\tau_{i,j}}(G)$.

Proof. The formulas i.a) and i.b) follow from Theorem 1, since we know (from i) of Theorem 4 that $P_{i,A,\pi} = \frac{\partial F}{\partial x_i}(a_{\pi(1)}, \ldots, a_{\pi(n)}) = \sum_{v_i \sim v_j} v_j$. Hence $\frac{\partial^2 F}{\partial x_i \partial x_j} x_i = 1$ if $v_i \sim v_j$ and $\frac{\partial^2 F}{\partial x_i \partial x_j} x_i = 0$ if v_i is not adjacent to v_j. Now we use $\pi^*(v_i) \geqslant \pi^*(v_j)$ in i.a) and i.b) and just check in each of the cases ii.a), ii.b), iii.a), iii.b) what is true: $\triangle E \geqslant 0$ or $\triangle E \leqslant 0$. $\square$

ALGORITHM 2. To maximize the energy of the labeled graph G transpose the labels in pairs of non-adjacent vertices v_i and v_j as long as there are such pairs that $\pi(^*v_i) > \pi^*(v_j)$ and $P_i < P_j$. Likewise, transpose the labels in pairs of adjacent vertices v_i and v_j as long as there are such pairs that $\pi^*(v_i) > \pi^*(v_j)$ and $P_i - \pi^*(v_j) < P_j - \pi^*(v_i)$.

REMARK. Algorithm 2 is just a special case of Algorithm 1. The reader will easily formulate the analogous version for the minimal rearrangement.

EXAMPLE 3. Using the described algorithm we can find the following labeling of the cubic graph with 8 vertices (Figure 2). By Theorem 5 the energy of this labeling cannot be increased by any transposition. Yet this does not prove that this is a maximal labeling!



$\pi(v_i)$	1	2	3	4	5	6	7	8
P_i	5+3+2 = 10	6+4+1 = 11	7+4+1 = 12	8+3+2 = 13	7+6+1 = 14	8+5+2 = 15	8+5+3 = 16	7+6+4 = 17

Figure 2: *Labeled graph (left) and potentials P_i of labels i.*

Using Theorem 3 and an induction argument we can prove the following generalization of rearrangement inequality (Lemma 1):

LEMMA 2. *Let $A = a_{i,j}$ be a matrix of labels such that $0 \leqslant a_{1,1} \leqslant a_{1,2} \leqslant \ldots \leqslant a_{1,n} \leqslant 0 \leqslant a_{2,1} \leqslant a_{2,2} \leqslant \ldots \leqslant a_{2,n} \ldots \leqslant 0 \leqslant a_{m,1} \leqslant a_{m,2} \leqslant \ldots \leqslant a_{m,n}$. Then $a_{1,1}a_{2,1}\ldots a_{m,1} + a_{1,2} + a_{2,2}\ldots a_{m,2} + \ldots a_{n,1}a_{n,2}\ldots a_{n,m} = f_{max}$ is the maximal value of a permutation function $f = F_A$, where $F = \sum_{i=1}^{m} a_{i,\pi(1)}\ldots a_{i,\pi(m)}$ is the sum of n monomials with m factors from different rows of a $m \times n$ matrix; different monomials have different factors $x_{i,j}$.*

Proof. The hypergraph H corresponding to the function F is a disjoint union of m complete graphs K_n (Figure 3 shows the maximal labeling of a hypergraph H corresponding to a permutation function with $m = 3$ and $n = 4$ with labels taken from sequences $a_1 = (1,5,9)$, $a_2 = (1,5,9)$, $a_3 = (3,7,11)$, $a_4 = (4,8,12)$). Now we use the induction argument. For $m = 1$ there is nothing to prove. If the theorem holds for some $m = k$, then it holds also for $k+1$. For it is clear (apply Theorem 3) that the largest m numbers must be the labels of the same copy of a hypergraph, corresponding to a monomial with n factors. Then we just use the induction hypothesis. □

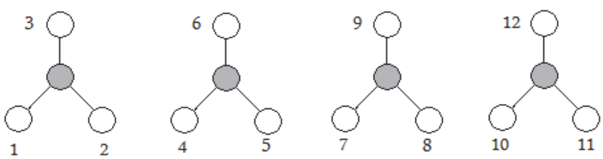


Figure 3: *Maximal labeling of a hypergraph H.*

3. Permutation inequalities $f \leqslant f_{max}$ obtained from graphs

In this section we find and prove some permutation inequalities $f \leqslant f_{max}$ (inequalities $f \geqslant f_{min}$ are harder) obtained from computing energies of various families of graphs.

