ON THE OPTIMALITY OF A CLASS OF ∆H MATRICES

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We derive a necessary condition for optimality of ∆H-1 matrices in $C_{nn}$, 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. ∆H MATRICES

According to [2], a ∆H matrix is a matrix which can be written as

$$G = D + DH - HD$$

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

$$G = D + DH - HD$$

$$G = [d_k; h_{ij}(d_k - d_j)]^n_i$$

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

For a matrix $A \in C_{nn}$ let us consider the optimisation problems

(*) $\max \|\text{Diag } T^* A T\|$; $TT^* = E$ (i.e., $T$ is unitary)

and

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

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

These problems involve ∆H matrices: if a diagonal matrix $D$ is a stationary point for problem (**), then $A$ must be a ∆H matrix with $\text{Diag}(A) = D$ (Theorem 3 in [2]). On the other hand, for a ∆H 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 ∆H matrix: $A = G = D + DH - HD$; in our previous papers we called it an optimal ∆H matrix. In the case $n = 2$, optimality means (Theorem 5 in [2]) that $G$ has the form

$$G = \begin{bmatrix} d_1 & h_{12} (d_1 - d_2) \\ h_{21} (d_2 - d_1) & d_2 \end{bmatrix}; \quad h_{12} = h_{21}; \quad |h_{12}| \leq \frac{1}{2}$$

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

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\[ \Delta H \] matrices also occur as limit points of a Jacobi sequence \( \{ A_n \} \), where the initial matrix \( A_0 \in C_{non} \) 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

\[
I_D = \{ (k, j) ; d_k = d_j \}
\]

(1.4)

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

\[
G(Z) = \sum_{k,j=1}^{n} \left| z_{kj} \right|^2 \left| d_k - d_j \right|^2 - \frac{1}{2} \sum_{k,j=1}^{n} h_{kj} \left( z_{ik} z_{kj} + z_{kj} z_{ij} \right) \begin{bmatrix} d_k & d_k & 1 \\ d_j & d_j & 1 \\ \end{bmatrix}
\]

\[
-\frac{1}{2} \sum_{i_1 \neq j_1}^{n} \left( h_{i_1} z_{i_1} + h_{j_1} z_{j_1} \right) \left( d_k - d_j \right) \left( d_k - d_j \right) \begin{bmatrix} d_k & d_k & 1 \\ d_j & d_j & 1 \\ \end{bmatrix}
\]

\[ \geq 0 \]

(1.5)

for all \( \left[ z_{i_1} \right]_{i=1}^{n} = Z \in C_{non} \), i.e., the hessian \( G(Z) \) is positive semi-definite on \( C_{non} \).

2. \( \Delta H \)-1 MATRICES IN \( C_{non} \)

A \( \Delta H \)-1 matrix in \( C_{non} \) is a matrix of the form

\[
G = \begin{bmatrix}
    d_1 & h_{12} (d_1 - d_2) & h_{13} (d_1 - d_2) & \cdots & h_{1n} (d_1 - d_2) \\
    h_{21} (d_2 - d_1) & d_2 & 0 & \cdots & 0 \\
    h_{31} (d_2 - d_1) & 0 & d_2 & \cdots & 0 \\
    \cdots & \cdots & \cdots & \cdots & \cdots \\
    h_{n1} (d_2 - d_1) & 0 & 0 & \cdots & d_2
\end{bmatrix} \\
; \quad h_{ik} = \bar{h}_{ik}
\]

(2.1)

with \( d_1 \neq d_2 \). Because

\[
d_1 \neq d_2 = d_3 = \ldots d_n
\]

(2.2)

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

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

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

(2.3)

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

\[
I_D = \{ (k, j) ; k, j = 2, \ldots, n \}
\]

(2.4)

so the hessian becomes
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\[ G(Z) = |d_1 - d_2|^2 \left[ \sum_{k=2}^{n} |z_{ik}|^2 + \sum_{k=2}^{n} |z_{k1}|^2 - 2 \sum_{k,j=2}^{n} h_{kj} z_{ik} z_{kj} \right] = \]
\[ = g(\ldots) = g_1(\ldots) - g_2(\ldots) \]
\[ = d_1 - d_2 \left[ \frac{1}{2} \left( \sum_{k=2}^{n} |z_{ik}|^2 - 2 \sum_{k,j=2}^{n} h_{kj} z_{ik} z_{kj} \right) \right] \]
\[ = |d_1 - d_2|^2 \left[ (1 - 2\|h\|)^2 \left( \sum_{k=2}^{n} |z_{ik}|^2 + \sum_{k=2}^{n} |z_{k1}|^2 \right) \right] \]

and

\[ g_2(\ldots) = 2|d_1 - d_2|^2 \left[ \sum_{k,j=2}^{n} h_{kj} z_{ik} z_{kj} + \sum_{k,j=2}^{n} h_{kj} z_{k1} z_{kj} \right] \]

