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OPTIMAL PLANE ROTATIONS FOR COMPLEX MATRICES

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1. Introduction

By the classical Jacobi method, applied to a symmetric matrix $A \in R^{n\times n}$ we obtain the unitary matrix U of the eigenvector of A as a product of plane rotations, while U^*AU proves to be diagonal. It is evident trying to extend this method to the complex non-Hermitian case, i.e. to find for $A \in C^{n\times n}$ as a product of complex plane rotations with maximum diagonal $\sum_{i=1}^{n} \mid U^*AU_{ii} \mid^2$.

Suppose that we are going to compute the optimal rotation in the i, j plane. This means that we have to do with the 2×2 matrix

$$\begin{bmatrix} a_{ii} & a_{ij} \\ a_{ji} & a_{jj} \end{bmatrix} \tag{1}$$

Thus we can restrict our investigations in Theorem 1 to 2×2 matrices. We use the following simplifying notation:

$$\begin{bmatrix} a_1 & b \\ c & a_2 \end{bmatrix} = \begin{bmatrix} a_{ii} & a_{ij} \\ a_{ji} & a_{jj} \end{bmatrix} \tag{2}$$

Our basic result is Theorem 1, giving the maximum possible increase (7) of the difference (3). (See also (11), the analogue to (7) in the general case). The formulae (6) - (10) for the maximum increase as well as for the optimal variables are expressed in terms of two real, three-dimensional vectors.

The matrix $B = U^*AU$, obtained in the course of complex plane rotations is, generally speaking, no more diagonal, but has a special structure: we refer to it, starting from [1], as a Δ^*H-matrix. We prove the result in [1] (that complex matrices having maximal diagonal with regard to complex plane rotations are exactly the Δ^*H-matrices) on the basis of (7), see Theorem 2.

Unfortunately, even the normal matrices cannot be diagonalized in this way, or equivalently: the normal Δ^*H-matrices are not necessarily diagonal. To illustrate this, a family of normal, nondiagonal Δ^*H-matrices is given (c.f. [2,p.237, Problem 10]).

2. Maximizing the diagonal of 2×2 matrices.

Let $A \in C^{2\times 2}$ be arbitrary, $U \in C^{2\times 2}$be unitary, and $\hat{A} = U^*AU$, where

$$A = \begin{bmatrix} a_1 & b \\ c & a_2 \end{bmatrix}, \; U = \begin{bmatrix} x & -\bar{y} \\ y & \bar{x} \end{bmatrix}, \; \hat{A} = \begin{bmatrix} \hat{a}_1 & \hat{b} \\ \hat{c} & \hat{a}_2 \end{bmatrix},$$

and $| x |^2 + | y |^2 = 1$.

We seek for that $x, y \in C$, for which $| b |^2 + | c |^2$ is minimum, or, equivalently, $| \hat{a}_1 |^2 + | \hat{a}_2 |^2$ is maximum. The equivalence is garanteed by $\| \hat{A} \|^2 = \| A \|^2$, where $\| \cdot \|$ denotes the Euclidean norm. Thus, the increase of the diagonal sum $| a_1 |^2 + | a_2 |^2$, due to x, y is equal to

$$\delta(x,y) = | \hat{a}_1 |^2 + | \hat{a}_2 |^2 - (| a_1 |^2 + | a_2 |^2) = | b |^2 + | c |^2 - (| \hat{b} |^2 + | \hat{c} |^2) \tag{3}$$

In the symmetric case $A = A^*$ we have $\hat{b}_{opt} = \hat{c}_{opt} = 0$ and $\max \delta(x,y) = 2 | b |^2$. Now, in the general case, we express the increase in terms of x, y.

