MATH50003
Numerical Analysis

III.4 Orthogonal and Unitary Matrices

Dr Sheehan Olver

Chapter III

Numerical Linear Algebra

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

LU factorisation: $A = LU$

PLU factorisation: $A = P^\top LU$

Cholesky factorisation: $A = LL^\top$

QR factorisation: $A = QR$

Motivation: least squares

For rectangular systems, find vector that matches "closest"

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

$$A\mathbf{x} \approx \mathbf{b}$$

by minimising

$$\|A\mathbf{x} - \mathbf{b}\|$$

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

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

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

$$U(n) = \{Q \in \mathbb{C}^{n\times n} : Q^\star Q = I\}.$$

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

Properties of orthogonal/unitary matrices

III.3.1 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:

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

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* $\theta \in \mathbb{R}$.

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

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

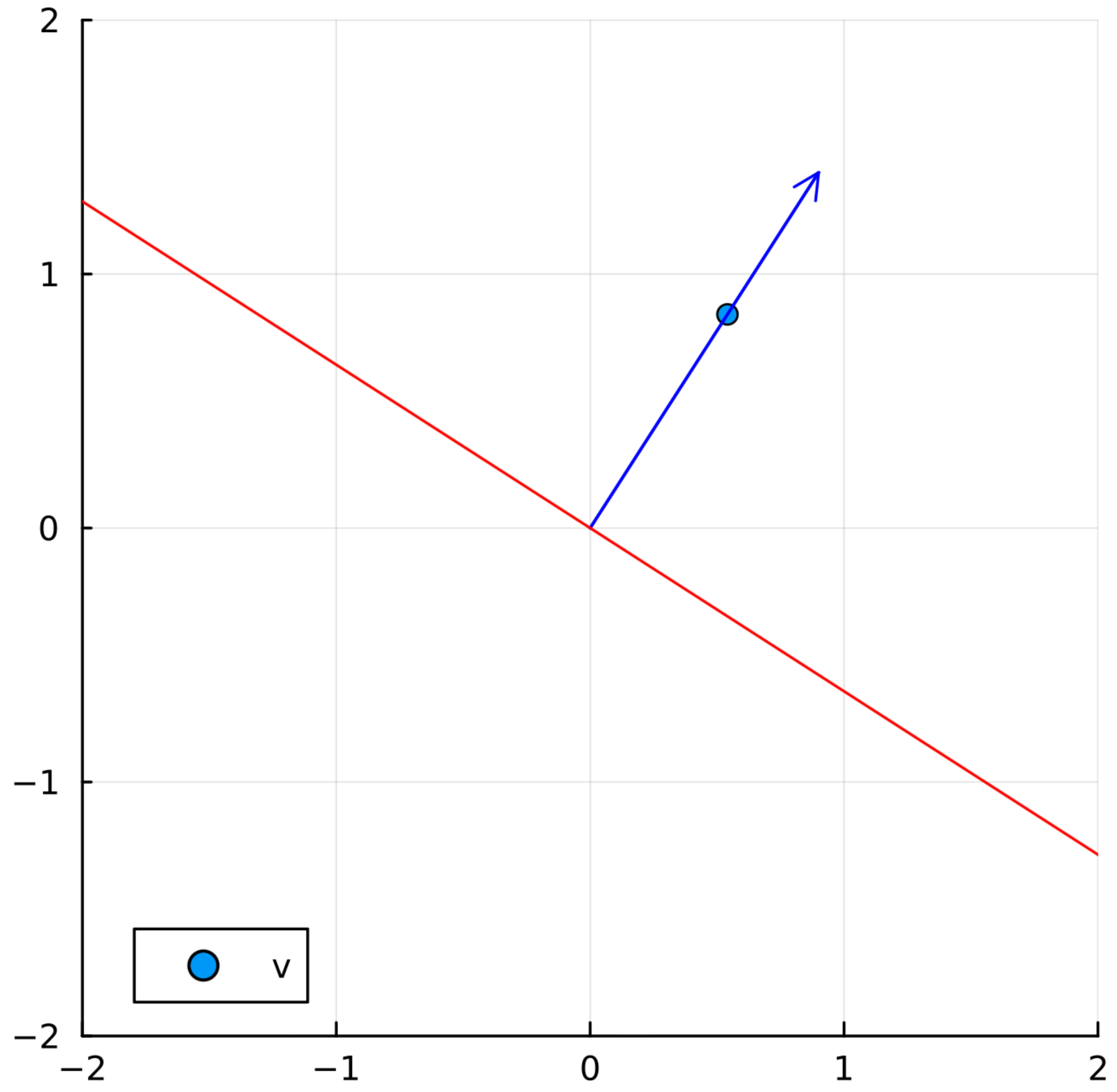
is a rotation matrix ($Q \in SO(2)$) satisfying

