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ON THE OPTIMALITY OF A CLASS OF ΔH MATRICES

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We derive a necessary condition for optimality of **ΔH**-1 matrices in $\mathbf{C}_{n\times n}$, which are defined in section 2. We show that for $n = 3$ this condition is also sufficient, and we state a conjecture for $n > 3$.

1. ΔH MATRICES

According to [2], a **ΔH** matrix is a matrix which can be written as

$$\mathbf{G} = \mathbf{D} + \mathbf{DH} - \mathbf{HD} \tag{1.1}$$

where: $\mathbf{D} = \mathrm{diag}(d_1,\ d_2,\ \ldots\ ,d_n)$ is a diagonal matrix and $\mathbf{H}$ is hermitean: $\mathbf{H}^* = \mathbf{H}$. An equivalent notation for $\mathbf{G}$ is

$$\mathbf{G} = \mathbf{D} + \mathbf{DH} - \mathbf{HD} \qquad\qquad \mathbf{G} = [d_k; h_{kj}(d_k - d_j)]_1^n \tag{1.2}$$

where $h_{kj}(d_k - d_j)$, $k \neq j$, are the off-diagonal entries.

For a matrix $\mathbf{A} \in \mathbf{C}_{n\times n}$ let us consider the optimisation problems

(*) $\max \left\| \mathrm{Diag}\ \mathbf{TAT}^* \right\|$; $\mathbf{TT}^* = \mathbf{E}$ (i.e., $\mathbf{T}$ is unitary)

and

(**) $\min \left\| \mathbf{A} - \mathbf{Z} \right\|$; $\mathbf{ZZ}^* - \mathbf{Z}^*\mathbf{Z} = \mathbf{0}$ (i.e., $\mathbf{Z}$ is normal)

Here $\mathrm{Diag}(\mathbf{A}) = \mathrm{diag}\left(a_{11}, a_{22},\ \ldots\ , a_{nn}\right)$ and $\left\|\mathbf{A}\right\| = \left(\sum_{k,j=1}^{n} \left| a_{kj} \right|^2 \right)^{1/2}$ is the Frobenius norm of the matrix $\mathbf{A}$.

These problems involve **ΔH** matrices: if a diagonal matrix **D** is a stationary point for problem (**) of the best normal approximation, then **A** must be a **ΔH** matrix with $\mathrm{Diag}\left(\mathbf{A}\right) = \mathbf{D}$ (Theorem 3 in [2]). On the other hand, for a **ΔH** matrix **A**, the identity matrix **E** is a stationary point for problem (*); the converse is not always true, but it holds when **E** is a second-order stationary point. When only global extrema are considered, then problems (*) and (**) are always equivalent (Theorem 5 in [1] and Theorem 1 in [2]).

If **E** is a global solution to (*) and/or **D** is a global solution to (**), then **A** must be a **ΔH** matrix: $\mathbf{A} = \mathbf{G} = \mathbf{D} + \mathbf{DH} - \mathbf{HD}$; in our previous papers we called it an *optimal* **ΔH** matrix. In the case $n = 2$, optimality means (Theorem 5 in [2]) that **G** has the form

$$\mathbf{G} = \begin{bmatrix} d_1 & h_{12}\left(d_1 - d_2\right) \\ h_{21}\left(d_2 - d_1\right) & d_2 \end{bmatrix}; \quad h_{12} = \bar{h}_{21}; \quad \left|h_{12}\right| \leq \frac{1}{2} \tag{1.3}$$

and is equivalent to the second-order stationary point condition.

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ΔH matrices also occur as limit points of a Jacobi sequence $\{\mathbf{A}_n\}$, where the initial matrix $\mathbf{A}_0 \in \mathbf{C}_{n\times n}$ is an arbitrary (normal or non-normal) matrix (Theorem 3 in [9]).