Lemma 1.

$$\delta(x,y) = 2 | f(x,y) |^2 - | a_1 - a_2 |^2 /2, \quad \text{where}$$
$$f(x,y) = (a_1 - a_2)(| x |^2 - 1/2) + b\bar{x}y + cx\bar{y}.$$

Proof: In view of the trace equality $\hat{a} + \hat{a}_2 = a_1 + a_2$ we have

$$| \hat{a}_1 |^2 + | \hat{a}_2 |^2 = | \hat{a}_1 |^2 + | a_1 + a_2 - \hat{a}_1 |^2 = 2 | \hat{a}_1 - (a_1 + a_2)/2 |^2 + | a_1 + a_2 |^2 /2$$
$$= | (a_1 - a_2)(| x |^2 - | y |^2)/2 + b\bar{x}y + cx\bar{y} |^2 + | a_1 + a_2 |^2 /2.$$

Finally, use $| x |^2 + | y |^2 = 1$ to get the result.

Remark 1. We can assume, that x is real and nonnegative. Indeed, if $\hat{x} = x \cdot sgn(\bar{x}), \hat{y} = y \cdot sgn(\bar{x})$, then $\delta(\hat{x}, \hat{y}) = \delta(x,y)$. Moreover,

$$x^2 \geq 1/2 \tag{4}$$

can also be assumed. To this end introduce, if necessary, $\hat{x} = | y |, \hat{y} = = -xy/ | y |$. Then $f(\hat{x}, \hat{y}) = -f(x,y)$, and $\delta(\hat{x}, \hat{y}) = \delta(x,y)$. Thus, the increase due to x, y is given by

$$\delta(x,y) = 2 | (a_1 - a_2)(x^2 - 1/2) + bxy + cx\bar{y} |^2 - | a_1 - a_2 |^2 /2 \tag{5}$$

Let us introduce the following real vectors:

$$p = \begin{bmatrix} Re(a_1 - a_2) \\ Re(b + c) \\ Im(c - b) \end{bmatrix}, q = \begin{bmatrix} Im(a_1 - a_2 \\ Im(b + c) \\ Re(b - c) \end{bmatrix}, w = \begin{bmatrix} x^2 - 1/2 \\ x \; Re \; y \\ x \; Im \; y \end{bmatrix} \tag{6}$$

We can now solve the maximum diagonal problem is terms of p and q.

Theorem 1. The maximum of $\delta(x, y)$, subject to $x \geq 1\sqrt{2}, y \in C$, and $x^2 + \mid y \mid^2 = 1$ is (c.f. (3) and (5)):

$$\delta = 1/4\{2(\mid b \mid^2 + \mid c \mid^2) - \mid a_1 - a_2 \mid^2 + \mid (a_1 - a_2)^2 + 4bc \mid\} \tag{7}$$

As for the optimal variables, see (6), (8), (9) and (10).

Remark 2. Denote by λ_1, λ_2 the eigenvalues of A. Comparising the different forms for the discriminant of A yields:

$$\mid \lambda_1 - \lambda_2 \mid^2 = \mid disA \mid = \mid (a_1 - a_2)^2 + 4bc \mid .$$

Thus, applying equality $a_1 + a_2 = \lambda_1 + \lambda_2$ we get the equivalent form

$$\delta = 1/2\{\mid b \mid^2 + \mid c \mid^2 + \mid \lambda_1 \mid^2 + \mid \lambda_2 \mid^2 - \mid a_1 \mid^2 - \mid a_2 \mid^2\}, \tag{7'}$$

being more suitable for generalizations.

Proof: The chain of equivalent problems, listed below, results in a 2×2 eigenvalue-problem, being easily solvable. The first problem to be solved is (see Lemma 1 and Remark 1):

(P1)

$$max \mid (a_1 - a_2)(x^2 - a/2) + bxy + cx\bar{y} \mid^2; x \geq 1/\sqrt{2}, y \in C, x^2 + \mid y \mid^2 = 1.$$

$$(Hint : Re\; f(x, y) = p^T w,\; Im\; f(x, y) = q^T w, \text{ hence}$$
$$\mid f(x, y) \mid^2 = (p^T w)^2 + (q^T w)^2 = w^T (pp^T + qq^T) w,$$
$$\text{and } \| w \|^2 = (x^2 - 1/2)^2 + x^2 \mid y \mid^2 = 1/4).$$

