MATH50003 Numerical Analysis

III.4 Orthogonal and Unitary Matrices

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Part III

Numerical Linear Algebra

Square

1. Structured matrices such as banded
2. LU and PLU factorisations for solving linear systems
3. Cholesky factorisation for symmetric positive definite
4. Orthogonal matrices such as Householder reflections
5. QR factorisation for solving least squares

rectangular

LU factorisation: $$A = LU$$

PLU factorisation: $$A = P^T LU$$

Cholesky factorisation: $$A = LL^T$$

$\in \mathbb{C}^{m \times n}$ where $m \geq n$

QR factorisation: $$\underbrace{A}_{} = \underbrace{Q}_{}\underbrace{R}_{}$$

$U(m) \subset \mathbb{C}^{m \times m}$

$R \in \mathbb{C}^{m \times n}$

"right" triangular

Motivation: least squares

For rectangular systems, find vector that matches "closest"

Given rectangular $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$, find $x \in \mathbb{R}^n$ such that

$$Ax \approx b$$

Can't solve $A\vec{x} = \vec{b}$ unless $\vec{b}$ is in colspan(A).

by minimising

$$\|\underbrace{A}_{QR}x - b\|$$

so $A\vec{x}$ is as close to $\vec{b}$ as possible. How? Via QR

Definition 17 (orthogonal/unitary matrix)**.** A square real matrix is *orthogonal* if its inverse is its transpose:

$$O(n) = \{Q \in \mathbb{R}^{n\times n} : Q^\top Q = I\} \qquad \Rightarrow \qquad Q^{-1} = Q^\top$$

A square complex matrix is *unitary* if its inverse is its adjoint:

$$U(n) = \{Q \in \mathbb{C}^{n\times n} : Q^\star Q = I\}. \qquad \Rightarrow \qquad Q^{-1} = Q^*$$

Here the adjoint is the same as the conjugate-transpose: $Q^\star := \bar{Q}^\top$.

Note $O(n) < U(n)$.

Both $O(n)$ & $U(n)$ groups.

Eg if $Q_1, Q_2 \in O(n)$ then $Q_1 Q_2 \in O(n)$ since

$$(Q_1 Q_2)^T (Q_1 Q_2) = Q_2^T \underbrace{\cancel{Q_1^T Q_1}}_{I} Q_2 = I.$$

Idea: write $Q \in O(n)$ as a product

$$Q = Q_1 Q_2 \,\text{———}\, Q_m$$

where Q_k are rotations or reflections

Properties of orthogonal/unitary matrices

$\boxed{\text{Proofs are in PS}}$

1. Norm-preservation: $Q \in U(n)$ & $\vec{x} \in \mathbb{C}^n$ then

$$\| Q\vec{x} \| = \| \vec{x} \|$$

2. eigenvals have abs value 1 (are on complex circle)

$$Q\vec{x} = \lambda \vec{x} \Rightarrow |\lambda| = 1$$

3. $Q \in O(n) \Rightarrow \det Q = \pm 1$

III.~~3~~4.1 Rotations

Rotations in $\mathbb{R}^2$ correspond to 2×2 orthogonal matrices

Definition 18 (Special Orthogonal and Rotations)**.** *Special Orthogonal Matrices* are

$$SO(n) := \{Q \in O(n) | \det Q = 1\}$$

And (simple) *rotations* are $SO(2)$.

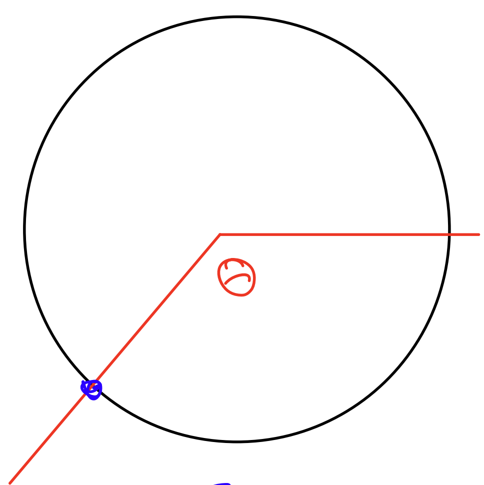
Definition 19 (two-arg arctan)**.** The two-argument arctan function gives the angle θ through the point $[a, b]^\top$, i.e.,

$$\sqrt{a^2+b^2}\begin{bmatrix}\cos\theta\\ \sin\theta\end{bmatrix} = \begin{bmatrix}a\\ b\end{bmatrix}.$$

