Extremal Representation for Non-diagonal Elements of Hermitian Matrix

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Abstract: The extremum representation for the non-diagonal element of Hermitian matrix through it's eigenvalues is presented in the paper. The expression for diagonal elements, corresponding to extreme non-diagonal elements, is obtained as well. There is an example of estimation for matrix eigenvalues by the use of non-diagonal elements.

Key words and phrases: eigenvalues problem, extremal representation, unitarily similar matrices, Hermitian matrix.
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It is known the following inequality for the spread of Hermitian matrix [1]:

$$\mathrm{S}(\mathbf{A}') \geq 2\left|A'_{ij}\right| \quad (i \neq j), \tag{1}$$

where $\mathrm{S}(\mathbf{A}') = \lambda_{\max} - \lambda_{\min}$ is the named spread; A'_{ij} in the right side is any non-diagonal element of given matrix. In this paper I make this result precise on the set of unitarily similar matrices

$$\mathbf{A}' = \boldsymbol{\beta}\mathbf{A}\boldsymbol{\beta}^*, \tag{2}$$

where $\boldsymbol{\beta}$ runs over the set of all unitary matrices; $\mathbf{A}$ is a given Hermitian matrix of the dimensionality n. Below, it was established that the left part of the inequality (1) is a precise upper bound of the right side under any $\boldsymbol{\beta}$. It was established as well, that if it holds next equality for the any non-diagonal element:

$$\mathrm{S}(\mathbf{A}') = 2\left|A'_{ij}\right|, \tag{3}$$

then corresponding diagonal elements are equal to

$$A'_{ii} = A'_{jj} = \frac{\lambda_{\max} + \lambda_{\min}}{2}. \tag{4}$$

In mechanics of rigid deformed bodies it is known the formula for extremal tangent stress at the given point of the body under various directions of

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elementary area, as well as the expression for normal stress on the area with extreme tangent stress. Similar relations were also obtained for shearing strain and stretch (refer to [2; §§5.16 and 6.5]). Named extremal relations, as a matter of fact, are the equalities (3) и (4) under $n = 3$. The expression (4) in the case of stress tensor **A** is written in the form

$$\sigma_n = \frac{\sigma_1 + \sigma_3}{2}$$

and let to obtain criteria of material's strength. Therefore, in the special case of $n = 3$ the result (4) is practically applicable.

The result (3) may be useful for evaluation of the eigenvalues of Hermitian matrices, that has been grounded at the end of this paper.

For what follows, it is convenient to renumber the eigenvalues of **A** so that $\lambda_1 = \lambda_{\max}$, $\lambda_2 = \lambda_{\min}$.

Theorem. For any non-diagonal element of the unitarily similar Hermitian matrix (2) we have an extremal representation:

$$\max_{\beta} \left| A'_{ij} \right| = \frac{\lambda_1 - \lambda_2}{2}, \tag{5}$$

where λ_1 is a maximum eigenvalue for matrix **A**; λ_2 is a minimum eigenvalue for this matrix. When the value $\left| A'_{ij} \right|$ reaches upper bound (5), there hold an equalities for diagonal elements:

$$A'_{ii} = A'_{jj} = \frac{\lambda_1 + \lambda_2}{2}. \tag{6}$$

Proof. By carrying out unitary transformation (2), one can attain a coincidence of any non-diagonal elements of initial and final matrices:

$$A'_{ij} = A_{rs}, \; i \neq j; \; r \neq s,$$

under following requirements for diagonal elements:

$$A'_{ii} = A_{rr}; \; A'_{jj} = A_{ss}.$$

Such transformation is attained by means of no more then two simple pivoting motions. A being of such transformation means that it is sufficient to prove the theorem under $i = 1$, $j = 2$.