PROPOSITION 3. *The energy of a complete graph $G = K_n$ on n vertices is for every labeling π of its vertices with labels from a given set A the same: $E_{A,\pi}(K_n) = (1/2)((\sum a_i)^2 - \sum a_i^2)$.*

Proof. We compute $E_{A,\pi}(K_n) = \sum_{v_i \sim v_j} \pi^*(v_i)\pi^*(v_j) = (1/2)\sum \pi^*(v_i)P_i = (1/2)((\sum a_i)^2 - \sum a_i^2)$. In the special case $A = \{1,2,\ldots,n\}$ we get by a straightforward calculation $E(K_n) = (n(n+1)/2)^2 - n(n+1)(2n+1)/6 = n(n+1)(3n^2-n-2)/24$. □

EXAMPLE. For $n \in \{1,2,3,4,5\}$ the values of $E(K_n)$ are $0,2,11,35,85$, and these are exactly the values obtained by our formula; they can be calculated also by the obvious recursive formula: $E(K_{n+1}) - E(K_n) = (n+1)(1+2+\ldots+n) = n(n+1)^2/2$.

PROPOSITION 4. *Let $G = K_{m,n-m}$ be a complete bipartite graph and let $a = \sum \pi(v_i) = a_1 + a_2 + \ldots + a_n$ be the sum of all the labels $a_i \in A$. If $x = \sum_{i=1}^m \pi(v_i)$ is the sum of the labels in one part, then the upper bound for the maximal energy of G is $E_{A,\pi}(K_{m,n-m}) = \sum x(A-x) \leqslant a^2/4$. This upper bound is attained if and only if $x = a - x = a/2$.*

Proof. $E_{A,\pi}(K_{m,n-m}) = (\sum_{i=1}^m \pi(v_i))(\sum_{i=m+1}^n \pi(v_i)) = \sum x(A-x) \leqslant a^2/4$, since this quadratic function attains its maximal value at $x = A/2 = A - x$. □

REMARK. The problem of finding maximal energy of a complete bipartite graph, labeled with nonnegative integers $a_1 \leqslant a_2 \ldots \leqslant a_n$ transforms to the *problem of partitions* (see Garey and Johnson, [4], p. 223): we know the value $a^2/4$ can be attained if and only if the set of labels A can be partitioned into two subsets with equal sums – and this is exactly the problem of partitions, which is NP-hard!

PROPOSITION 5. *Let $a_1 \geqslant \ldots \geqslant a_n \geqslant 0$ and let $f : \mathbb{R}^n \to \mathbb{R}^n$ be defined with the formula: $f(x_1,\ldots,x_n) := x_1x_2 + x_2x_3 + \ldots + x_{n-1}x_n$. Then for any $\{x_1,\ldots,x_n\} = \{a_1,\ldots,a_n\}$ the maximal value f_{max} of f is given by the right side of the inequality: $f(x_1,\ldots,x_n) = x_1x_2 + x_2x_3 + \ldots + x_{n-1}x_n \leqslant a_1a_2 + \sum_{i=1}^{n-2} a_ia_{i+2}$.*

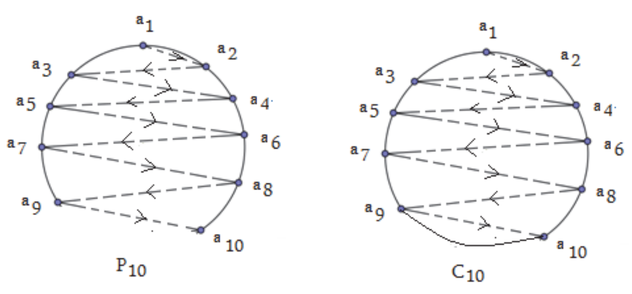


Figure 4: *Maximal labelings of the path P_{10} and the cycle C_{10}.*

Proof. The proposition claims that the maximal energy of the path P_n, labeled with non-negative numbers a_i, equals $a_1a_2 + \sum_{i=1}^{n-2} a_ia_{i+2}$. (see Figure 4 left); this interpretation immediately reveals also the maximal energy of the cycle on n points:

$E_{max}(C_n) = E_{max}(P_n) + a_{n-1}a_n$. We can assume $n \geqslant 3$. The proof is divided in five steps:

i) Suppose $(x_1, x_2, \ldots, x_n)$ is a maximal permutation. Then $a_1 \neq x_1$, otherwise the transposition of x_1 and x_2 would increase the value of f for $(a_1 - x_2)x_3 \geqslant 0$ and in that case the rearrangement $(x_1, x_2, \ldots, x_n)$ would not be maximal. Likewise $a_1 \neq x_n$. Hence $a_1 = x_j$ for some j such that $0 < j < n$.