It can be defined in terms of the standard arctan as follows:

$$\operatorname{atan}(b,a) := \begin{cases} \operatorname{atan}\frac{b}{a} & a>0\\ \operatorname{atan}\frac{b}{a}+\pi & a<0 \text{ and } b>0\\ \operatorname{atan}\frac{b}{a}-\pi & a<0 \text{ and } b<0\\ \pi/2 & a=0 \text{ and } b>0\\ -\pi/2 & a=0 \text{ and } b<0 \end{cases}$$

this case



$$\vec{x} = \begin{bmatrix}a\\ b\end{bmatrix} = \begin{bmatrix}-1\\ -\sqrt{3}\end{bmatrix} = \begin{bmatrix}\cos\theta\\ \sin\theta\end{bmatrix}$$

Eg.

$$\operatorname{atan}(b,a) = \operatorname{atan}(-\sqrt{3}, -1)$$

$$= \operatorname{atan}\sqrt{3} - \pi$$

$$= \frac{\pi}{3} - \pi = -\frac{2\pi}{3}$$

Proposition 7 (simple rotation). *A 2×2 rotation matrix through angle θ is*

$$Q_\theta := \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}.$$

We have $Q \in SO(2)$ if and only if $Q = Q_\theta$ for some $\theta \in \mathbb{R}$.

Proof $\quad Q_\theta \in SO(2) \qquad$ Write $\quad c, s = \cos\theta, \sin\theta,$

so

$$Q_\theta = \begin{bmatrix} c & -s \\ s & c \end{bmatrix}$$

then

$$Q_\theta^T Q_\theta = \begin{bmatrix} c & s \\ -s & c \end{bmatrix}\begin{bmatrix} c & -s \\ s & c \end{bmatrix} = \begin{bmatrix} c^2+s^2 & -sc+cs \\ 0 & s^2+c^2 \end{bmatrix}$$

$$= I.$$

Also $\quad \det Q_\theta = c^2 + s^2 = 1.$

$$\boxed{Q \in SO(2) \Rightarrow \exists\, \theta \text{ s.t. } Q = Q_\theta}$$

Write

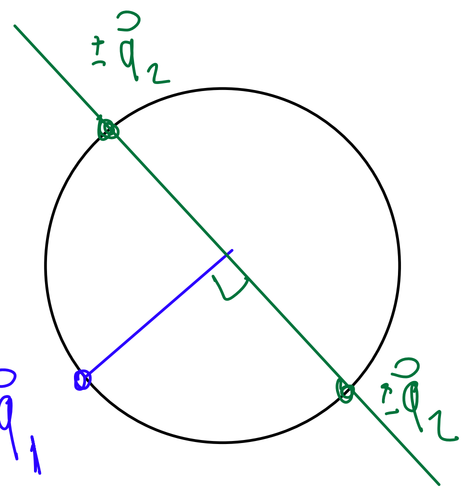
new def for c, s

$$Q = \left[\vec q_1 \,\middle|\, \vec q_2\right] = \begin{bmatrix} c & t \\ s & d \end{bmatrix}$$

We know

$$Q^TQ = I \Rightarrow \|\vec q_k\| = 1 \quad \& \quad \underbrace{\vec q_1^{\,T} \vec q_2}_{\text{orthogonal}} = 0$$

$$\begin{bmatrix} \vec q_1^{\,T} \vec q_1 & \vec q_1^{\,T} \vec q_2 \\ q_2^T q_1 & q_2^T q_2 \end{bmatrix}$$



$$\begin{bmatrix} c \\ s \end{bmatrix} = \vec q_1$$

ie $\vec q_2 = \pm \begin{bmatrix} -s \\ c \end{bmatrix}$

But $+1 = \det Q = cd - st = \pm(c^2 + s^2)$

must be +

$$\Rightarrow \quad \vec{q}_2 = \begin{bmatrix} -s \\ c \end{bmatrix}$$

ie, $\quad c = \cos\theta, \quad s = \sin\theta \quad$ for $\quad \theta = \operatorname{atan}(s, c)$.