We can also establish that there exists such unitary transformation, that

$$\mathbf{A}' = \left(\begin{array}{cc|c} \frac{\lambda_1 + \lambda_2}{2} & \frac{\lambda_1 - \lambda_2}{2} & \\ \frac{\lambda_1 - \lambda_2}{2} & \frac{\lambda_1 + \lambda_2}{2} & \mathbf{O} \\ \hline \multicolumn{2}{c|}{\mathbf{O}^{\mathrm{T}}} & \mathbf{\Lambda}_{n-2} \end{array} \right), \tag{7}$$

where block $\mathbf{\Lambda}_{n-2}$ is formed by eigenvalues of matrix **A**:

$$\mathbf{\Lambda}_{n-2} = \mathrm{diag}\{\lambda_3, \dots, \lambda_n\};$$

block **O** is zero rectangular matrix of corresponding dimensionality. One can obtain matrix (7) by two consequent transformations: in the beginning go over to main axises of matrix **A**, to get $\mathbf{A}' = \mathrm{diag}\{\lambda_1, \lambda_2, \lambda_3, \dots, \lambda_n\}$, and then execute simple pivoting motion by means of a matrix

$$\beta = \left(\begin{array}{cc|c} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} & \mathbf{O} \\ \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & \\ \hline \multicolumn{2}{c|}{\mathbf{O}^{\mathrm{T}}} & \mathbf{E}_{n-2} \end{array} \right),$$

where $\mathbf{E}_{n-2}$ is a unit matrix of an order specified by the index.

Thus, the set of unitarily similar matrices may be specified by a transform (2), where matrix **A** is the right part of expression (7).

It follows from the said that we can reformulate the theorem in following terms:

$$\max_{\beta} |A'_{12}| = \frac{\lambda_1 - \lambda_2}{2}, \tag{8}$$

where $\mathbf{A}'$ is obtained by unitary transform of matrix **A**, defined by (7). If upper bound is reached, then it holds:

$$A'_{11} = A'_{22} = \frac{\lambda_1 + \lambda_2}{2}. \tag{9}$$

To prove this statement we represent element A'_{12} by means of formula (2), where substitute the matrix **A** from the expression (7):

$$A'_{12} = \sum_{k,l=1}^{n} \beta_{1k}\beta^*_{2l} A_{kl} =$$

$$= (\beta_{11}\beta^*_{21} + \beta_{12}\beta^*_{22}) \frac{\lambda_1 + \lambda_2}{2} + (\beta_{12}\beta^*_{21} + \beta_{11}\beta^*_{22}) \frac{\lambda_1 - \lambda_2}{2} + \sum_{k=3}^{n} \beta_{1k}\beta^*_{2k}\lambda_k . \tag{10}$$

Orthogonality of a rows of matrix $\boldsymbol{\beta}$ means that

$$\beta^*_{2*}\beta_{1*} \equiv \beta_{11}\beta^*_{21} + \beta_{12}\beta^*_{22} + \sum_{k=3}^{n} \beta_{1k}\beta^*_{2k} = 0. \tag{11}$$

Consequently

$$A'_{12} = (\beta_{12}\beta^*_{21} + \beta_{11}\beta^*_{22}) \frac{\lambda_1 - \lambda_2}{2} + \sum_{k=3}^{n} \beta_{1k}\beta^*_{2k} \left(\lambda_k - \frac{\lambda_1 + \lambda_2}{2} \right);$$

$$|A'_{12}| \le |\beta_{12}\beta^*_{21} + \beta_{11}\beta^*_{22}| \frac{\lambda_1 - \lambda_2}{2} + \sum_{k=3}^{n} |\beta_{1k}\beta^*_{2k}| \cdot \left| \lambda_k - \frac{\lambda_1 + \lambda_2}{2} \right|. \tag{12}$$

Under chosen numbering of eigenvalues, we have:

$$-\frac{\lambda_1-\lambda_2}{2}\le\lambda_k-\frac{\lambda_1+\lambda_2}{2}\le\frac{\lambda_1-\lambda_2}{2},\quad k=\overline{3,n}. \tag{13}$$

By replacing of values $\lambda_k-\frac{\lambda_1+\lambda_2}{2}$ in the inequality (12) with the proper estimates from (13), we obtain:

$$|A'_{12}|\le\left(\left|\beta_{12}\beta^*_{21}+\beta_{11}\beta^*_{22}\right|+\sum_{k=3}^{n}\left|\beta_{1k}\beta^*_{2k}\right|\right)\frac{\lambda_1-\lambda_2}{2}. \tag{14}$$

For what follows, we introduce vectors

$$\mathbf{a}^{\mathrm{T}}=\left(|\beta_{12}|,|\beta_{11}|,|\beta_{13}|,\ldots,|\beta_{1n}|\right);\ \ \mathbf{b}^{\mathrm{T}}=\left(|\beta_{21}|,|\beta_{22}|,|\beta_{23}|,\ldots,|\beta_{2n}|\right).$$

