A majorization method for localizing graph topological indices

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Abstract

This paper presents a unified approach for localizing some relevant graph topological indices via majorization techniques. Through this method, old and new bounds are derived and numerical examples are provided, showing how former results in the literature could be improved.

Key Words: Majorization; Schur-convex functions; Graphs; Topological indices.

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1 Introduction and preliminaries

Optimization problems involving Schur-convex or Schur-concave functions have received much attention in the literature providing some useful applications in different fields: for example they became a convenient tool to localize eigenvalues of a real spectrum matrix ([1], [21]) or more generally to obtain bounds for an arbitrary order statistic distribution ([3]). More recently some issues related to the structural properties of graphs, characterized in terms of invariants, have been explored solving suitable optimization problems via majorization techniques ([2], [7]).

The aim of this paper is to explore this approach, showing that it is a powerful tool for achieving, through a unified scheme, many well-known bounds of some graph topological indices that can be expressed in terms of Schur-convex or Schur-concave functions. One major advantage of this technique is to set up a strategy for improving these bounds as well as to obtain new ones. We start recalling some basic definitions on majorization. More details can be found in [18].

Definition 1 Given two vectors \( y, z \in D = \{ x \in \mathbb{R}^n : x_1 \geq x_2 \geq \cdots \geq x_n \} \), the majorization order \( y \preceq z \) means:

\[
\begin{align*}
\langle y, s^k \rangle &\leq \langle z, s^k \rangle, \quad k = 1, \ldots, (n-1) \\
\langle y, s^n \rangle &\leq \langle z, s^n \rangle
\end{align*}
\]

where \( \langle \cdot, \cdot \rangle \) is the inner product in \( \mathbb{R}^n \) and \( s^j = [1, 1, \cdots, 1, 0, 0, \cdots, 0] \), \( j = 1, 2, \cdots, n \).

Definition 2 Given a set \( S \subseteq D \cap \{ x \in \mathbb{R}^n : \langle x, s^n \rangle = a \} \), a vector \( x^*(S) \in S \) (\( x_*(S) \in S \)) is said to be the maximal (minimal) vector in \( S \) with respect to the majorization order if \( x \preceq x^*(S) \) (\( x_*(S) \preceq x \)) for each \( x \in S \).
Since the upper and lower level sets:
\[ U(z) = \{ x \in S_a : z \leq x \} , \quad L(z) = \{ x \in S_a : x \leq z \} \]
are closed, the existence of maximal and minimal elements of \( S \) are ensured by its compactness. In \[1\], \[2\] and \[18\], the extremal vectors for some closed subsets of
\[ \Sigma_a = \{ x \in \mathbb{R}^n : x_1 \geq x_2 \geq \ldots \geq x_n \geq 0 \} \cap \{ x \in \mathbb{R}^n : \langle x, s^n \rangle = a \} \]
have been computed. In particular in \[2\] the maximal and minimal elements of
\[ S_a = \Sigma_a \cap \{ x \in \mathbb{R}^n : M_i \geq x_i \geq m_i, i = 1, \ldots, n \} \]
where \( M_1 \geq M_2 \geq \cdots \geq M_n, m_1 \geq m_2, \ldots \geq m_n \), have been derived, studying also the extremal vectors of some subsets of \( S_a \) of particular interest:
\[ S^1_a = \Sigma_a \cap \{ x \in \mathbb{R}^n : M \geq x_1 \geq x_2 \geq \cdots \geq x_n \geq m \} \]  \( \text{(see also [18])} \)
\[ S^2_a = \Sigma_a \cap \{ x \in \mathbb{R}^n : x_i \geq a, i = 1, \ldots, h, 1 \leq h \leq n, \alpha \leq \frac{a}{h} \} \]  \( \text{(see also [1])} \)
\[ S^3_a = \Sigma_a \cap \{ x \in \mathbb{R}^n : x_i \leq \alpha, i = h + 1, \ldots, n, 1 \leq h \leq (n - 1), \alpha < a \}; \]  \( \text{(see also [1])} \)

\[ S_a^{(h)} = \Sigma_a \cap \{ x \in \mathbb{R}^n : M_1 \geq x_1 \geq \cdots \geq x_h \geq m_1, M_2 \geq x_{h+1} \geq \cdots \geq x_n \geq m_2, m_i < M_i, i = 1, 2 \}. \]  \( \text{(4)} \)