We will now state the second order optimality condition for problem (**) when the solution to the problem is a diagonal matrix **D**. We consider the general case, when not all diagonal entries of **D** are distinct, i.e. $d_k = d_j$ for $k \neq j$ is allowed. Let

$$I_D = \{(k,j); d_k = d_j\} \tag{1.4}$$

Clearly, the pairs $\{(k,k)\}$ belong to the set I_D. The second order optimality condition is (Theorem 2 in [5]):

$$G(\mathbf{Z}) = \sum_{k,j=1}^{n} \left| z_{kj} \right|^2 \cdot \left| d_k - d_j \right|^2 - \frac{1}{2} \sum_{k,l,j=1}^{n} h_{kj} \left(z_{lk}\overline{z}_{lj} + z_{jl}\overline{z}_{kl} \right) \begin{vmatrix} \overline{d}_k & d_k & 1 \\ \overline{d}_l & d_l & 1 \\ \overline{d}_j & d_j & 1 \end{vmatrix} -$$
$$- \frac{1}{2} \sum_{(k,j)\in I_D} \left| \sum_{l=1}^{n} \left(h_{kl} z_{lj} + h_{lj} z_{kl} \right) \left(d_k - d_l \right) \right|^2 - \frac{1}{2} \sum_{(k,j)\in I_D} \left| \sum_{l=1}^{n} \left(h_{kl} z_{lj} + h_{lj} z_{kl} \right) \left(\overline{d}_k - \overline{d}_l \right) \right|^2 \geq 0 \tag{1.5}$$

for all $\left[z_{kj} \right]_1^n = \mathbf{Z} \in \mathbf{C}_{n\times n}$, i.e., the hessian $G(\mathbf{Z})$ is positive semi- definite on $\mathbf{C}_{n\times n}$.

2. ΔH-1 MATRICES IN $\mathbf{C}_{n\times n}$

A **ΔH-1** matrix in $\mathbf{C}_{n\times n}$ is a matrix of the form

$$\mathbf{G} = \begin{bmatrix} d_1 & h_{12}(d_1 - d_2) & h_{13}(d_1 - d_2) & \cdots & h_{1n}(d_1 - d_2) \\ h_{21}(d_2 - d_1) & d_2 & 0 & \cdots & 0 \\ h_{31}(d_2 - d_1) & 0 & d_2 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ h_{n1}(d_2 - d_1) & 0 & 0 & \cdots & d_2 \end{bmatrix}; \quad h_{1k} = \overline{h}_{k1} \tag{2.1}$$

with $d_1 \neq d_2$. Because

$$d_1 \neq d_2 = d_3 = \ldots d_n \tag{2.2}$$

D could be viewed as a non trivial “maximal” degenerate diagonal matrix.

Theorem 1. *For a* **ΔH-1** *matrix* (2.1), *condition* (1.5) *is equivalent to*

$$\|h\| = \left(\sum_{k=2}^{n} \left| h_{1k} \right|^2 \right)^{1/2} \leq \frac{1}{2}; \quad h = \left(h_{12}, h_{13}, \ldots, h_{1n} \right). \tag{2.3}$$

Proof**.** First, for a **ΔH-1** matrix all determinants in (1.5) are zero and, on the other hand,

$$I_D = \{ \, (k,j) \; ; \; k,j = 2,\ldots \, , \; n \} \tag{2.4}$$

so the hessian becomes

$$
\begin{aligned}
G(\mathbf{Z}) &= |d_1 - d_2|^2 \left[\sum_{k=2}^{n} |z_{1k}|^2 + \sum_{k=2}^{n} |z_{k1}|^2 - 2 \sum_{k,j=2}^{n} \left| h_{k1} z_{1j} + h_{1j} z_{k1} \right|^2 \right] = \\
&= g\left(z_{12}, \dots, z_{1n};\ z_{21}, \dots, z_{n1}\right) = \\
&= g_1\left(z_{12}, \dots, z_{1n};\ z_{21}, \dots, z_{n1}\right) - g_2\left(z_{12}, \dots, z_{1n};\ z_{21}, \dots, z_{n1}\right)
\end{aligned}
\tag{2.5}
$$