These vectors have a unit Euclidean norm:

$$\|\mathbf{a}\|=\sqrt{\mathbf{a}^*\mathbf{a}}=1;\quad \|\mathbf{b}\|=\sqrt{\mathbf{b}^*\mathbf{b}}=1, \tag{15}$$

and, by using Cauchy-Schwartz inequality, we get an estimate for the expression in parentheses from the right part of (14):

$$(\ldots)\le\mathbf{a}^*\mathbf{b}\le\|\mathbf{a}\|\cdot\|\mathbf{b}\|=1. \tag{16}$$

Thus, value $|A'_{12}|$ can't be greater then $\frac{\lambda_1-\lambda_2}{2}$, though reaches it in accordance with expression (7). Therefore, equality (8) is proved.

Remark next. Since there hold inequalities (14) and (16), we see that if the value $|A'_{12}|$ reaches upper bound (8), then holds $\mathbf{a}^*\mathbf{b}=\|\mathbf{a}\|\cdot\|\mathbf{b}\|$, i.e. vectors $\mathbf{a}$ and $\mathbf{b}$ turn out to be collinear. Therefore, by taking into account the relations (15), we establish:

$$|\beta_{12}|=|\beta_{21}|;\ |\beta_{11}|=|\beta_{22}|;\ |\beta_{13}|=|\beta_{23}|;\ \ldots;\ |\beta_{1n}|=|\beta_{2n}|. \tag{17}$$

Equalities (9) are proved by means of relations for elements of matrix $\boldsymbol{\beta}$, ensuring the condition

$$|A'_{12}|=\frac{\lambda_1-\lambda_2}{2}. \tag{18}$$

We shall obtain these relations. We confine our consideration to the element A'_{11}. Likewise the formula (10), one can obtain:

$$A'_{11}=\sum_{k,l=1}^{n}\beta_{1k}\beta^*_{1l}A_{kl}=$$

$$=(\beta_{11}\beta^*_{11}+\beta_{12}\beta^*_{12})\frac{\lambda_1+\lambda_2}{2}+(\beta_{11}\beta^*_{12}+\beta_{12}\beta^*_{11})\frac{\lambda_1-\lambda_2}{2}+\sum_{k=3}^{n}\beta_{1k}\beta^*_{1k}\lambda_k. \tag{19}$$

In the beginning we consider the case of isolated eigenvalues λ_1 and λ_2, when

$$\lambda_2<\lambda_k<\lambda_1,\quad k=\overline{3,n}.$$

and therefore holds:

$$-\frac{\lambda_1-\lambda_2}{2}<\lambda_k-\frac{\lambda_1+\lambda_2}{2}<\frac{\lambda_1-\lambda_2}{2}, \quad k=\overline{3,n}. \tag{20}$$

In the case of

$$\sum_{k=3}^{n}\left|\beta_{1k}\beta_{2k}^{*}\right|>0, \tag{21}$$

from inequalities (20) and evaluation (12) we obtain a strict inequality (compare with (14)):

$$\left|A'_{12}\right|<\left(\left|\beta_{12}\beta_{21}^{*}+\beta_{11}\beta_{22}^{*}\right|+\sum_{k=3}^{n}\left|\beta_{1k}\beta_{2k}^{*}\right|\right)\frac{\lambda_1-\lambda_2}{2}.$$

As far as expression in parentheses does not exceed a unit, this inequality disagrees to condition (18). Consequently, the inequality (21) is impossible, and, by using the equalities (17), we establish:

$$\beta_{1k}=\beta_{2k}=0,\ k=\overline{3,n}. \tag{22}$$

Both inequalities (16) now become equalities, and we can see:

$$\left|\beta_{12}\beta_{21}^{*}+\beta_{11}\beta_{22}^{*}\right|=\left|\beta_{12}\right|\left|\beta_{21}\right|+\left|\beta_{11}\right|\left|\beta_{22}\right|=1.$$

Module of a sum of two complex numbers was discovered to be equal to a sum of their modules. Hence, main values of these numbers' arguments coincide:

$$\alpha\equiv\arg\left(\beta_{12}\beta_{21}^{*}\right)=\arg\left(\beta_{11}\beta_{22}^{*}\right).$$