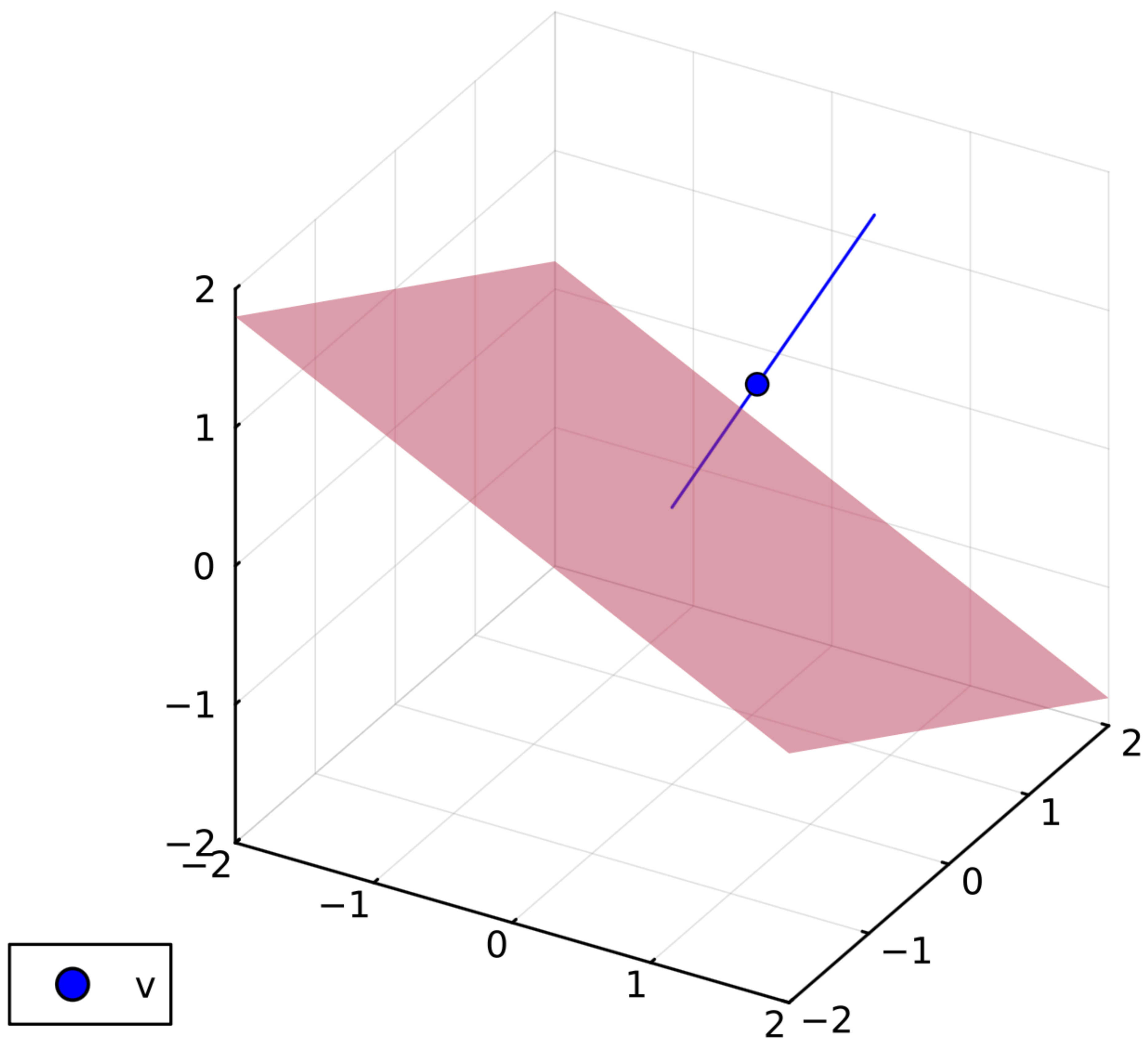
$$Q \begin{bmatrix} a \\ b \end{bmatrix} = \sqrt{a^2+b^2} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Example 15 (rotating a vector)**.**

