

# Householder Method for Tridiagonalization: Ver. 1.0

Taisuke Ozaki, RCIS, JAIST

August 17, 2007

The Householder method [1] is a way of transforming a Hermitian matrix  $B$  to a real symmetric tridiagonalized matrix  $B_{\text{TD}}$ . 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

$$|\mathbf{b}\rangle = |\mathbf{b}_r\rangle + i|\mathbf{b}_i\rangle. \quad (1)$$

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

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

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

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

where let us assume that

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

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

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

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

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

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

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

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

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

with  $a_r$  and  $a_i$  given by

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

and

$$a_i = \langle \mathbf{b}_i | \mathbf{s} \rangle. \quad (10)$$

Then, it is verified that

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

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

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

By defining

$$|\mathbf{p}\rangle \equiv B |\mathbf{v}\rangle, \quad (13)$$

Eq. (12) becomes

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

Moreover, by defining

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

we have a compact form:

$$Q^\dagger B Q = B - |\mathbf{v}\rangle\langle \mathbf{q}| - |\mathbf{q}\rangle\langle \mathbf{v}|. \quad (16)$$

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

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

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

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

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  $B_{\text{TD}}$  is given by

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

## References

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