By taking into consideration two first equalities (17), we come to forms:

$$\beta_{12}=\beta_{21}e^{i\alpha};\ \ \beta_{11}=\beta_{22}e^{i\alpha}. \tag{23}$$

By using the expressions (22), (23), we convert the scalar product (11) as follows:

$$\beta_{2*}^{*}\beta_{1*}=\beta_{11}\beta_{21}^{*}+\beta_{12}\beta_{22}^{*}=\beta_{11}\beta_{12}^{*}e^{i\alpha}+\beta_{12}\beta_{11}^{*}e^{i\alpha}=0.$$

Hence

$$\beta_{11}\beta_{12}^{*}+\beta_{12}\beta_{11}^{*}=0. \tag{24}$$

In formula (19) the first sum in parentheses is the norm of first row of matrix β, i.e.

$$\beta_{11}\beta_{11}^{*}+\beta_{12}\beta_{12}^{*}=1. \tag{25}$$

By substitution (22), (24) and (25) into the formula (19), we get required equality (8).

Let now in the set of eigenvalues $\lambda_3,\dots,\lambda_n$ one value is a greatest number λ_1, and one is a least number λ_2, i.e. under given numbers $r > 2$, $s > 2$ we have:

$$\begin{gathered}\lambda_r=\lambda_1;\ \lambda_s=\lambda_2;\\ \lambda_2<\lambda_k<\lambda_1,\ \text{if}\ \ k\neq 1,2,r,s.\end{gathered} \tag{26}$$

Let us generalize the proof of equalities (8) for this case. Instead of the estimate (12), now we have:

$$\left|A'_{12}\right| \le \left|\beta_{12}\beta^*_{21} + \beta_{11}\beta^*_{22} + \beta_{1r}\beta^*_{2r} - \beta_{1s}\beta^*_{2s}\right| \frac{\lambda_1 - \lambda_2}{2} + \sum_{\substack{k>2,\\ k\ne r,s}} \left|\beta_{1k}\beta^*_{2k}\right| \cdot \left|\lambda_k - \frac{\lambda_1 + \lambda_2}{2}\right|.$$

Under assuming that

$$\sum_{\substack{k>2,\\ k\ne r,s}} \left|\beta_{1k}\beta^*_{2k}\right| > 0,$$

we obtain in this case the strict inequality

$$\left|A'_{12}\right| < \left(\left|\beta_{12}\beta^*_{21} + \beta_{11}\beta^*_{22} + \beta_{1r}\beta^*_{2r} - \beta_{1s}\beta^*_{2s}\right| + \sum_{\substack{k>2,\\ k\ne r,s}} \left|\beta_{1k}\beta^*_{2k}\right| \right) \frac{\lambda_1 - \lambda_2}{2}. \qquad (27)$$

As before, in the case under consideration the relations (16) take place, but dots denote now the expression in parentheses from the formula (27). So the inequality (27) is impossible under the condition (18). Consequently

$$\beta_{1k} = \beta_{2k} = 0,\ k > 2, k \ne r,s, \qquad (28)$$

and under the condition (18) we obtain:

$$\begin{aligned} &\left|\beta_{12}\beta^*_{21} + \beta_{11}\beta^*_{22} + \beta_{1r}\beta^*_{2r} - \beta_{1s}\beta^*_{2s}\right| = \\ &= \left|\beta_{12}\right|\left|\beta_{21}\right| + \left|\beta_{11}\right|\left|\beta_{22}\right| + \left|\beta_{1r}\right|\left|\beta_{2r}\right| + \left|\beta_{1s}\right|\left|\beta_{2s}\right| = 1. \end{aligned} \qquad (29)$$

Here we can establish again an equality of addends' arguments in the first module:

$$\alpha \equiv \arg\left(\beta_{12}\beta^*_{21}\right) = \arg\left(\beta_{11}\beta^*_{22}\right) = \arg\left(\beta_{1r}\beta^*_{2r}\right) = \arg\left(-\beta_{1s}\beta^*_{2s}\right),$$

and instead of expressions (23) we get:

$$\beta_{12} = \beta_{21}e^{i\alpha};\ \ \beta_{11} = \beta_{22}e^{i\alpha};\ \ \beta_{1r} = \beta_{2r}e^{i\alpha};\ \ \beta_{1s} = -\beta_{2s}e^{i\alpha}. \qquad (30)$$