**Definition 3** A symmetric function \( \phi : A \to \mathbb{R}, A \subseteq \mathbb{R}^n \), is said to be Schur-convex on \( A \) if \( x \preceq y \) implies \( \phi(x) \leq \phi(y) \). If in addition \( \phi(x) < \phi(y) \) for \( x \preceq y \) but \( x \) is not a permutation of \( y \), \( \phi \) is said to be strictly Schur-convex on \( A \). A function \( \phi \) is (strictly) Schur-concave on \( A \) if \( -\phi \) is (strictly) Schur-convex on \( A \).

Given an interval \( I \subseteq \mathbb{R} \), and a (strictly) convex function \( g : I \to \mathbb{R} \), the function \( \phi(x) = \sum_{i=1}^n g(x_i) \) is (strictly) Schur-convex on \( I^n = I \times I \times \cdots \times I \). The corresponding result holds if \( g \) is (strictly) concave on \( I^n \).

From the order preserving property of Schur-convex functions, the solution of some constrained nonlinear optimization problems of particular interest can be obtained in a straightforward way. More precisely, the problem we face is the following:

\[ \begin{aligned}
\text{max} \quad & (\min) \ \phi(x) \\
\text{subject to} \quad & x \in S
\end{aligned} \]  \( \text{(P)} \)

where \( S \subseteq \mathbb{R}^n \) is a generic subset which admits maximal vector \( x^*(S) \) and minimal vector \( x_*(S) \) with respect to the majorization order. If the objective function \( \phi \) is Schur-convex, the maximum and the minimum are attained in \( x^*(S) \) and \( x_*(S) \) respectively; the opposite holds if \( \phi \) is a Schur-concave function. This enable us to solve problem (P) in a more direct way, avoiding the standard approach of Lagrange multipliers. In the next section we illustrate how the procedure above can be successfully applied to get upper and lower bounds for some relevant topological indices, which found applications in many fields varying from chemistry to network analysis.
2 Majorization and bounds for graph topological indices.

Let us firstly recall some basic graph notations and concepts to be used later. For more details refer to [8] and [10]. Let \( G = (V, E) \) be a simple, connected, undirected graph where \( V = \{v_1, ..., v_n\} \) is the set of vertices and \( E \subseteq V \times V \) the set of edges. We consider graphs with fixed order \( |V| = n \) and fixed size \( |E| = m \). Denote by \( \pi = (d_1, d_2, ..., d_n) \) the degree sequence of \( G \), where \( d_i \) is the degree of vertex \( v_i \), arranged in non increasing order \( d_1 \geq d_2 \geq \cdots \geq d_n \). It is well known that \( \sum_{i=1}^{n} d_i = 2m \) and that if \( G \) is a tree, i.e. a connected graph without cycles, \( m = n - 1 \). Let \( A(G) \) be the adjacency matrix of \( G \) and \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \) be the set of (real) eigenvalues of \( A(G) \). The matrix \( L(G) = D(G) - A(G) \) is called Laplacian matrix of \( G \), where \( D(G) \) is the diagonal matrix of vertex degrees. Let \( \mu_1 \geq \mu_2 \geq \cdots \geq \mu_n \) be the eigenvalues of \( L(G) \). The following properties of spectra of \( A(G) \) and \( L(G) \) are well known :

\[
\sum_{i=1}^{n} \lambda_i = 0; \quad \sum_{i=1}^{n} \lambda_i^2 = 2m; \\
\sum_{i=1}^{n} \mu_i = 2m; \quad \mu_1 \geq 1 + \frac{d_1}{n} \geq \frac{2m}{n}; \quad \mu_n = 0, \mu_{n-1} > 0.
\]