$(P2)$ $$max\; w^T (pp^T + qq^T) w, w \in \mathcal{R}, \| w \| = 1/2.$$

$(P3)$ $$(pp^T + qq^T) w = \lambda w, \lambda \to max, \| w \| = 1/2.$$

$$(P4)\quad \begin{bmatrix} \| p \|^2 & p^T q \\ p^T q & \| q \|^2 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \lambda \begin{bmatrix} \alpha \\ \beta \end{bmatrix}, \lambda \to max, w = \alpha p + \beta q, \| w \| = 1/2.$$

The larger root of the characteristic equation

$$det \begin{vmatrix} \| p \|^2 - \lambda & p^T q \\ p^T q & \| q \|^2 - \lambda \end{vmatrix} = 0$$

is equal to

$$= 1/2\{\| p \|^2 + \| q \|^2 + ((\| p \|^2 - \| q \|^2)^2 + (2p^T q)^2)^{1/2}\} \tag{8}$$

With the optimal variables, from (P3) we have $| f(x,y) |^2 = w^T(pp^T + qq^T)w = \lambda \| w \|^2 = \lambda/4$, thus by Lemma 1:

$$\delta(x,y) = 2 \mid f(x,y) \mid^2 - \mid a_1 - a_2 \mid^2 /2 = (\lambda - \mid a_1 - a_2 \mid^2)/2,$$

and in view of (8),

$$4\delta(x,y) = \| p \|^2 + \| q \|^2 + ((\| p \|^2 - \| q \|^2)^2 + (2p^T q)^2)^{1/2} - 2 \mid a_1 - a_2 \mid^2$$

Use now the indentitites

$$Re\ uv = Re\ u\ Re\ v - Im\ u\ Im\ v,$$

$$Im\ uv = Re\ u\ Im\ v + Im\ u\ Re\ v$$

to get

$$\| p \|^2 + \| q \|^2 = \mid a_1 - a_2 \mid^2 + 2(\mid b \mid^2 + \mid c \mid^2),$$

$$\| p \|^2 - \| q \|^2 = Re((a_1 - a_2)^2 + 4bc),$$

$$2p^T q = Un((a_1 - a_2)^2 + 4bc),$$

showing that (7) is true.

Determine the optimal vector w, as the solution of (P4). If $b = c = 0$, then there is no increase (see (7)), and hence $w = (1/2, 0, 0)^T$ can be taken.

(This corresponds to $x = 1, y = 0$ i.e. $U = I$. If $|b|^2 + |c|^2 \neq 0$, then $\|p\|^2 + \|q\|^2 \neq 0$ also is valid. The formulae for w are (apart from normalizing):

$$\begin{aligned}
a)\ p^T q = 0 :\ & a0)\ \|p\| = \|q\|: w = \alpha p + \beta q = 0 \text{ arbitrary} \\
& a1)\ \|p\| > \|q\|: w = p \\
& a2)\ \|p\| < \|q\|: w = q \\
b)\ p^T q \neq 0 :\ & b1)\ \|p\| \geq \|q\|: w = (\lambda - \|q\|^2)p + p^T q \cdot q \\
& b2)\ \|p\| < \|q\|: w = p^T q \cdot q + (\lambda - \|p\|^2)q
\end{aligned} \tag{9}$$

After this, w is to be normalized in accordance with

$$\|w\| = 1/2; \quad w_1 \geq 0.$$

Finally, x and y can be determined as:

$$x = (w_1 + 1/2)^{1/2}, \quad y = (w_2 + iw_3)/x. \tag{10}$$

Remark 3. The generic formulae b1) and b2) in (9) are - after normalizing - identical. We distiguished between them only for the sake of numerical stability. For the same reason we propose to apply the power method to the matrix in (P4) for determining w.