After substitution of equalities (28), (30) into the condition of orthogonality (11), we get the expression (compare with (24)):

$$\beta_{11}\beta^*_{12} + \beta_{12}\beta^*_{11} + \beta_{1r}\beta^*_{1r} - \beta_{1s}\beta^*_{1s} = 0. \qquad (31)$$

In this case the formula (19) is transformed to the form:

$$\begin{aligned} A'_{11} &= (\beta_{11}\beta^*_{11} + \beta_{12}\beta^*_{12})\frac{\lambda_1 + \lambda_2}{2} + (\beta_{11}\beta^*_{12} + \beta_{12}\beta^*_{11})\frac{\lambda_1 - \lambda_2}{2} + \beta_{1r}\beta^*_{1r}\lambda_r + \\ &+ \beta_{1s}\beta^*_{1s}\lambda_s = (\beta_{11}\beta^*_{11} + \beta_{12}\beta^*_{12} + \beta_{1r}\beta^*_{1r} + \beta_{1s}\beta^*_{1s})\frac{\lambda_1 + \lambda_2}{2} + \\ &+ (\beta_{11}\beta^*_{12} + \beta_{12}\beta^*_{11} + \beta_{1r}\beta^*_{1r} - \beta_{1s}\beta^*_{1s})\frac{\lambda_1 - \lambda_2}{2}. \end{aligned} \qquad (32)$$

The last expression is obtained by the substitutions:

$$\lambda_r = \frac{\lambda_1 + \lambda_2}{2} + \frac{\lambda_1 - \lambda_2}{2};\ \ \lambda_s = \frac{\lambda_1 + \lambda_2}{2} - \frac{\lambda_1 - \lambda_2}{2}.$$

If we make a substitution (31) into the last expression of formula (32), then, taking into account that the first row of matrix $\boldsymbol{\beta}$ is normalized by a unit, we obtain required equality (9).

We have considered the case when an order of both greatest and least eigenvalues is 2 (according to assumptions (26)). Cases of any other orders for these eigenvalues do not require special consideration because of their evidence.

Theorem is proved.

Besides of theoretical significance, the proved theorem can have practical interest for evaluation of the eigenvalues of Hermitian matrices. It follows from the theorem, that for the non-negatively definite matrix the greatest eigenvalue can't be less then double module of non-diagonal element:

$$\lambda_1 \geq 2\left|A_{ij}\right| \ (i \neq j) \text{ , if } \mathbf{A} \geq 0. \tag{33}$$

Besides, next estimate for the minimum eigenvalue follows from the proved theorem:

$$\lambda_2 \leq \lambda_1 - 2\left|A'_{ij}\right| \ (i \neq j). \tag{34}$$

This estimate might be useful for badly conditioned positively definite matrices, because algorithms of eigenvalues' calculation for such matrices lose stability if any eigenvalue is close to zero [3].

Example. Give the estimates of values λ_1, λ_2 for non-negatively definite matrix

$$\mathbf{A} = \begin{pmatrix} 5 & 1 & -2 & 4 \\ 1 & 4 & 1 & 1 \\ -2 & 1 & 3 & -2 \\ 4 & 1 & -2 & 4 \end{pmatrix}.$$

Since for the Hermitian matrix $\lambda_1 \geq A_{ii}$, in given case we have $\lambda_1 \geq 5$. Known relation for Euclidean norm of a matrix gives more strong estimate:

$$\lambda_1 \geq \frac{\|\mathbf{A}\|_E}{\sqrt{n}} = 5.48 .$$

From the relation (33) we obtain $\lambda_1 \geq 8$.

By solving the characteristic equation for given matrix one can get the following eigenvalues: $\lambda_1 = 9.87$, $\lambda_2 = 0.42$. Known estimate $\lambda_2 \leq A_{ii}$ holds in given case $\lambda_2 \leq 3$. By means of formula (34) we can estimate this eigenvalue more precisely: $\lambda_2 \leq 1.87$. Without exact value λ_1 we also can use formula (34) together with evaluation $\lambda_1 \leq \|\mathbf{A}\|_E = 10.96$. We obtain: $\lambda_2 \leq \|\mathbf{A}\|_E - 2\left|A'_{ij}\right| \leq 2.96$.

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THE ABSTRACT

A.I. Rusakov. Extremal Representation for Non-diagonal Elements of Hermitian Matrix.

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