Proposition 8 (rotation of a vector). *The matrix*

No trig!

$$Q = \frac{1}{\sqrt{a^2+b^2}} \begin{bmatrix} a & b \\ -b & a \end{bmatrix}$$

is a rotation matrix ($Q \in SO(2)$) *satisfying*

$$Q \underbrace{\begin{bmatrix} a \\ b \end{bmatrix}}_{\vec{x}} = \underbrace{\sqrt{a^2+b^2}}_{\|\vec{x}\|} \underbrace{\begin{bmatrix} 1 \\ 0 \end{bmatrix}}_{\vec{e}_1}$$

Proof $Q \in SO(2)$ since:

$$Q^T Q = \frac{1}{a^2+b^2} \begin{bmatrix} a & -b \\ b & a \end{bmatrix} \begin{bmatrix} a & b \\ -b & a \end{bmatrix} = \begin{bmatrix} a^2+b^2 & 0 \\ 0 & a^2+b^2 \end{bmatrix} \frac{1}{a^2+b^2}$$

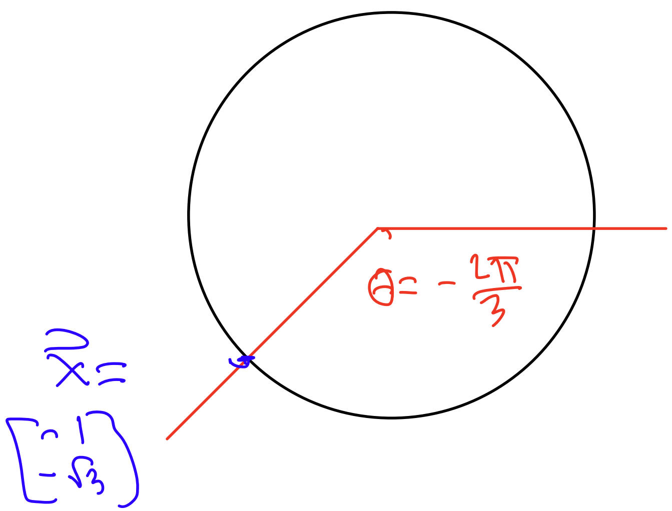
$$= I$$

& $\det Q = \dfrac{a^2+b^2}{a^2+b^2} = 1,$

Also $\quad Q\begin{bmatrix} a \\ b \end{bmatrix} = \frac{1}{\sqrt{a^2+b^2}}\begin{bmatrix} a & b \\ -b & a \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \frac{1}{\sqrt{a^2+b^2}}\begin{bmatrix} a^2+b^2 \\ 0 \end{bmatrix}$

Example 15 (rotating a vector).

$$\vec{x} = \begin{bmatrix} -1 \\ -\sqrt{3} \end{bmatrix} =: \begin{bmatrix} a \\ b \end{bmatrix}$$



$\boxed{\text{Method 1}}$ Use

$$Q_{-\theta} = \begin{bmatrix} \cos\frac{2\pi}{3} & -\sin\frac{2\pi}{3} \\ \sin\frac{2\pi}{3} & \cos\frac{2\pi}{3} \end{bmatrix}$$

Lots of trig?

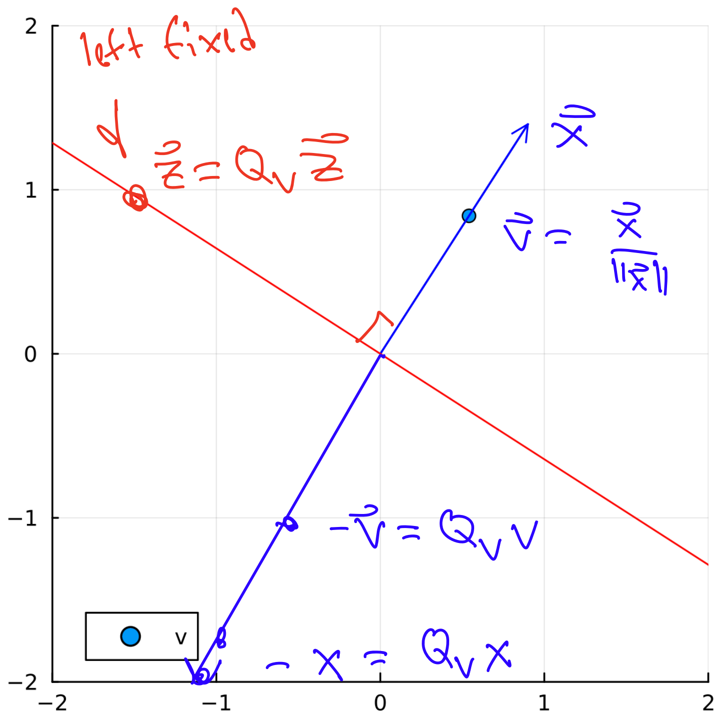
$\boxed{\text{Method 2}}$ $\quad Q := \frac{1}{\sqrt{1+3}}\begin{bmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix}$