ii) At each side of the greatest number $a_1 = x_j$ in the maximal rearrangement $(b_m, b_{m-1}, \ \ldots, b_1, a_1, c_1, , \ldots, c_{k-1}, c_k)$ the numbers decrease towards both end positions: $b_m \leqslant b_{m-1} \leqslant \ldots \leqslant b_1 \leqslant a_n \geqslant c_1 \geqslant \ldots \geqslant c_{k-1} \geqslant c_k$. For suppose $b_i \geqslant b_1$ for some $i > 1$. Then the permutation $(b_i, b_{i-1}, \ldots, b_1) \to (b_1, \ldots, b_{i-1}, b_i)$ increases the value of f for $b_i a_n + b_1 b_{i+1} - (b_1 a_n + b_i b_{i+1}) = (b_i - b_1)(a_n - b_{i+1}) \geqslant 0$. So $b_1 = max\{b_1, \ldots, b_m\}$. Likewise we prove $b_2 = max\{b_2, \ldots, b_m\}$ etc., hence $b_j \geqslant b_{j+1}$ for all j. Exactly the same reasoning for c-numbers gives the inequalities: $c_j \geqslant c_{j+1}$ for all j.

iii) Let $(b_m, b_{m-1}, \ldots, b_1, a_1, c_1, \ldots, c_{k-1}, c_k)$ be a maximal rearrangement. If $b_1 \leqslant c_1$ then ii) implies $c_1 = a_2$, since $c_1 \geqslant b_1 \geqslant b_i$ and $c_1 \geqslant c_j$. Likewise, ii) implies $a_3 \in \{b_1, c_2\}$. It must be $b_1 = a_3$, since $f(b_m, \ldots, b_1, a_1, c_1, c_2, \ldots, c_k) - f(c_k, \ldots, c_2, b_1, a_1, c_1, b_1, \ldots, b_m) = a_1(b_1 - c_2) + c_1(c_2 - b_1) = (a_1 - c_1)(b_1 - c_2) \geqslant 0$ only if $b_1 \geqslant c_2$.

iv) If $c_{i+1} \leqslant b_i \leqslant c_i$ in a maximal rearrangement, then $c_{i+2} \leqslant b_{i+1} \leqslant c_{i+1}$. This is proved as follows: $b_{i+1} \leqslant c_{i+1}$ must be true, since only then the value of f on the rearrangement with permuted and reflected parts $(b_m, \ldots, b_{i+1})$ and $(c_{i+1}, \ldots, c_k)$ is smaller: $f(b_m, \ldots, b_{i+1}, b_i, \ldots, b_1, a_1, c_1, \ldots, c_i, c_{i+1}, \ldots, c_k) - f(c_k, \ldots, c_{i+1}, b_i, \ldots, b_1, a_1, c_1, \ldots, c_i, b_{i+1}, \ldots b_m) = b_i(b_{i+1} - c_{i+1}) + c_i(c_{i+1} - b_{i+1}) = (b_i - c_i)(b_{i+1} - c_{i+1}) \geqslant 0$.

Likewise $c_{i+2} \leqslant b_{i+1}$ must be true, since only in that case the value of f on the rearrangement with permuted and reflected parts $(b_m, \ldots, b_{i+1})$ and $(c_{i+2}, \ldots, c_k)$ is smaller: $f(b_m, \ldots, b_{i+1}, b_i, \ldots, b_1, a_1, c_1, \ldots, c_i, c_{i+1}, \ldots, c_k) - f(c_k, \ldots, c_{i+1}, b_i, \ldots, b_1, a_1, c_1, \ldots, c_i, b_{i+1}, \ldots, b_m) = b_i(b_{i+1} - c_{i+1}) + c_i(c_{i+1} - b_i) = (b_i - c_{i+1})(b_{i+1} - c_{i+2}) \geqslant 0$.

v) Consequently $c_i = a_{2i}$ and $b_i = a_{2i+1}$. There are just two rearrangements giving the maximal value of f, obtained from each other by a reflection symmetry. The smallest two numbers a_n and a_{n-1} lie at the end positions. □

Proposition 5 can be generalized to infinite paths (infinite in both directions) and to *subdivided stars* $S_{m,n}$ with m rays and $mn+1$ vertices (defined by Hartsfield [6]). Notice that a path P_{2n+1} with $2n+1$ vertices is the same as the star $S_{n,n}$ with $m = 2$ rays.