Notice that most of the topological indices of graphs are formulated by strictly Schur-convex (Schur-concave) functions of the degree sequence as well as the eigenvalues of \( A(G) \) or \( L(G) \). The corresponding bounds are generally expressed in terms of size and order of \( G \) but they can take also into account the degrees of one or more vertices of \( G \). With respect to the degree sequence, one of the most popular index is the General Randić index:

\[
R_\alpha(G) = \sum_{(v_i, v_j) \in E} (d_i d_j)^\alpha,
\]

where \( \alpha \) is a non zero real number (see [4]). Setting a specific value for \( \alpha \), some very well known indices can be obtained: for example, \( \alpha = 1 \) corresponds to the Zagreb index \( M_2(G) \) (see [19]) while \( \alpha = -\frac{1}{2} \) and \( \alpha = -1 \) to the branching indices (see [20]). In the recent paper [24], the sum-connectivity index has been proposed and in [6] it has been extended to the Generalized sum-connectivity index defined as follows:

\[
\chi_\alpha(G) = \sum_{(v_i, v_j) \in E} (d_i + d_j)^\alpha.
\]

Note that for \( \alpha = 1 \) we obtain the first Zagreb index \( M_1(G) = \sum_{v_i, v_j \in E} (d_i + d_j) = \sum_{v_i \in E} d_i^2 \). Other frequently used indices involve Schur-convex or Schur-concave functions of the eigenvalues of \( A(G) \) and \( L(G) \). We recall, among the others:

1. Energy index: \( E(G) = \sum_{i=1}^{n} |\lambda_i| \) ([9])
2. \( s_\alpha(G) = \sum_{i=1}^{n-1} \mu_i^\alpha, \alpha \neq 0, 1 \) ([15], [20])
3. Kirchhoff index $Kf(G) = n \sum_{i=1}^{n-1} \frac{1}{\mu_i} = ns_{-1}(G)$ \((\ref{23}, \ref{23})\)

4. Laplacian Estrada index $LEE(G) = \sum_{i=1}^{n} e^{\mu_i}$ \((\ref{22}, \ref{28})\)

In the next section we present theoretical results on upper and lower bounds for the indices previously mentioned, recovering well known bounds and improving, in some cases, the existing ones of the literature. We postpone to Section 3 some numerical examples.

2.1 General Randic index

The generalized Randic index can be equivalently expressed as:

$$R_\alpha(G) = \sum_{(v_i, v_j) \in E} (d_i d_j)^\alpha = \frac{1}{2} \left( \sum_{(v_i, v_j) \in E} (d_i^{\alpha} + d_j^{\alpha})^2 - \sum_{i=1}^{n} d_i^{2\alpha+1} \right).$$

Let $\pi = (d_1, d_2, \ldots, d_n)$ be a fixed degree sequence and $x \in \mathbb{R}^m$ be the vector whose components are $d_i^{\alpha} + d_j^{\alpha}$, with $(v_i, v_j) \in E$. Hence, taking into account that $\sum_{i=1}^{n} d_i^{2\alpha+1}$ is a constant, $R_\alpha(G)$ is a Schur convex function of the degree sequence of $G$ and it is minimal (maximal) if and only $f(x) = \sum_{i=1}^{m} x_i^2 = \|x\|_2^2$ is minimal (maximal). Extending the result proved in \cite{17}, it is possible to show that

$$\sum_{i=1}^{m} x_i = \sum_{(v_i, v_j) \in E} (d_i^{\alpha} + d_j^{\alpha}) = \sum_{i=1}^{n} d_i^{\alpha+1}$$

and thus $\sum_{i=1}^{m} x_i$ is a constant. Hence, considering a subset $S$ of $\Sigma_a \subseteq \mathbb{R}^m$, where $a = \sum_{i=1}^{n} d_i^{\alpha+1}$, which admits $x_*(S)$ and $x^*(S)$ as extremal vectors with respect to the majorization order, the function $f$ attains its minimum and maximum on $S$ at $f(x_*(S))$ and $f(x^*(S))$, respectively. The general Randic index can be consequently bounded as follows:

$$\frac{\|x_*(S)\|_2^2 - \sum_{i=1}^{n} d_i^{2\alpha+1}}{2} \leq R_\alpha(G) \leq \frac{\|x^*(S)\|_2^2 - \sum_{i=1}^{n} d_i^{2\alpha+1}}{2}. \tag{6}$$

Clearly different numerical bounds can be derived, if we characterize suitably the set $S$. The structure of $S$, among the typology of sets given in \cite{11,14}, will depend on the information available on the degree sequence of $G$.