Associated with the form $g(\ldots)$, except for the positive factor $|d_1 - d_2|^2$, is the hermitean matrix

\[ \Omega_1(h) = \begin{bmatrix} (1 - 2\|h\|)E & -2h^* h \\ -2h h^* & (1 - 2\|h\|)E \end{bmatrix} = \begin{bmatrix} E & 0 \\ 0 & E \end{bmatrix} - 2 \begin{bmatrix} 0 & h^* h \\ h h^* & 0 \end{bmatrix} \]

The characteristic equation of the matrix

\[ \Omega_2 = \begin{bmatrix} 0 & h^* h \\ h h^* & 0 \end{bmatrix} \]

is

\[ \chi^{2(n-2)}(k^2 - \|h\|^4) = 0 \]

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

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

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 $B$ let us denote

\[ Kom_{h+B}(B) = \{ X; \ X^* = X, \ XB = BX \} \]

and, for a hermitian matrix $H$, let $\delta(H)$ be its spectral diameter: $\delta(H) = y_{\text{max}} - y_{\text{min}}$, where $y_{\text{max}}$ and $y_{\text{min}}$ are, respectively, the largest and the smallest eigenvalues of $H$. Further, with
\[
\delta(H, B) = \inf \left\{ \delta(H - X) : X \in \text{Kom}_H(B) \right\}
\]  
(2.13)

Theorem 5 in [8] states that a sufficient condition for a normal matrix \(B\) to be the best normal approximation (in Frobenius norm) for the matrix \(A = B + BH - HB\) is
\[
\delta(H, B) \leq 1.
\]  
(2.14)

For a \(\Delta H\)-1 matrix \(G\), let us take
\[
B = \text{diag} \left( d_1, d_2, \ldots, d_2 \right).
\]  
(2.15)

Then every matrix \(X\) in \(\text{Kom}_H(B)\) can be expressed as
\[
X = \begin{bmatrix} x_1 & 0 \\ 0 & X_1 \end{bmatrix} X_1^* = X_1,
\]  
(2.16)

hence the matrix \(H - X\) will essentially have the form
\[
H - X = \begin{bmatrix} x_1 & h \\ h^* & X_2 \end{bmatrix} X_2^* = X_2
\]  
(2.17)

Now, if we consider the canonical decomposition of \(X_2\): \(X_2 = T \text{diag} \left( x_2, \ldots, x_n \right) T^*; TT^* = E\), the result stated will follow from

**Lemma 1:** We have
\[
\delta\left( \begin{bmatrix} x_1 & h \\ h^* & X_2 \end{bmatrix} \right) = \delta\left( \begin{bmatrix} x_1 & u \\ x_2 & 0 \\ u & \ddots & 0 \\ 0 & 0 & \cdots & 0 \end{bmatrix} \right),
\]  
(2.18)

where \(u = hT^*\).

The point here is that
\[
\|h\| = \|hT^*\| = \|u\|.
\]

3. THIRD ORDER \(\Delta H\)-1 MATRICES

We will show that for third order \(\Delta H\)-1 matrices
\[
G = \begin{bmatrix}
d_1 & h_{12} (d_1 - d_2) & h_{13} (d_1 - d_2) \\
h_{21} (d_2 - d_1) & d_2 & 0 \\
h_{31} (d_2 - d_1) & 0 & d_2
\end{bmatrix}; \quad h_{kl} = \bar{h}_{kl}
\]  
(3.1)

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

To this aim, consider the characteristic equation
\[
y^3 - p_1 y^2 + p_2 y - p_3 = 0
\]  
(3.2)

of the matrix.
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\[
H_x = \begin{bmatrix}
x_1 & h_{12} & h_{13} \\
h_{12} & x_2 & 0 \\
h_{13} & 0 & x_3
\end{bmatrix}
\]  

(3.3)

and the problem

\[
\min \{ (y^\max - y^\min) ; \quad (x_1, x_2, x_3) \in \mathbb{R}^3 \}
\]  

(3.4)

where $y^\max$ and $y^\min$ are the largest and, respectively, the smallest eigenvalues. Putting

\[
q_1 = s = x_1 + x_2 + x_3, \quad q_2 = x_1x_2 + x_1x_3 + x_2x_3, \quad q_3 = x_1x_2x_3
\]  

(3.5)

we get

\[
p_1 = q_1 = s \\
p_2 = q_2 - |h_{12}|^2 - |h_{13}|^2 \\
p_3 = q_3 - |h_{12}|^2 x_3 - |h_{13}|^2 x_2
\]  

(3.6)

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

\[
y_1 = y_1^\max = -y_2^\min = -y_3^\min
\]  

(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

\[
y^3 + p_2 y = 0 \\
p_3 y^2 + p_1 = 0
\]  

(3.8)

which lead to

\[
\mathbf{I} \quad y^2 + q_2 - \|h\|^2 = 0 \\
\mathbf{II} \quad q_1 y^2 - |h_{12}|^2 x_2 - |h_{13}|^2 x_3 + q_3 = 0
\]  

(3.9)

From $\mathbf{I}$ 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

\[
x_1 + x_2 = 0, \quad x_1 + x_3 = 0 \quad \text{or} \quad x_2 + x_3 = 0
\]  

(3.10)

then $q_2 \leq 0$.