with

$$
\begin{aligned}
& g_1\left(z_{12}, \dots, z_{1n};\ z_{21}, \dots, z_{n1}\right) = \\
&= |d_1 - d_2|^2 \left[\sum_{k=2}^{n} |z_{1k}|^2 + \sum_{k=2}^{n} |z_{k1}|^2 - 2 \sum_{k,j=2}^{n} |h_{k1}|^2 |z_{1j}|^2 - 2 \sum_{k,j=2}^{n} |h_{1j}|^2 |z_{k1}|^2 \right] = \\
&= |d_1 - d_2|^2 \left[\left(1 - 2\|h\|\right)^2 \left(\sum_{k=2}^{n} |z_{1k}|^2 + \sum_{k=2}^{n} |z_{k1}|^2 \right) \right]
\end{aligned}
\tag{2.6}
$$

and

$$
g_2\left(z_{12}, \dots, z_{1n}; z_{21}, \dots, z_{n1}\right) = 2|d_1 - d_2|^2 \left[\sum_{k,j=2}^{n} \bar{h}_{1k} \bar{h}_{1j} z_{1j} \bar{z}_{k1} + \sum_{k,j=2}^{n} h_{1j} h_{1k} z_{k1} \bar{z}_{1j} \right]
\tag{2.7}
$$

Associated with the form $g\left(z_{12}, \dots, z_{1n}; z_{21}, \dots, z_{n1}\right)$, except for the positive factor $|d_1 - d_2|^2$, is the hermitean matrix

$$
\Omega_1(h) = \begin{bmatrix} \left(1 - 2\|h\|^2\right)\mathbf{E} & -2h^*\bar{h} \\ -2h^T h & \left(1 - 2\|h\|^2\right)\mathbf{E} \end{bmatrix} = \left(1 - 2\|h\|^2\right) \begin{bmatrix} \mathbf{E} & \mathbf{0} \\ \mathbf{0} & \mathbf{E} \end{bmatrix} - 2 \begin{bmatrix} \mathbf{0} & h^*\bar{h} \\ h^T h & \mathbf{0} \end{bmatrix}
\tag{2.8}
$$

The characteristic equation of the matrix

$$
\Omega_2 = \begin{bmatrix} \mathbf{0} & h^*\bar{h} \\ h^T h & \mathbf{0} \end{bmatrix}
\tag{2.9}
$$

is

$$
x^{2(n-2)} \left(x^2 - \|h\|^4 \right) = 0
\tag{2.10}
$$

and the nonzero roots are $\|h\|^2$ and $-\|h\|^2$; therefore, the eigenvalues of the matrix $\Omega_1(h)$ are

$$
1 - 4\|h\|^2,\quad 1 \quad \text{and,} \quad 1 - 2\|h\|^2 \quad [2(n-2) \text{ times}].
\tag{2.11}
$$

Hence, the matrix $\Omega_1(h)$ is positive semi-definite if and only if $1 - 4\|h\|^2 \geq 0$, that is, $\|h\| \leq 1/2$. ■

In order to show that the condition $\|h\| \leq 1/2$ is also sufficient for global optimality in problem (**) we should invoke Theorem 5 in [8]. For a normal matrix $\mathbf{B}$ let us denote

$$
Kom_H(\mathbf{B}) = \left\{ \mathbf{X};\ \mathbf{X}^* = \mathbf{X},\ \mathbf{XB} = \mathbf{BX} \right\}
\tag{2.12}
$$

and, for a hermitiean matrix $\mathbf{H}$ let $\delta(\mathbf{H})$ be its spectral diameter: $\delta(\mathbf{H}) = y_{\max} - y_{\min}$, where $y_{\max}$ and $y_{\min}$ are, respectively, the largest and the smallest eigenvalues of $\mathbf{H}$. Further, with

$$\delta(\mathbf{H},\mathbf{B}) = \inf\left\{\delta(\mathbf{H}-\mathbf{X})\ ;\ \mathbf{X}\in \mathit{Kom}_H(\mathbf{B})\right\} \tag{2.13}$$