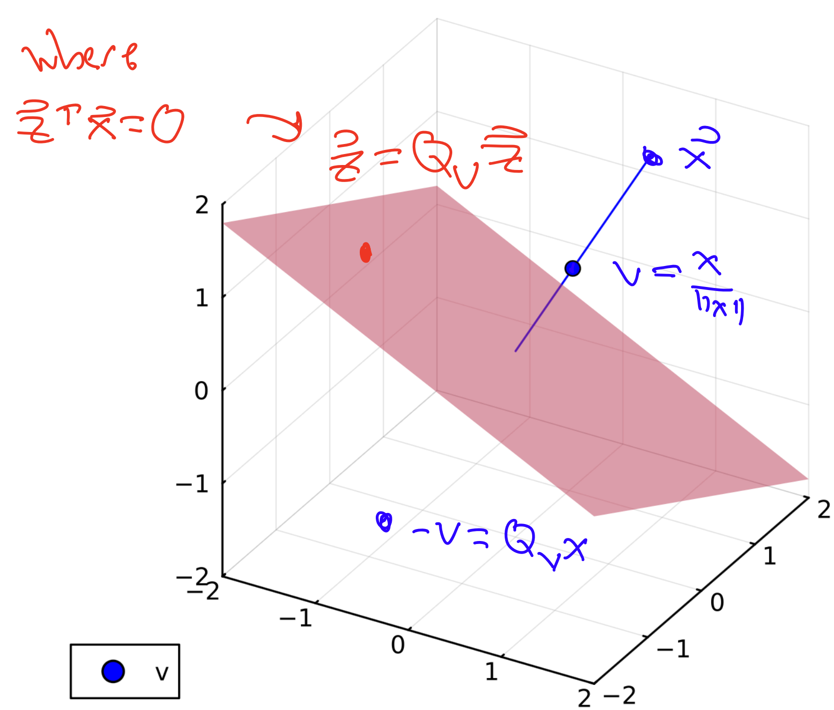
so that

$$Q\begin{bmatrix}-1\\-\sqrt{3}\end{bmatrix} = \frac{1}{2}\begin{bmatrix}-1 & -\sqrt{3}\\ \sqrt{3} & -1\end{bmatrix}\begin{bmatrix}-1\\-\sqrt{3}\end{bmatrix} = \begin{bmatrix}2\\0\end{bmatrix}$$

III.4.2 Reflections

Every unit vector corresponds to a $\underbrace{\text{reflection}}_{Q_{\vec v}}$, which is unitary





Definition 20 (reflection matrix)**.** Given a unit vector $\boldsymbol{v} \in \mathbb{C}^n$ (satisfying $\|\boldsymbol{v}\| = 1$), define the corresponding *reflection matrix* as:

$$\underbrace{Q_{\boldsymbol{v}}}_{Q :=} := I - \underbrace{2\boldsymbol{v}\boldsymbol{v}^\star}_{\text{outer product}}$$

Properties

Symmetry ① $Q^* = (I - 2vv^*)^* = I - 2vv^* = Q$

Unitary ② $Q^*Q = Q^2 = (I - 2vv^*)(I - 2vv^*)$

$= I - 4vv^* + 4v\underbrace{(v^*v)}_{=1}v^* = I$

③ $Q\vec{v} = (I - 2vv^*)v$

$= v - 2v\underbrace{(v^*v)}_{=1} = -v$

ie $\vec{v}$ is an eigenvector of Q w/ ev -1.

4 $\quad W := \vec{v}^{\perp} = \underbrace{\{ \vec{w} \in \mathbb{C}^n : \vec{w}^* \vec{v} = 0 \}}_{\text{dim } n-1}$

For all $\vec{w} \in W$

$$Q w = w - 2\vec{v}\underbrace{(v^* w)}_{=0} = \vec{w}.$$

5 $\quad \det Q = (-1)\underbrace{(1 \text{———} 1)}_{\substack{n-1 \text{ evs} \\ \text{of } 1}} = -1$