Remark 4. The Hermitian case is included in a1). (Note, that in this case not only $p^T q = 0$, but $q = 0$ also holds). From (7) we have $\delta = 2|b|^2$, which is identical with the maximum possible increase in the case $A = A^*$. Therefore, in view of the restriction $x \geq 1/\sqrt{2}$, the classical Jacobi method, and the Jacobi-like method based on Theorem 1 are in case of Hermitian matrices identical!

For completeness, we describe the k-th iteration step of this Jacobi-like method, omitting for simplicity the index k. Note that the maximum increase δ_{ij} in the i,j plane can be determined from (7) taking into account (2).

The Jacobi-like iteration step:

Determine the indices i,j from

$$\begin{aligned}
\delta &= 1/4\{2(|a_{ij}|^2 + |a_{ji}|^2) - |a_{ii} - a_{jj}|^2 + |(a_{ii} - a_{jj})^2 + 4a_{ij}a_{ji}|\} \\
&= max\{\delta_{i'j'}; 1 \leq i' < j' \leq n\},
\end{aligned} \tag{11}$$

and execute a rotation $A \to U^*AU$ in the i,j plane with

$$U = U_{ij}(x,y) = \begin{array}{cc} \begin{array}{cccc} & i, & j & \end{array} & \\ \begin{bmatrix} 1 & & & \\ & x & -\bar{y} & \\ & y & x & \\ & & & 1 \end{bmatrix} & \begin{array}{c} \\ i \\ j \\ \\ \end{array} \end{array} \qquad (12)$$

where x and y are given by (6), (8), and (10), c.f. (2).

3. Characterization of the plane rotation-optimal matrices

The above theorem enables us to characterize the 2×2 matrices, for which the sum $| a_1 |^2 + | a_2 |^2$ cannot be increased, i.e. $\delta(x,y) = 0$ is local maximum. In this way we obtain a new proof for [1, Th. 6]. We need the following concepts.

Definition 1. [1, Def. 1.] $A \in C^{n \times n}$ is a ΔH-matrix, iff

$$a_{ij} = h_{ij}(a_{ii} - a_{jj}), \ \ h_{ij} = \bar{h}_{ji} \ \text{ for } \ i \neq j.$$

For brevity we use the following notation:

Definition 2. $A \in C^{n \times n}$ is a $\Delta^* H$-matrix, iff A is ΔH-matrix, and

$$| h_{ij} | \leq 1/2, \ \ 1 \leq i \neq j \leq n.$$

In order to emphasize, that increasing can only be realized via plane rotations, we introduce the following definition:

Definition 3. $A \in C^{n \times n}$ is plane rotation-optimal, or, in a word: pro-optimal, iff for every plane rotation $U = u_{ij}(x,y) \in C^{n \times n}$ of the form (12) we have $\sum_{i=1}^{n} | \hat{a}_{ii} |^2 \leq \sum_{i=1}^{n} | a_{ii} |^2$, where $\hat{A} = U^* A U = (\hat{a}_{ij})$.

Theorem 2. [1, Th. 6.] $A \in C$ is pro-optimal, iff A is $\Delta^* H$-matrix.

Proof: Note that both properties can be "decomposed into properties of second order", more precisely A is pro-optimal (or: A is $\Delta^* H$-matrix), iff its any block of the form (1) is pro-optimal (or: $\Delta^* H$-matrix). Therefore it is sufficient to prove the theorem for $n = 2$. We use again the simple notation (2).

Necessity: First we rewrite the definition of $\Delta^* H$ in terms of the matrix elements. In view of Definition 2 we become that

$$b = (a_1 - a_2)h, \quad c = (a_2 - a_1)h, \quad | h | \leq 1/2 \tag{13}$$

is equivalent to

$$| b | = | c |, \quad bc = -\epsilon^2 | b |^2, \quad 4 | b |^2 \leq | a_1 - a_2 |^2, \tag{13'}$$

where $\epsilon = sgn(a_1 - a_2)$.