Theorem 5 in [8] states that a sufficient condition for a normal matrix $\mathbf{B}$ to be the best normal approximation (in Frobenius norm) for the matrix $\mathbf{A}=\mathbf{B}+\mathbf{BH}-\mathbf{HB}$ is

$$\delta(\mathbf{H},\mathbf{B}) \le \mathbf{1}\ . \tag{2.14}$$

For a **ΔH-1** matrix $\mathbf{G}$, let us take

$$\mathbf{B} = \operatorname{diag}\left(d_1, d_2, \dots,\ d_2\right)\ . \tag{2.15}$$

Then every matrix $\mathbf{X}$ in $\mathit{Kom}_H(\mathbf{B})$ can be expressed as

$$\mathbf{X} = \begin{bmatrix} x_1 & \mathbf{0} \\ \mathbf{0} & X_1 \end{bmatrix}\ \ X_1^* = X_1\,, \tag{2.16}$$

hence the matrix $\mathbf{H}-\mathbf{X}$ will essentially have the form

$$\mathbf{H}-\mathbf{X} = \begin{bmatrix} x_1 & h \\ h^* & \mathbf{X}_2 \end{bmatrix}\ \ \mathbf{X}_2^* = \mathbf{X}_2 \tag{2.17}$$

Now, if we consider the canonical decomposition of $\mathbf{X}_2$: $\mathbf{X}_2 = \mathbf{T}\operatorname{diag}\ (x_2,\dots,\ x_n)\mathbf{T}^*$; $\mathbf{TT}^* = \mathbf{E}$, the result stated will follow from

Lemma 1: *We have*

$$\delta\left(\begin{bmatrix} x_1 & h \\ h^* & \mathbf{X}_2 \end{bmatrix}\right) = \delta\left(\begin{bmatrix} x_1 & & \mathbf{u} & \\ & x_2 & & 0 \\ \mathbf{u}^* & & \ddots & 0 \\ & 0 & 0 & x_n \end{bmatrix}\right), \tag{2.18}$$

where $\mathbf{u} = h\mathbf{T}^*$.

The point here is that

$$\|h\| = \left\|h\mathbf{T}^*\right\| = \|\mathbf{u}\|\ .$$

3. THIRD ORDER ΔH-1 MATRICES

We will show that for third order **ΔH-1** matrices

$$\mathbf{G} = \begin{bmatrix} d_1 & h_{12}(d_1-d_2) & h_{13}(d_1-d_2) \\ h_{21}(d_2-d_1) & d_2 & 0 \\ h_{31}(d_2-d_1) & 0 & d_2 \end{bmatrix};\quad h_{k1} = \overline{h}_{1k} \tag{3.1}$$

the condition $\|h\| = \left(|h_{12}|^2 + |h_{13}|^2\right)^{1/2} \le \dfrac{1}{2}$ uniquely identifies global extrema in problems (*) and (**).

To this aim, consider the characteristic equation

$$y^3 - p_1 y^2 + p_2 y - p_3 = 0 \tag{3.2}$$

of the matrix

$$\mathbf{H}_x = \begin{bmatrix} x_1 & h_{12} & h_{13} \\ \overline{h}_{12} & x_2 & 0 \\ \overline{h}_{13} & 0 & x_3 \end{bmatrix} \tag{3.3}$$

and the problem

$$\min\{(y_{\max} - y_{\min});\quad (x_1, x_2, x_3) \in \mathbf{R}^3\} \tag{3.4}$$

where $y_{\max}$ and $y_{\min}$ are the largest and, respectively, the smallest eigenvalues. Putting

$$q_1 = s = x_1 + x_2 + x_3, \quad q_2 = x_1x_2 + x_1x_3 + x_2x_3, \quad q_3 = x_1x_2x_3 \tag{3.5}$$

we get

$$\begin{aligned} p_1 &= q_1 = s \\ p_2 &= q_2 - |h_{12}|^2 - |h_{13}|^2 \\ p_3 &= q_3 - |h_{12}|^2 x_3 - |h_{13}|^2 x_2 \end{aligned} \tag{3.6}$$