For the particular case $\alpha = 1$, which corresponds to the Zagreb index $M_2$, this methodology was applied in \cite{7}, and, more recently, in \cite{2} where the authors get sharper bounds for the index $M_2$, valid for a particular class of graphs having exactly $h$ pendant vertices, i.e. vertices with degree one, with degree sequence

$$\pi = (d_1, \ldots, d_{n-h}, 1, \ldots, 1). \tag{7}$$

Starting from (6), the following results allow to compute the Randic index corresponding to a generic $\alpha$, for a class of graphs with $h$ pendant vertices and degree sequence given by \cite{7}. Let us
assume, furthermore, that the degree sequence $\pi$ is such that:

$$
\begin{align*}
1 + d_1^\alpha &\leq d_{n-h}^\alpha + d_{n-h-1}^\alpha & \text{for } \alpha > 0 \\
d_{n-h}^\alpha + d_{n-h-1}^\alpha &\leq 1 + d_1^\alpha & \text{for } \alpha < 0.
\end{align*}
$$

(8)

These conditions, always satisfied for $\alpha = -1$, assure that the $h$ components of $x$, corresponding to pendant nodes, are separated from the others. Moreover, since the components of $x$ are arranged in nonincreasing order, for $\alpha > 0$, they are assigned to the last $h$ positions of the vector $x$ while, for $\alpha < 0$, to the first $h$ positions of the vector $x$. Being interested in bounds for the branching indices associated to $\alpha = -\frac{1}{2}$ and $\alpha = -1$, in the sequel we only focus on negative values of $\alpha$. It is easy to see that the choice of a degree sequence equal to (7), combined with (5), lead us to face the following set of type (4):

$$
S = \{ x \in \mathbb{R}^m : 1 + d_1^\alpha \leq x_h \leq \cdots \leq x_1 \leq d_{n-h}^\alpha + 1, \\
d_2^\alpha + d_2^\alpha \leq x_m \leq \cdots \leq x_{h+1} \leq d_{n-h}^\alpha + d_{n-h-1}^\alpha, \quad (x, s^m) = \sum_{i=1}^{n} d_i^{\alpha+1} \}
$$

(9)

whose maximal and minimal elements with respect to the majorization order can be computed by corollaries 3 and 10 in [2]. Let us notice that both inequalities in (4) are attained if and only if the set $S$ reduces to a singleton. This is the case when $d_1 = d_{n-h}$, i.e. when all non pendant vertices have the same degree (see [2] for some significant examples).

2.2 Generalized sum-connectivity index

Let $\pi$ be a fixed degree sequence and $x \in \mathbb{R}^m$ be the vector whose components are $(d_i + d_j)$, $(v_i, v_j) \in E$. The function $f(x) = \sum_{i=1}^{m} x_i^\alpha$ is strictly Schur-convex for $\alpha > 1$ or $\alpha < 0$, while it is strictly Schur-concave for $0 < \alpha < 1$. Thus, taking into account that $\sum_{i=1}^{m} x_i = \sum_{i=1}^{n} d_i^\alpha$ is a constant, considering a subset $S$ of $\Sigma_a$, where $a = \sum_{i=1}^{n} d_i^\alpha$ for $\alpha > 1$ or $\alpha < 0$ we get

$$
\|x_*(S)\|_\alpha \leq \chi_a(G) \leq \|x^*(S)\|_\alpha,
$$

(10)

where $\|\|_\alpha$ stands for the $l_\alpha$-norm. For $0 < \alpha < 1$, the bounds are exchanged.

2.3 Energy index

Let us point out that $E(G) = \sum_{i=1}^{n} |\lambda_i| = \sum_{i=1}^{n} \sqrt{\lambda_i^2}$ and thus this index is a Schur-concave function of the variables $\lambda_i^2$, $i = 1, \cdots, n$. Furthermore $\sum_{i=1}^{n} \lambda_i^2 = 2m$. Let $x_i = \lambda_i^2$, $i = 1, \cdots, n$. It is well known that $\lambda_1 \geq \frac{2m}{n}$. If a sharper lower bound for $\lambda_1$ is available, i.e. $\lambda_1 \geq k(\geq \frac{2m}{n})$, we have $x_1 \geq k^2 \geq (\frac{2m}{n})^2 \geq \frac{2m}{n}$. The minimal element of the set

$$
S = \Sigma_a \cap \{ x \in \mathbb{R}^n : x_1 \geq k^2 \}
$$

where $a = 2m$, is given, using Corollary 14 in [2], by:

$$
x_*(S) = \left[ k^2, \frac{2m - k^2}{n-1}, \cdots, \frac{2m - k^2}{n-1} \right].
$$
Thus
\[ E(G) \leq k + \sqrt{(n-1)(2m-k^2)}. \]

