Householder Method for Tridiagonalization: Ver. 1.0

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August 17, 2007

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

$$|\mathbf{b}\rangle = |\mathbf{b}_r\rangle + i|\mathbf{b}_i\rangle. \tag{1}$$

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

$$|\mathbf{s}\rangle = \begin{pmatrix} s \\ 0 \\ \cdot \\ \cdot \\ 0 \end{pmatrix} + i \begin{pmatrix} 0 \\ 0 \\ \cdot \\ \cdot \\ 0 \end{pmatrix}. \tag{2}$$

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

$$Q^\dagger = I - \alpha^* |\mathbf{v}\rangle\langle\mathbf{v}|, \tag{3}$$

where let us assume that

$$|\mathbf{s}\rangle = Q^\dagger |\mathbf{b}\rangle. \tag{4}$$

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

$$|\mathbf{v}\rangle = \frac{1}{\alpha^* \langle \mathbf{v}|\mathbf{b}\rangle} \left(|\mathbf{b}\rangle - |\mathbf{s}\rangle \right). \tag{5}$$

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

$$|\mathbf{v}\rangle = \beta \left(|\mathbf{b}\rangle - |\mathbf{s}\rangle \right) = \beta |\mathbf{u}\rangle. \tag{6}$$

If $\mathbf{v}$ is normalized, β is given by

$$\begin{aligned} \beta &= \frac{1}{\sqrt{(\langle \mathbf{b}| - \langle \mathbf{s}|)(|\mathbf{b}\rangle - |\mathbf{s}\rangle)}}, \\ &= \frac{1}{\sqrt{\langle \mathbf{b}|\mathbf{b}\rangle + \langle \mathbf{s}|\mathbf{s}\rangle - \langle \mathbf{b}|\mathbf{s}\rangle - \langle \mathbf{s}|\mathbf{b}\rangle}}, \\ &= \frac{1}{\sqrt{2s^2 - \langle \mathbf{b}|\mathbf{s}\rangle - \langle \mathbf{s}|\mathbf{b}\rangle}}. \end{aligned} \tag{7}$$

Comparing Eqs. (5) with (6) and making use of Eq. (7), we have

$$\alpha^* = \frac{2a_r}{a_r^2 + a_i^2}(a_r - i a_i) \tag{8}$$

with a_r and a_i given by

$$a_r = \frac{1}{2}\left(2s^2 - \langle \mathbf{b}|\mathbf{s}\rangle - \langle \mathbf{s}|\mathbf{b}\rangle\right) \tag{9}$$

and

$$a_i = \langle \mathbf{b}_i|\mathbf{s}\rangle. \tag{10}$$

Then, it is verified that

$$\begin{aligned} QQ^\dagger &= (I - \alpha|\mathbf{v}\rangle\langle\mathbf{v}|)\,(I - \alpha^*|\mathbf{v}\rangle\langle\mathbf{v}|)\,, \\ &= I - \alpha^*|\mathbf{v}\rangle\langle\mathbf{v}| - \alpha|\mathbf{v}\rangle\langle\mathbf{v}| + \alpha\alpha^*|\mathbf{v}\rangle\langle\mathbf{v}|\mathbf{v}\rangle\langle\mathbf{v}|, \\ &= I - \frac{(2a_r)^2}{a_r^2 + a_i^2}|\mathbf{v}\rangle\langle\mathbf{v}| + \frac{(2a_r)^2}{a_r^2 + a_i^2}|\mathbf{v}\rangle\langle\mathbf{v}|, \\ &= I. \end{aligned} \tag{11}$$

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

$$\begin{aligned} Q^\dagger BQ &= (I - \alpha^*|\mathbf{v}\rangle\langle\mathbf{v}|)\,B\,(I - \alpha|\mathbf{v}\rangle\langle\mathbf{v}|)\,, \\ &= B - \alpha^*|\mathbf{v}\rangle\langle\mathbf{v}|B - \alpha B|\mathbf{v}\rangle\langle\mathbf{v}| + \alpha^*\alpha|\mathbf{v}\rangle\langle\mathbf{v}|B|\mathbf{v}\rangle\langle\mathbf{v}|. \end{aligned} \tag{12}$$