It is now easy to see that we can always choose x_1, x_2 and x_3 such that

$$y_1 = y_{\max} = -y_{\min} = -y_3 \tag{3.7}$$

with y_2 between y_1 and y_3: $y_1 \geq y_2 \geq -y_1$. Equation (3.2) has the roots $y_1 = -y_3$ and $y_2 = s$. Besides, y_1 and y_3 verify the equations

$$\begin{aligned} y^3 + p_2 y &= 0 \\ p_1 y^2 + p_3 &= 0 \end{aligned} \tag{3.8}$$

which lead to

$$\begin{aligned} &\mathbf{I} \qquad y^2 + q_2 - \|h\|^2 = 0 \\ &\mathbf{II} \qquad q_1 y^2 - |h_{13}|^2 x_2 - |h_{12}|^2 x_3 + q_3 = 0 \end{aligned} \tag{3.9}$$

From **I** we get $y^2 = \|h\|^2 - q_2$. If $x_1 = x_2 = x_3 = 0$ we have the solution $y_{\max} = y_0 = \|h\|^2$. We shall prove that this is a global solution to problem (3.4), i.e. that $q_2 \leq 0$ for any other values x_1, x_2, x_3. To this end, we show that the contrary assumption, $q_2 > 0$, leads to a contradiction.

Lemma 2: *If either*

$$x_1 + x_2 = 0, \quad x_1 + x_3 = 0 \quad \text{or} \quad x_2 + x_3 = 0 \tag{3.10}$$

then $q_2 \leq 0$.

Proof (for $x_1 + x_2 = 0$). If $x_2 = -x_1$ then

$$q_2 = x_3(x_1 + x_2) - x_1^2 = -x_1^2 \leq 0 \tag{3.11}$$

Lemma 3: *If* $q_2 > 0$ *then*

$$\operatorname{sgn}(x_1 + x_2) = \operatorname{sgn}(x_1 + x_3) = \operatorname{sgn}(x_2 + x_3) = \operatorname{sgn}(x_1 + x_2)(x_1 + x_3)(x_2 + x_3)\,. \tag{3.12}$$

Proof. We have

$$\begin{aligned}(x_1+x_2)(x_1+x_3)&=x_1^2+q_2>0\\(x_1+x_2)(x_2+x_3)&=x_2^2+q_2>0\\(x_1+x_3)(x_2+x_3)&=x_3^2+q_2>0\end{aligned} \tag{3.13}$$

Lemma 4: *The identity*

$$q_1q_2-q_3=(x_1+x_2)(x_1+x_3)(x_2+x_3) \tag{3.14}$$

holds.

Proof. Obvious.

Suppose now $x_1\neq 0$ and let

$$x_1=x,\quad x_2=t_2x,\quad x_3=t_3x\ . \tag{3.15}$$

From Lemma 3 we have

$$\operatorname{sgn}(1+t_2)=\operatorname{sgn}(1+t_2)=\operatorname{sgn}(1+t_3)=\operatorname{sgn}(t_2+t_3)(1+t_2)(1+t_3)\ . \tag{3.16}$$

By multiplying **I** (in 3.8) by $s=q_1$ and deducting **II**, y is eliminated; using (3.15) we obtain

$$\begin{aligned}R&=q_1q_2-q_3-\|h\|^2q_1+|h_{12}|^2x_3+|h_{13}|^2x_2=\\&=(1+t_2)(1+t_3)(t_2+t_3)\ \ x^3-(|h_{12}|^2+|h_{13}|^2)(1+t_2+t_3)\ \ x+|h_{12}|^2t_3x+|h_{13}|^2t_2x=0\end{aligned} \tag{3.17}$$

and a straightforward computation yields

$$x^2=\frac{|h_{12}|^2(1+t_2)+|h_{13}|^2(1+t_3)}{(1+t_2)(1+t_3)(t_2+t_3)}\ . \tag{3.18}$$

