Householder Method for Tridiagonalization: Ver. 1.0

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The Householder method [1] is a way of transforming a Hermitian matrix $B$ to a real symmetric tridiagonalized matrix $B_{TD}$. Let $b$ be a column vector of $B$, and consider that the vector $b$ consists of the real part $b_r$ and the imaginary part $b_i$ as

$$|b\rangle = |b_r\rangle + i|b_i\rangle. \quad (1)$$

Also let us introduce a vector $s$ of which real part has just one non-zero component $s(= \sqrt{(b b^*)})$ and imaginary part is a zero vector as

$$|s\rangle = \begin{pmatrix} s \\ 0 \\ \vdots \\ 0 \end{pmatrix} + i \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}. \quad (2)$$

Then, consider a mirror transform $Q^\dagger$ bridging the two vectors $b$ and $s$ by

$$Q^\dagger = I - \alpha^*|v\rangle\langle v|, \quad (3)$$

where let us assume that

$$|s\rangle = Q^\dagger b). \quad (4)$$

Putting Eq. (3) into Eq. (4), and solving it with respect to $|v\rangle$, we have

$$|v\rangle = \frac{1}{\alpha^* (v|b)} (|b\rangle - |s\rangle). \quad (5)$$

Thus, Eq. (5) allows us to write $|v\rangle$ as

$$|v\rangle = \beta (|b\rangle - |s\rangle) = \beta |u\rangle. \quad (6)$$

If $v$ is normalized, $\beta$ is given by

$$\beta = \frac{1}{\sqrt{(b|b) - (s|b) - (s|s)}} = \frac{1}{\sqrt{(b^* b) + (s|b) - (b|s) - (s|s)}} = \frac{1}{\sqrt{2s^2 - (s|b) - (s|s)}}. \quad (7)$$
Comparing Eqs. (5) with (6) and making use of Eq. (7), we have

\[ \alpha^* = \frac{2a_r}{a_r^2 + a_i^2}(a_r - ia_i) \]  

(8)

with \( a_r \) and \( a_i \) given by

\[ a_r = \frac{1}{2}\left(2s^2 - \langle b|s\rangle - \langle s b\rangle\right) \]  

(9)

and

\[ a_i = \langle b_i|s\rangle. \]  

(10)

Then, it is verified that

\[ QQ^\dagger = (I - \alpha|v\rangle\langle v|)(I - \alpha^*|v\rangle\langle v|), \]

\[ = I - \alpha^*|v\rangle\langle v| - \alpha|v\rangle\langle v| + \alpha\alpha^*|v\rangle\langle v|\langle v|\langle v|, \]

\[ = I - \frac{(2a_r)^2}{a_r^2 + a_i^2}|v\rangle\langle v| + \frac{(2a_r)^2}{a_r^2 + a_i^2}|v\rangle\langle v|, \]

\[ = I. \]  

(11)

Thus, the transformation \( Q^\dagger BQ \) for the Hermitian matrix \( B \) is a similarity transformation, and given by

\[ Q^\dagger BQ = (I - \alpha^*|v\rangle\langle v|) B (I - \alpha^*|v\rangle\langle v|), \]

\[ = B - \alpha^*|v\rangle\langle v| B - \alpha^*|v\rangle\langle v| B + \alpha^*|v\rangle\langle v| B |v\rangle\langle v|. \]  

(12)

By defining

\[ |p\rangle \equiv B|v\rangle, \]  

(13)

Eq. (12) becomes

\[ Q^\dagger BQ = B - \alpha^*|v\rangle\langle p| - \alpha|p\rangle\langle v| + \alpha^*\alpha|v\rangle\langle v| |p\rangle\langle v|, \]

\[ = B - \alpha^*|v\rangle \left(|p\rangle - \frac{\alpha}{2}|v\rangle|p\rangle\langle v|\right) - \alpha \left(|p\rangle - \frac{\alpha^*}{2}|v\rangle|p\rangle\right) \langle v|. \]  

(14)

Moreover, by defining

\[ |q\rangle \equiv \alpha \left(|p\rangle - \frac{\alpha^*}{2}|v\rangle|p\rangle\right), \]  

(15)

we have a compact form:

\[ Q^\dagger BQ = B - |v\rangle|q\rangle - |q\rangle\langle v|. \]  

(16)

For the numerical stability, we furthermore modify Eq. (16) as shown below. Let us introduce a vector \( p' \) as.

\[ |p'\rangle = \frac{B|u\rangle}{|u|^2}. \]  

(17)
Then, \( \mathbf{p} \) can be written by \( \mathbf{p}' \) as

\[
|\mathbf{p}\rangle = \frac{|\mathbf{v}\rangle}{\sqrt{2a_r}},
\]

\[
= \frac{|\mathbf{u}\rangle}{\sqrt{2a_r}},
\]

\[
= \frac{|\mathbf{p}'\rangle}{\sqrt{2a_r}},
\]

\[
= \frac{\sqrt{2a_r}}{2}|\mathbf{p}'\rangle.
\]

Also, noting that

\[
|\mathbf{v}\rangle = \frac{1}{\sqrt{2a_r}}|\mathbf{u}\rangle,
\]

\( \mathbf{q} \) can be rewritten by

\[
|\mathbf{q}\rangle = \alpha\frac{\sqrt{2a_r}}{2} \left( |\mathbf{p}'\rangle - \frac{\alpha^*}{4a_r}|\mathbf{u}\rangle\langle\mathbf{u}|\mathbf{p}'\rangle \right).
\]

Putting Eqs. (19) and (20) into Eq. (16), we have

\[
Q^\dagger BQ = B - |\mathbf{u}\rangle\langle\mathbf{u}| - |\mathbf{q}'\rangle\langle\mathbf{q}'| - |\mathbf{q}\rangle\langle\mathbf{q}| - |\mathbf{q}'\rangle\langle\mathbf{q}'|.
\]

with \( \mathbf{q}' \) defined by

\[
|\mathbf{q}'\rangle = \frac{\alpha}{2} \left( |\mathbf{p}'\rangle - \frac{\alpha^*}{4a_r}|\mathbf{u}\rangle\langle\mathbf{u}|\mathbf{p}'\rangle \right),
\]

where

\[
|\mathbf{p}'\rangle = \frac{1}{a_r}|\mathbf{u}\rangle.
\]

The transformation by Eq. (21) can be applied to each column vector step by step in which the place occupied by \( s \) in Eq. (2) is shifted one by one. Then, the tridiagonalized matrix \( B_{TD} \) is given by

\[
B_{TD} = Q_{n-1}^\dagger Q_{n-2}^\dagger \cdots Q_3^\dagger Q_2^\dagger Q_1^\dagger B Q_1 Q_2 Q_3 \cdots Q_{n-2} Q_{n-1}.
\]

References