By defining

$$|\mathbf{p}\rangle \equiv B|\mathbf{v}\rangle, \tag{13}$$

Eq. (12) becomes

$$\begin{aligned} Q^\dagger BQ &= B - \alpha^*|\mathbf{v}\rangle\langle\mathbf{p} - \alpha|\mathbf{p}\rangle\langle\mathbf{v}| + \alpha^*\alpha|\mathbf{v}\rangle\langle\mathbf{v}|\mathbf{p}\rangle\langle\mathbf{v}|, \\ &= B - \alpha^*|\mathbf{v}\rangle\left(\langle\mathbf{p}| - \frac{\alpha}{2}\langle\mathbf{v}|\mathbf{p}\rangle\langle\mathbf{v}|\right) - \alpha\left(|\mathbf{p}\rangle - \frac{\alpha^*}{2}|\mathbf{v}\rangle\langle\mathbf{v}|\mathbf{p}\rangle\right)\langle\mathbf{v}|. \end{aligned} \tag{14}$$

Moreover, by defining

$$|\mathbf{q}\rangle \equiv \alpha\left(|\mathbf{p}\rangle - \frac{\alpha^*}{2}|\mathbf{v}\rangle\langle\mathbf{v}|\mathbf{p}\rangle\right), \tag{15}$$

we have a compact form:

$$Q^\dagger BQ = B - |\mathbf{v}\rangle\langle\mathbf{q}| - |\mathbf{q}\rangle\langle\mathbf{v}|. \tag{16}$$

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

$$|\mathbf{p}'\rangle = \frac{B|\mathbf{u}\rangle}{\frac{|\mathbf{u}|^2}{2}}. \tag{17}$$

Then, $\mathbf{p}$ can be written by $\mathbf{p}'$ as

$$\begin{aligned} |\mathbf{p}\rangle &= B|\mathbf{v}\rangle, \\ &= \frac{B|\mathbf{u}\rangle}{\sqrt{2a_r}}, \\ &= \frac{|\mathbf{p}'\rangle a_r}{\sqrt{2a_r}}, \\ &= \frac{\sqrt{2a_r}}{2}|\mathbf{p}'\rangle. \end{aligned} \tag{18}$$

Also, noting that

$$|\mathbf{v}\rangle = \frac{1}{\sqrt{2a_r}}|\mathbf{u}\rangle, \tag{19}$$

$\mathbf{q}$ can be rewritten by

$$|\mathbf{q}\rangle = \alpha\frac{\sqrt{2a_r}}{2}\left(|\mathbf{p}'\rangle - \frac{\alpha^*}{4a_r}|\mathbf{u}\rangle\langle\mathbf{u}|\mathbf{p}'\rangle\right). \tag{20}$$

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

$$Q^\dagger BQ = B - |\mathbf{u}\rangle\langle\mathbf{q}'| - |\mathbf{q}'\rangle\langle\mathbf{u}| \tag{21}$$

with $\mathbf{q}'$ defined by

$$|\mathbf{q}'\rangle = \frac{\alpha}{2}\left(|\mathbf{p}'\rangle - \frac{\alpha^*}{4a_r}|\mathbf{u}\rangle\langle\mathbf{u}|\mathbf{p}'\rangle\right), \tag{22}$$

where

$$|\mathbf{p}'\rangle = \frac{1}{a_r}B|\mathbf{u}\rangle. \tag{23}$$

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

$$B_{\mathrm{TD}} = Q_{n-1}^\dagger Q_{n-2}^\dagger \cdots Q_3^\dagger Q_2^\dagger Q_1^\dagger B Q_1 Q_2 Q_3 \cdots Q_{n-2} Q_{n-1}. \tag{24}$$

References

[1] A. S. Householder, J. ACM **5**, 339 (1958).