In the case of bipartite graphs, since \( \lambda_1 = -\lambda_n \), we have \( x_1 = x_2 \) and thus we face the set
\[ S = \Sigma_a \cap \{ x \in \mathbb{R}^n : x_i \geq k^2, i = 1, 2 \} \]
whose minimal element becomes
\[ x_*(S) = \left[ k^2, k^2, \frac{2m^2 - 2k^2}{n-2}, \ldots, \frac{2m^2 - 2k^2}{n-2} \right] \]
and as a consequence
\[ E(G) \leq 2k + \sqrt{(n-2)(2m^2 - 2k^2)}. \]

For \( k = \frac{2m}{n} \) we get the bounds in [11] and [12], while for \( k = \frac{\sum_{i=1}^{n} d_i}{n} \) the bounds in [27]. Different choices of \( k \) allow to obtain all the other bounds in [16] and a new bound for \( E(G) \) as soon as a sharper lower bound of \( \lambda_1 \) is available.

### 2.4 Laplacian indices

1. Let \( s_\alpha(G) = \sum_{i=1}^{n-1} \mu_i^\alpha, \alpha \neq 0, 1 \) be the index given by the sum of the \( \alpha \)-th power of the non zero Laplacian eigenvalues and consider the set
\[ S = \Sigma_a \cap \{ \mu \in \mathbb{R}^{n-1} : \mu_1 \geq 1 + d_1 \} \]
where \( a = \sum_{i=1}^{n-1} \mu_i = 2m \) and \( \Sigma_a \subseteq \mathbb{R}^{n-1} \). Since \( \frac{2m}{n-1} \leq (1 + d_1) \), by Corollary 14 in [2] it follows that the minimal element of \( S \) is
\[ x_*(S) = \left[ 1 + d_1, \frac{2m - 1 - d_1}{n-2}, \ldots, \frac{2m - 1 - d_1}{n-2} \right]. \]

Taking into account the Schur-convexity or Schur-concavity of the functions \( s_\alpha(G) \), the bounds in [26], Theorem 3 can be easily derived. The same approach can be used to find the bounds for bipartite graphs given in [26], Theorem 5, observing that in this case \( \mu_1 \geq 2 \sqrt{\frac{\sum_{i=1}^{n} d_i^2}{n}} \).

The bounds in [26], Theorem 3 can be also improved taking into account further information on the localization of the eigenvalues. For instance, since \( \mu_2 \geq d_2 \) (see [4]), we can consider the set
\[ S = \Sigma_a \cap \{ \mu \in \mathbb{R}^{n-1} : \mu_1 \geq 1 + d_1, \mu_2 \geq d_2 \} \]
whose minimal element, computed applying Theorem 8 in [2], is given by
\[ x_*(S) = \left[ 1 + d_1, d_2, \frac{2m - 1 - d_1 - d_2}{n-3}, \ldots, \frac{2m - 1 - d_1 - d_2}{n-3} \right]. \]
Thus
\[
\begin{cases}
    s_\alpha(G) \geq (1 + d_1)^\alpha + d_2^\alpha + \frac{(2m-1-d_1-d_2)^\alpha}{(n-3)^{\alpha-1}} & \alpha > 1, \alpha < 0 \\
    s_\alpha(G) \leq (1 + d_1)^\alpha + d_2^\alpha + \frac{(2m-1-d_1-d_2)^\alpha}{(n-3)^{\alpha-1}} & 0 < \alpha < 1
\end{cases}
\] \tag{12}

2. Notice that bounds on the Kirchhoff index $K_f(G) = n \sum_{i=1}^{n-1} \frac{1}{\mu_i} = ns_{-1}(G)$ can be easily derived by bounds on $s_{-1}(G)$. In particular, using the set (11) we get
\[
K_f(G) \geq n \left( \frac{1}{1 + d_1} + \frac{1}{d_2} + \frac{(n-3)^2}{(2m-1-d_1-d_2)} \right). \tag{13}
\]