PROPOSITION 6. *Let* $a_1 \geqslant \ldots \geqslant a_n \geqslant \ldots \ \geqslant 0$, $\sum_{i=1}^{\infty} a_i = A < \infty$ *and let we have the equality of sets* $\{x_i \mid i \in \mathbb{Z}\} = \{a_j \mid j \in \mathbb{N}\}$. *Then* $\sum_{i=-\infty}^{\infty} x_i x_{i+1} \leqslant a_1 a_2 + \sum_{j=1}^{\infty} a_j a_{j+2}$.

Proof. We just repeat the steps ii), iii), iv) and v) of the proof of Proposition 5 (step i) is unnecessary, since there are no leaves in this case). We can imagine this maximal rearrangement on the number line: place a_1 at 0, a_{2i-1} at i, and a_{2i} at $-i$ (Figure 5). □

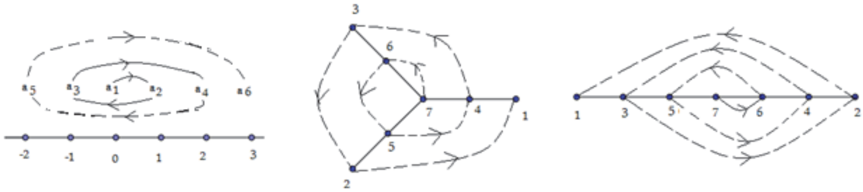


Figure 5: *Spiral-shaped maximal rearrangement on the number line, in the star $S_{3,2}$ with $m=3$ rays, and in the star $S_{2,3}$ with $m=2$ rays (or a path P_7).*

PROPOSITION 7. *The maximal value of the permutation function $f(x_0,x_{1,1},x_{2,1},\ldots,x_{m,1},x_{1,2},x_{2,2},\ldots,x_{m,2},\ldots,x_{1,n},x_{2,n},\ldots,x_{m,n}) = x_0\sum_{i=1}^m x_{i,1} + \sum_{i=1}^m \sum_{j=1}^{n-1} x_{i,j}x_{i,j+1}$ whose domain consists of all permutations of numbers $a_1 \geqslant \ldots \geqslant a_{mn+1} \geqslant 0$ is given by the permutation $(a_1,a_2,\ldots,a_{mn+1})$, hence $f_{max} = a_1\sum_{i=1}^m a_{i+1} + \sum_{i=1}^{mn-m} a_i a_{i+m}$.*

Proof. The greatest number a_1 must be in the center of the star: $x_0 = a_1$, surrounded by $a_2,\ldots,a_{m+1}$. As in step ii) of the proof of Proposition 5 we prove that the labels decrease from the center to the m leaves. Using Lemma 1 and induction we see that $x_{i,1} \geqslant x_{i,2} \geqslant \ldots \geqslant x_{i,m} \geqslant x_{i+1,m}$, hence $x_{1,1} \geqslant x_{1,2} \geqslant \ldots \geqslant x_{1,m} \geqslant x_{2,1} \geqslant x_{2,2} \geqslant \ldots \geqslant x_{2,m} \geqslant \ \ldots \ x_{n,1} \geqslant x_{n,2} \geqslant \ldots \geqslant x_{n,m}$, thus the maximal rearrangement is $(a_1,a_2,\ldots,a_{mn+1})$. □

REMARK. This maximal rearrangement can be obtained also by a "greedy algorithm" [8]: Place a_1 in the center of the star. Imagine it as an atom with m free bonds, and other a_i as atoms with two (or one) free bonds. Then for each $i \in \{1,2,\ldots,n\}$ connect a_i with the greatest a_j still having a free bond.

PROPOSITION 8. *Let $a_1 \geqslant a_2 \geqslant \ldots \geqslant a_n \geqslant 0$. The maximal and minimal energy of any tree T_n with n points lye between the maximal and minimal energy of a star $S_{n,2} = K_{1,n-1}$: $a_n(a_1+\ldots a_{n-1}) = E_{min}(S_{n,2}) \leqslant E_{min}(T_n) \leqslant E_{max}(T_n) \leqslant E_{max}(S_{n,2}) = a_1(a_2+\ldots a_n)$.*

Proof. We can assume $n \geqslant 3$ (the cases T_1 and T_2 are trivial). First let us prove $E_{max}(T_n) \leqslant E_{max}(S_{n,2})$. Placing a_1 in the center of the star $S_{n,2}$ we see $E_{max}(S_{n,2}) = a_1(a_2+\ldots a_n)$. If there is any leaf v_i in T_n not adjacent to v labeled a_1, replace the edge connecting v_i and its only adjacent vertex with an edge connecting v_i with v; this increases the energy of the tree. Repeat this replacements until all leafs are adjacent to v. An analogous proof with the label a_n in the center of the star shows that $E_{min}(S_{n,2}) \leqslant E_{min}(T_n)$. □

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