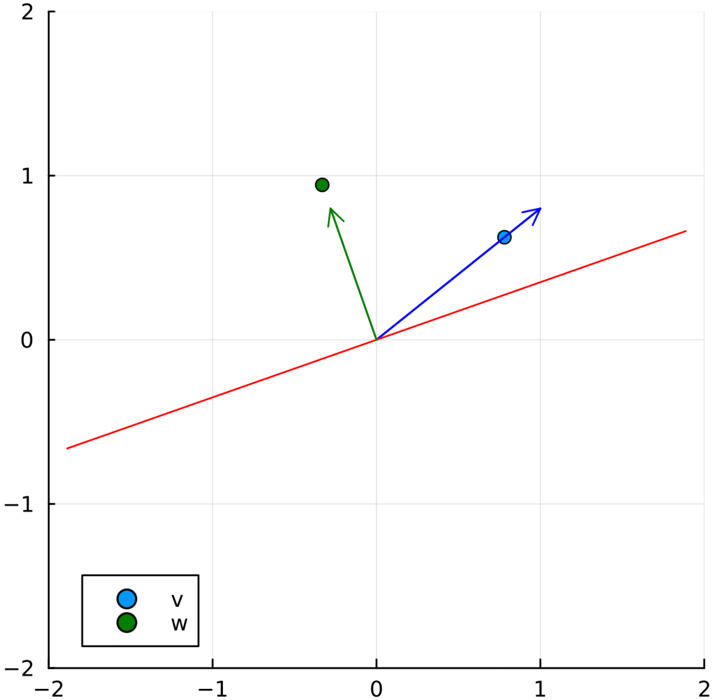
product of eigenvalues

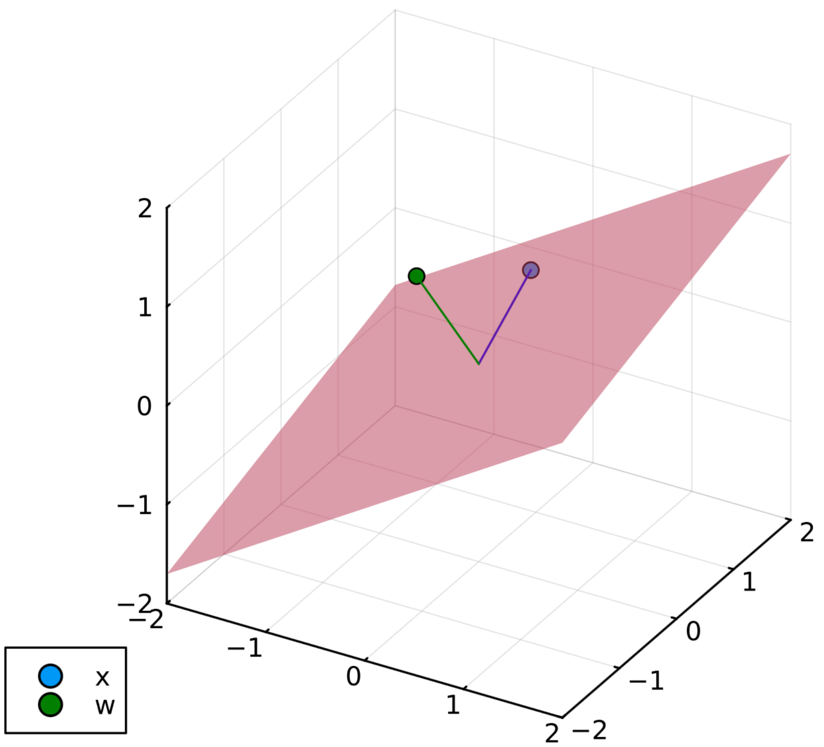
$$\Rightarrow Q \notin SO(n).$$

Example 16 (reflection through 2-vector)**.**

Householder reflections

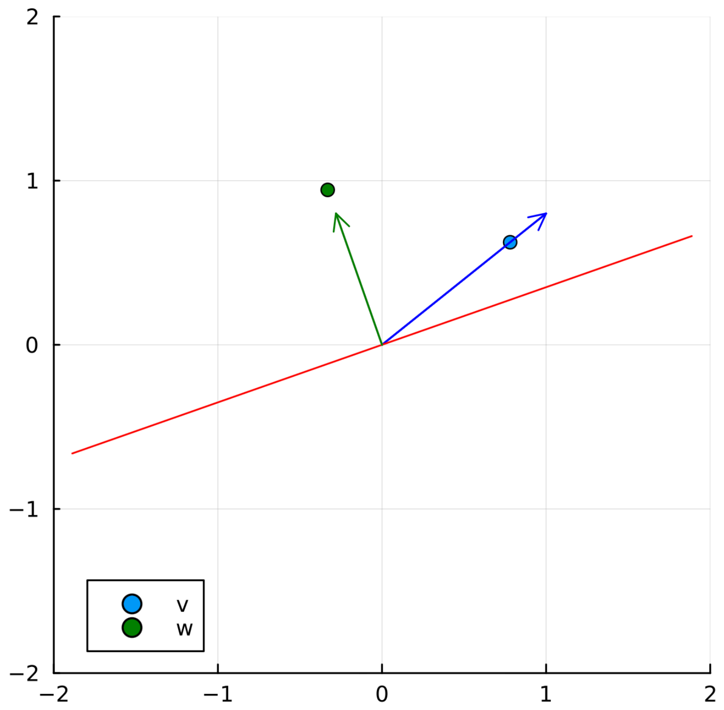
Reflect to the x-axis

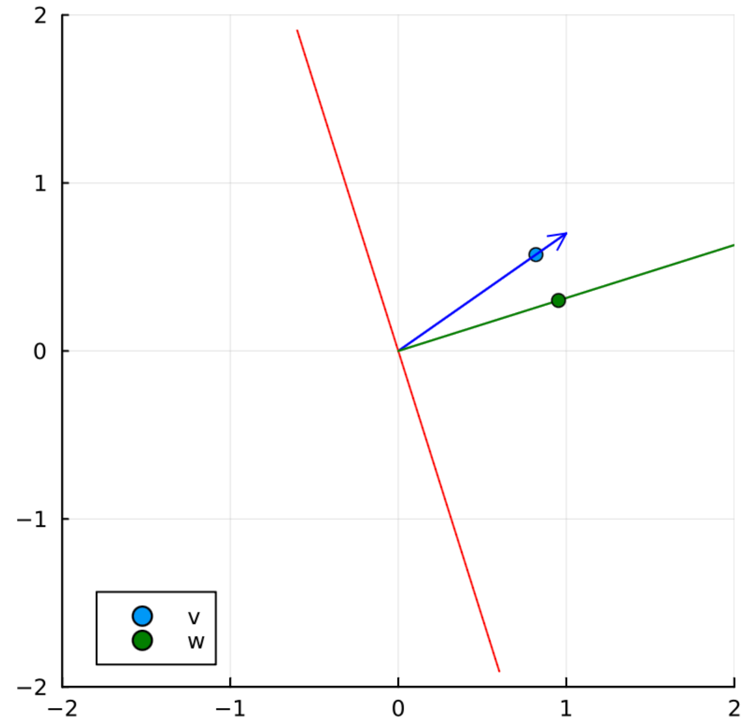




Householder reflections

Reflect to the x-axis (2 ways)





Definition 21 (Householder reflection, real case)**.** For a given vector $\boldsymbol{x} \in \mathbb{R}^n$, define the Householder reflection

$$Q_{\boldsymbol{x}}^{\pm,\mathrm{H}} := Q_{\boldsymbol{w}}$$

for $\boldsymbol{y} = \mp\|\boldsymbol{x}\|\boldsymbol{e}_1 + \boldsymbol{x}$ and $\boldsymbol{w} = \frac{\boldsymbol{y}}{\|\boldsymbol{y}\|}$. The default choice in sign is:

$$Q_{\boldsymbol{x}}^{\mathrm{H}} := Q_{\boldsymbol{x}}^{-\mathrm{sign}(x_1),\mathrm{H}}.$$

Definition 22 (Householder reflection, complex case)**.** For a given vector $\boldsymbol{x} \in \mathbb{C}^n$, define the Householder reflection as

$$Q_{\boldsymbol{x}}^{\mathrm{H}} := Q_{\boldsymbol{w}}$$

for $\boldsymbol{y} = \operatorname{csign}(x_1)\|\boldsymbol{x}\|\boldsymbol{e}_1 + \boldsymbol{x}$ and $\boldsymbol{w} = \frac{\boldsymbol{y}}{\|\boldsymbol{y}\|}$, for $\operatorname{csign}(z) = \mathrm{e}^{\mathrm{i}\arg z}$.

Lemma 6 (Householder reflection maps to axis, complex case)**.** *For* $\boldsymbol{x} \in \mathbb{C}^n$,

$$Q_{\boldsymbol{x}}^{\mathrm{H}}\boldsymbol{x} = -\operatorname{csign}(x_1)\|\boldsymbol{x}\|\boldsymbol{e}_1$$