From **I** we obtain

$$y^2=\|h\|^2-q_2=|h_{12}|^2+|h_{13}|^2-(t_1+t_2+t_2t_3)\,x^2 \tag{3.19}$$

or, by (3.18),

$$y^2=\frac{|h_{13}|^2t_2^2(1+t_3)+|h_{12}|^2t_3^2(1+t_2)}{(1+t_2)(1+t_3)(t_2+t_3)}\ . \tag{3.20}$$

Now we are ready to prove the following result

Theorem 2: *For a* **ΔH-1** *matrix* (3.1), *the condition*

$$\|h\|=\left(|h_{12}|^2+|h_{13}|^2\right)^{1/2}\leq\frac{1}{2} \tag{3.21}$$

is necessary and sufficient for **D** *to be a global extremum in problems* (*) *and* (**).

Proof. We only have to show that a contradiction occurs when assuming $q_2>0$. To this end, we relay on the inequality $y_1^2\geq q_1^2$ (hence $y_1^2\geq s^2$). Let us estimate

$$E = s^2 - y_1^2 = (1+t_2+t_3)\quad x^2 - y_1^2 =$$
$$= |h_{12}|^2 \frac{(1+t_2)\left[(1+t_2+t_3)^2 - t_3^2\right]}{(1+t_2)(1+t_3)(t_2+t_3)} + |h_{13}|^2 \frac{(1+t_3)\left[(1+t_2+t_3)^2 - t_2^2\right]}{(1+t_2)(1+t_3)(t_2+t_3)} =$$
$$= |h_{12}|^2 \left[\frac{(1+t_2)^2}{(1+t_3)(t_2+t_3)} + \frac{1+t_2}{1+t_3}\right] + |h_{13}|^2 \left[\frac{(1+t_3)^2}{(1+t_2)(t_2+t_3)} + \frac{1+t_3}{1+t_2}\right] \tag{3.22}$$

which should be negative. But, as can be seen from Lemma 3 and the associated relations (3.16), each term in the above sum is non negative.

Now, we only have to consider the special case $x_1 = 0$, when system (3.9) takes the form

$$y^2 + x_2 x_3 - \|h\|^2 = 0 \tag{3.23}$$

$$(x_2 + x_3)\, y^2 - |h_{12}|^2 x_3 - |h_{13}|^2 x_2 = 0 \;. \tag{3.24}$$

We can assume $x_2 \neq 0$. Then, with $x_2 = x, \quad x_3 = kx$, by eliminating y in (3.23) and (3.24), we get

$$x^2 = \frac{k|h_{12}|^2 + |h_{13}|^2}{k(1+k)} \;. \tag{3.25}$$

For $y^2 = \|h\|^2 - x_2 x_3$ the computation yields

$$y^2 = \frac{k|h_{12}|^2 + |h_{13}|^2}{1+k} \tag{3.26}$$

while for $s^2 - y_1^2$ we obtain the expression

$$s^2 - y_1^2 = |h_{12}|^2 \frac{2k+1}{k(1+k)} + |h_{13}|^2 \frac{(2+k)k}{1+k} \;. \tag{3.27}$$

which should be negative. But the condition $q_2 = kx^2 \geq 0$ implies $k \geq 0$, hence all terms in (3.27) are non negative. The contradiction also proves the theorem in this special case.

Conjecture. In accordance with Theorems 1 and 2 one can expect that the condition

$$\|h\| = \left(|h_{12}|^2 + |h_{13}|^2 + \ldots + |h_{1n}|\right)^{1/2} \leq \frac{1}{2}$$

is necessary and sufficient for D to be a global optimum in problems (*) and (**) for an arbitrary **ΔH-1** matrix in $\mathbf{C}_{n\times n}$.

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