Let now A be pro-optimal, i.e. $\delta = max\delta(x, y) = 0$ (see (7)). The inequality $| (a_1 - a_2)^2 + 4bc | \geq | a_1 - a_2 |^2 - 4 | bc |$ implies

$$0 = \delta \geq (| b | - | c |)^2/2,$$

giving $| b | = | c |$. From $\delta = 0$ we immediately have $4 | b |^2 \leq | a_1 - a_2 |^2$. Finally, from $\delta = 0$ again, it follows that

$$| a_1 - a_2 |^2 - 4 | b |^2 = | (a_1 - a_2)^2 + 4bc | = | \epsilon^2 | a_1 - a_2 |^2 + 4bc | =$$

$$|| a_1 - a_2 |^2 + \bar{\epsilon}^2 bc |,$$

whence by the "equality part" of the triangle inequality we have

$$\hat{\epsilon}^2 bc = - | b |^2, \quad i.e.\ bc = -\epsilon^2 | b |^2 .$$

Sufficiency: Let A be $\Delta^* H$-matrix, i.e. it holds (13). Then the maximum possible increase of the diagonal, multiplied by 4 is:

$$\begin{aligned} 4\delta &= 2(| b |^2 + | c |^2) - | a_1 - a_2 |^2 + | (a_1 - a_2)^2 + 4bc | \\ &= 4 | a_1 - a_2 |^2 | h |^2 - | a_1 - a_2 |^2 + | (a_1 - a_2)^2 + 4(a_1 - a_2)^2 | h |^2 | \\ &= | a_1 - a_2 |^2 (4 | h |^2 - 1) + | a_1 - a_2 |^2 | 1 - 4 | h |^2 | = 0, \text{ q.e.d.} \end{aligned}$$

Example: We give an example for normal, pro-optimal matrices without being diagonal. First consider the following problem: "Problem [2,p.237]: Let $A = (a_{k\ell}) \in C^{n \times n}$ be the normal matrix with

$$a_{k\ell} = \begin{cases} -(n-2)/2e^{2ij_k}, & \ell = k, \\ e^{i(j_k + j_\ell)}, & \ell \neq k, \end{cases}$$

where $\gamma_p = (p-1)\pi/n, 1 \le p \le n$. Prove that, for $n \ge 6$ there is no complex analogue of the classical Jacobi method, which decreases the square sum of the moduli of the nondiagonal elements."

Denote the above defined matrix by A_n. In light of the above theorem, we have to show that A_n is $\Delta^* H$-matrix for $n \ge 6$. Indeed, using (13'), a direct calculation leads to the result that A_n is ΔH-matrix for every $n > 2$, moreover, A_n is $\Delta^* H$-matrix, iff $\cos\,(2(j_k - j_\ell)) \le 1 - 8/(n-2)^2, 1 \le k \ne 1 \le n$, i.e. A_n is $\Delta^* H$-matrix, iff $\cos(2\pi/n) \le 1 - 8/(n-2)^2$.

This inequality is fulfilled for $n \ge 6$, specially for $n = 6$ the equality is true. Thus, the statement of [2] is proved: the matrices $A_n, n \ge 6$ are pro-optimal, therefore cannot be increased by any complex plane rotations.

Finally, we refer to an interesting phenomenon: In the practice the Jacobi-like method applied to A_n converges after all to the diagonal matrix of the eigenvalues! This is true, of course, only owing to the rounding errors. Nevertheless this means that, the local maximum of the diagonal sum $\sum_{i=1}^{n} | a_{ii} |^2$ is for some pro-optimal matrices fairly instable, and a little perturbation - due to the rounding errors - leads to the global maximum. It is worth noting that for determining the vector w, we applied the power method (the von Mises iteration) instead of the formulae (9).

Further informations on the normal $\Delta^* H$-matrices and a list of references can be found in [3].

Summary

Complex square matrices having maximal diagonal with regard to plane rotations can be characterized by means of their 2×2 blocks [1]. Here we give explicite formulae for the optimal plane rotations needed to maximizing the diagonal (Theorem 1). This enables us to give an alternative proof for [1; Th. 6], see Theorem 2. Finally, an example for normal matrices will be given.

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