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

\[
q_2 = x_3(x_1 + x_2) - x_1^2 = -x_1^2 \leq 0
\]  

(3.11)

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

\[
\text{sgn}(x_1 + x_2) = \text{sgn}(x_1 + x_3) = \text{sgn}(x_2 + x_3) = \text{sgn}(x_1 + x_2)(x_1 + x_3)(x_2 + x_3)
\]  

(3.12)
Proof. We have
\begin{align}
(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{align}
(3.13)

Lemma 4: The identity
\[ q_1 q_2 - q_3 = (x_1 + x_2)(x_1 + x_3)(x_2 + x_3) \]
(3.14)
holds.

Proof. Obvious.

Suppose now \( x_1 \neq 0 \) and let
\[ x_1 = x, \quad x_2 = t_2 x, \quad x_3 = t_1 x. \]
(3.15)
From Lemma 3 we have
\[ \text{sgn}(1+ t_2) = \text{sgn}(1+ t_2) = \text{sgn}(1+ t_3) = \text{sgn}(1+ t_3)(1+ t_2)(1+ t_1). \]
(3.16)
By multiplying I (in 3.8) by \( s = q_1 \) and deducting II, \( y \) is eliminated; using (3.15) we obtain
\[ R = q_1 q_2 - q_3 - \|h\|^2 q_1 + |h_{12}|^2 x_3 + |h_{13}|^2 x_2 = \]
\[ = (1+ t_2)(1+ t_3)(t_2 + t_3) x^3 - (|h_{12}|^2 + |h_{13}|^2)(1+ t_2 + t_3) x + |h_{12}|^2 t_3 x + |h_{13}|^2 t_2 x = 0 \]
(3.17)
and a straightforward computation yields
\[ x^2 = \frac{|h_{12}|^2 (1+ t_2) + |h_{13}|^2 (1+ t_3)}{(1+ t_2)(1+ t_3)(t_2 + t_3)}. \]
(3.18)
From I we obtain
\[ y^2 = \|h\|^2 - q_2 = |h_{12}|^2 + |h_{13}|^2 - (t_1 + t_2 + t_2 t_3) x^2 \]
(3.19)
or, by (3.18),
\[ y^2 = \frac{|h_{13}|^2 t_2^2 (1+ t_3) + |h_{12}|^2 t_2^2 (1+ t_2)}{(1+ t_2)(1+ t_3)(t_2 + t_3)}. \]
(3.20)
Now we are ready to prove the following result

Theorem 2: For a \( \Delta H \)-1 matrix (3.1), the condition
\[ \|h\| = \left( |h_{12}|^2 + |h_{13}|^2 \right)^{1/2} \leq \frac{1}{2} \]
(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 \( y_i^2 \geq q_i^2 \) (hence \( y_i^2 \geq s^2 \)). Let us estimate
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\[ E = s^2 - y_1^2 = (1 + t_2 + t_3) \quad x^2 - y_1^2 = \]
\[ = |h_{12}|^2 \left( \frac{(1 + t_2)^2}{(1 + t_2)(1 + t_3)(t_2 + t_3)} \right) + |h_{13}|^2 \left( \frac{(1 + t_3)^2}{(1 + t_2)(1 + t_3)(t_2 + t_3)} \right) \]
\[ = |h_{12}|^2 \left( \frac{(1 + t_2)^2 + 1 + t_2}{(1 + t_2)(t_2 + t_3)} \right) + |h_{13}|^2 \left( \frac{(1 + t_3)^2 + 1 + t_3}{(1 + t_2)(t_2 + t_3)} \right) \]
\[
\text{(3.22)}
\]

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

\[ y^2 + x_2 x_3 - |h|^2 = 0 \]
\[
\text{(3.23)}
\]

\[(x_2 + x_3) y^2 - |h_{12}|^2 x_3 - |h_{13}|^2 x_2 = 0 . \]
\[
\text{(3.24)}
\]

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

\[ x^2 = \frac{k |h_{12}|^2 + |h_{13}|^2}{k(1 + k)} . \]
\[
\text{(3.25)}
\]

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

\[ y^2 = \frac{k |h_{12}|^2 + |h_{13}|^2}{1 + k} \]
\[
\text{(3.26)}
\]

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

\[ s^2 - y_1^2 = |h_{12}|^2 \left( \frac{2k + 1}{k(1 + k)} \right) + |h_{13}|^2 \left( \frac{(2 + k)k}{1 + k} \right) . \]
\[
\text{(3.27)}
\]

which should be negative. But the condition $q_k = k x^2 \geq 0$ 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

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

is necessary and sufficient for $D$ to be a global optimum in problems (*) and (**) for an arbitrary $\Delta H$ matrix in $C_{\Delta H}$.

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