3. The Laplacian Estrada index $LEE(G) = \sum_{i=1}^{n} e^{\mu_i}$ is a Schur-convex function of the Laplacian eigenvalues. Thus, proceeding as before we can easily recover the bounds in [23], Remark 2. Furthermore, if we use the set (11), we find the bound:
\[
LEE(G) \geq 1 + e^{1+d_1} + e^{d_2} + (n-3)e^{\frac{2m-1-d_1-d_2}{n-3}}. \tag{14}
\]

3 Numerical examples

In this section we provide some numerical examples to illustrate our results and to show that, at least for the considered cases, we achieve sharper bounds with respect to recent literature.

i) General Randic index

Let us consider a tree $T$ with the degree sequence $\pi = (5, 3, 3, 3, 3, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1)$. We start exploring the Randic index $R(T)$, with $\alpha = -\frac{1}{2}$. The comparison (see Table 1) with bounds in [13] shows that bounds obtained by applying Corollary 3 and 10 in [2] always perform better:

| Ref. | Lower                        | Upper                        |
|------|------------------------------|------------------------------|
| [13] | 5.891249 (see Theorem 2.6)   | 7.486884 (see Theorem 2.24)  |
| [2]  | 6.768317                     | 7.064497                     |

Table 1: Lower and upper bounds for $R(T)$.  


For the case with $\alpha = -1$ and the tree $T$ with the same degree sequence, making a comparison with the result in [13], Theorem 3.7, we get

| Ref | Lower | Upper |
|-----|-------|-------|
| [13] | 1 | 4.888889 |
| [2]  | 3.2 | 3.666667 |

Table 2: Lower and upper bounds for $R_{-1}(T)$.

ii) Generalized sum-connectivity index

Let us consider a graph with degree sequence $\pi = (3, 2, 2, 1)$ and pick $\alpha = -5$. Since, in this case, $n$ is even, we make a comparison (see Table 3) between the results in [6] and those obtained from Corollary 3 in [2]. We can present here also the case when $n$ is odd, always choosing $\alpha = -5$. For a tree with the following degree sequence $\pi = (4, 4, 4, 3, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1)$, computing the bounds (see Table 4) we have:

| Ref. | Upper |
|------|-------|
| [6]  | $9.207015 \times 10^{-3}$ (see Theorem 1) |
| [2]  | $5.075226 \times 10^{-3}$ (see Corollary 3) |

Table 3: Upper bounds for $\chi_\alpha(G)$ with $n$ even.

For this index, making a comparison (see Table 5) between the result obtained by applying the lower bound obtained in equation (13) and the one derived from [25], Proposition 1, we have

| Ref. | Lower |
|------|-------|
| [25] | 12.5 |

Table 5: Lower bounds for $Kf(G)$. 

iii) Laplacian indices

Let us consider a graph whose degree sequence is $\pi = (3, 2, 2, 1)$.

a) Kirchhoff index

For this index, making a comparison (see Table 5) between the result obtained by applying the lower bound obtained in equation (13) and the one derived from [25], Proposition 1, we have

| Ref. | Lower |
|------|-------|
| [25] | 12.5 |

Table 5: Lower bounds for $Kf(G)$.
b) Laplacian Estrada index

In this case, we draw a comparison between the application of formula (14) and the result provided in [22], Proposition 3.4 (see Table 6)

| Ref | Lower |
|-----|-------|
| [22] | 59.90761 |
| formula (14) | 68.42377 |

Table 6: Lower bounds for \( LEE(G) \).

4 Conclusion

In this paper we present a unified approach for localizing some relevant graph topological indices, based on the optimization of Schur-convex or Schur-concave functions. Our results have been derived through the characterization of extremal vectors with respect to the majorization order, under suitable constraints. We have shown that classical results can be recovered and sometimes improved. Our theoretical approach paves the way to find new bounds, by taking advantage of further information that can be extracted from the graph \( G \), that allows us to define tighter sets \( S \) for performing the optimization problem. Finally, other topological indices can be localized whenever they can be expressed as Schur-convex or Schur-concave functions.

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