III.4.2 Reflections

Every unit vector corresponds to a reflection, which is unitary





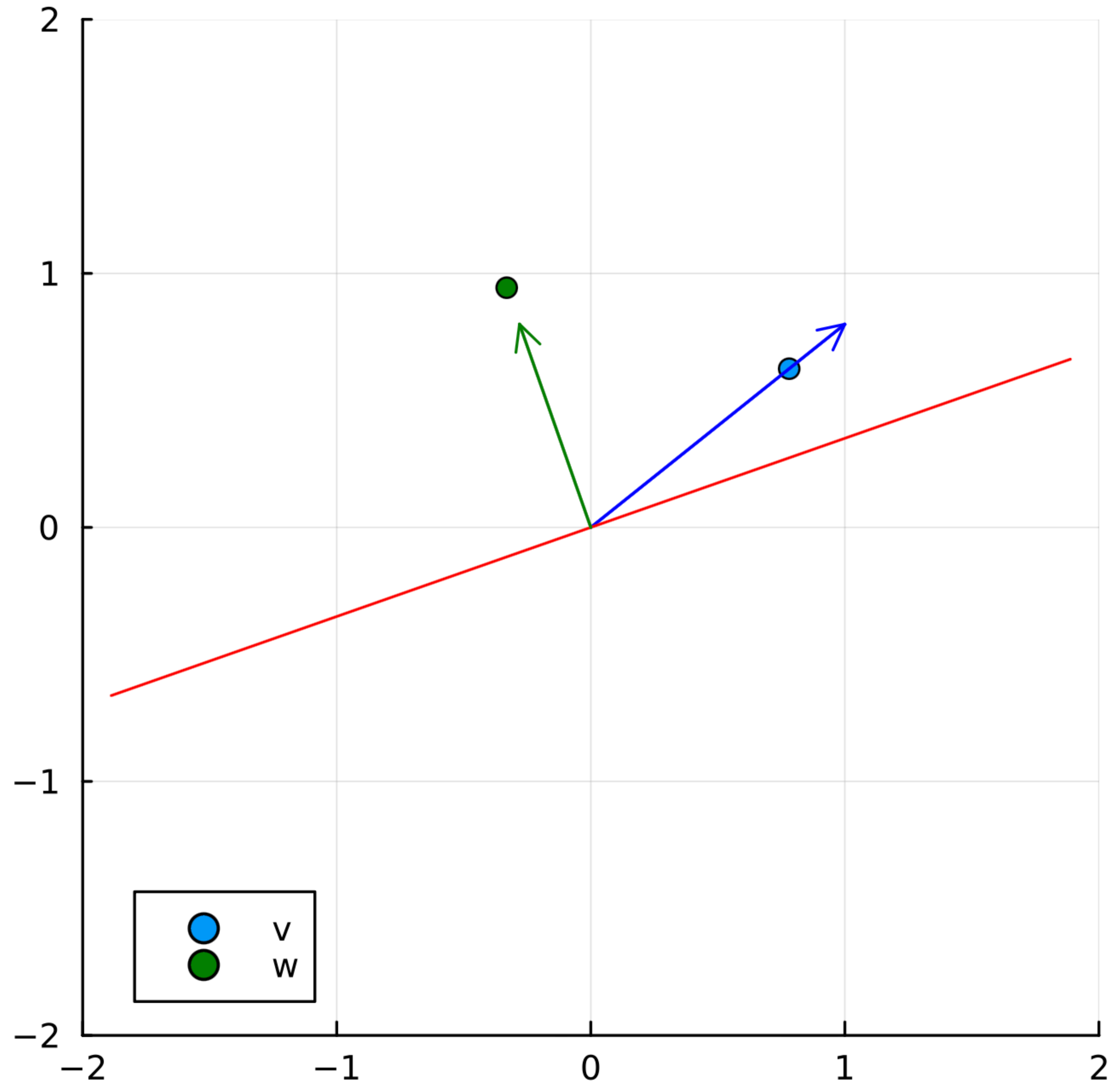
Definition 20 (reflection matrix)**.** Given a unit vector $\boldsymbol{v} \in \mathbb{C}^n$ (satisfying $\|\boldsymbol{v}\| = 1$), define the corresponding *reflection matrix* as:

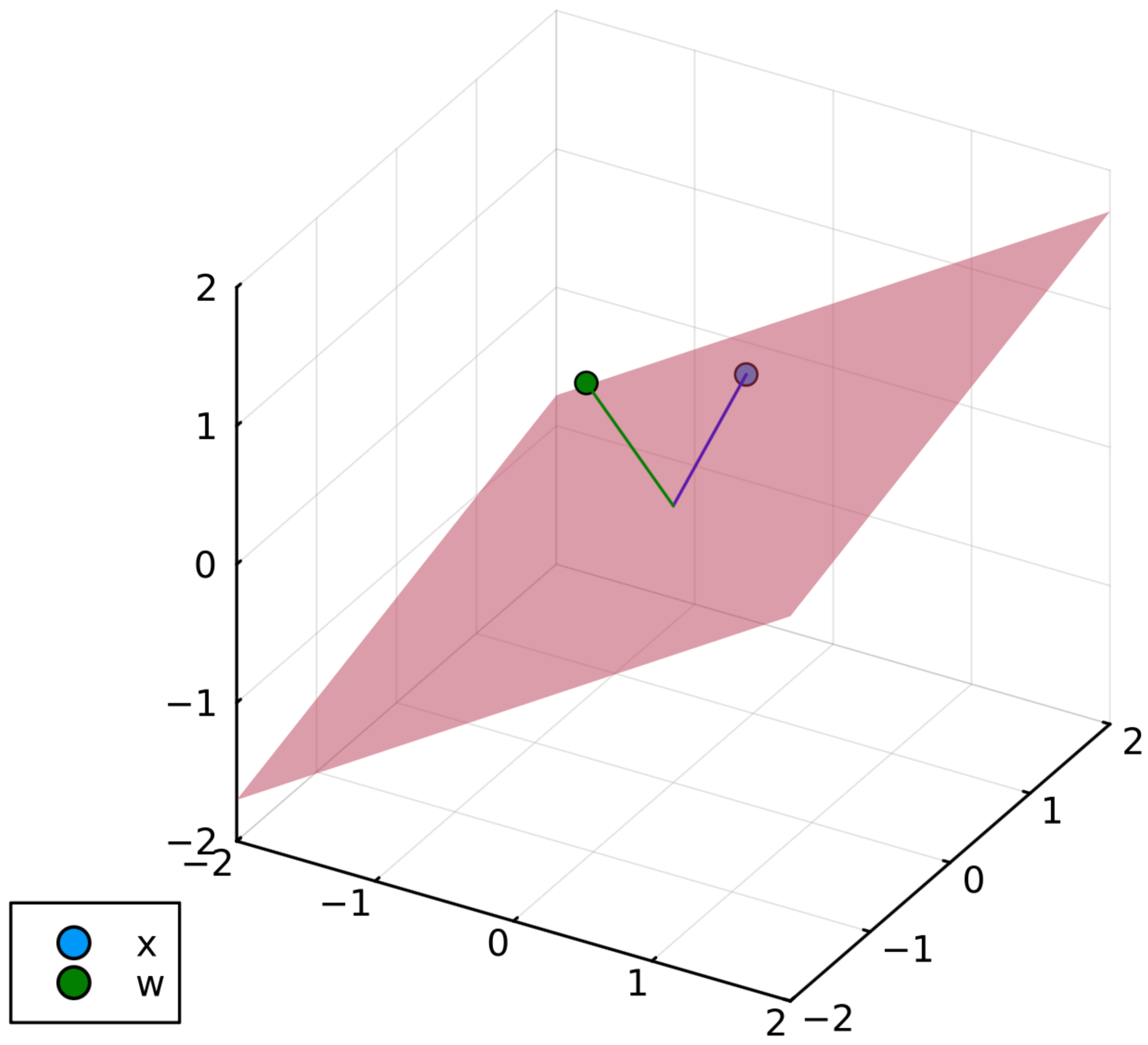
$$Q_{\boldsymbol{v}} := I - 2\boldsymbol{v}\boldsymbol{v}^\star$$

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

Householder reflections

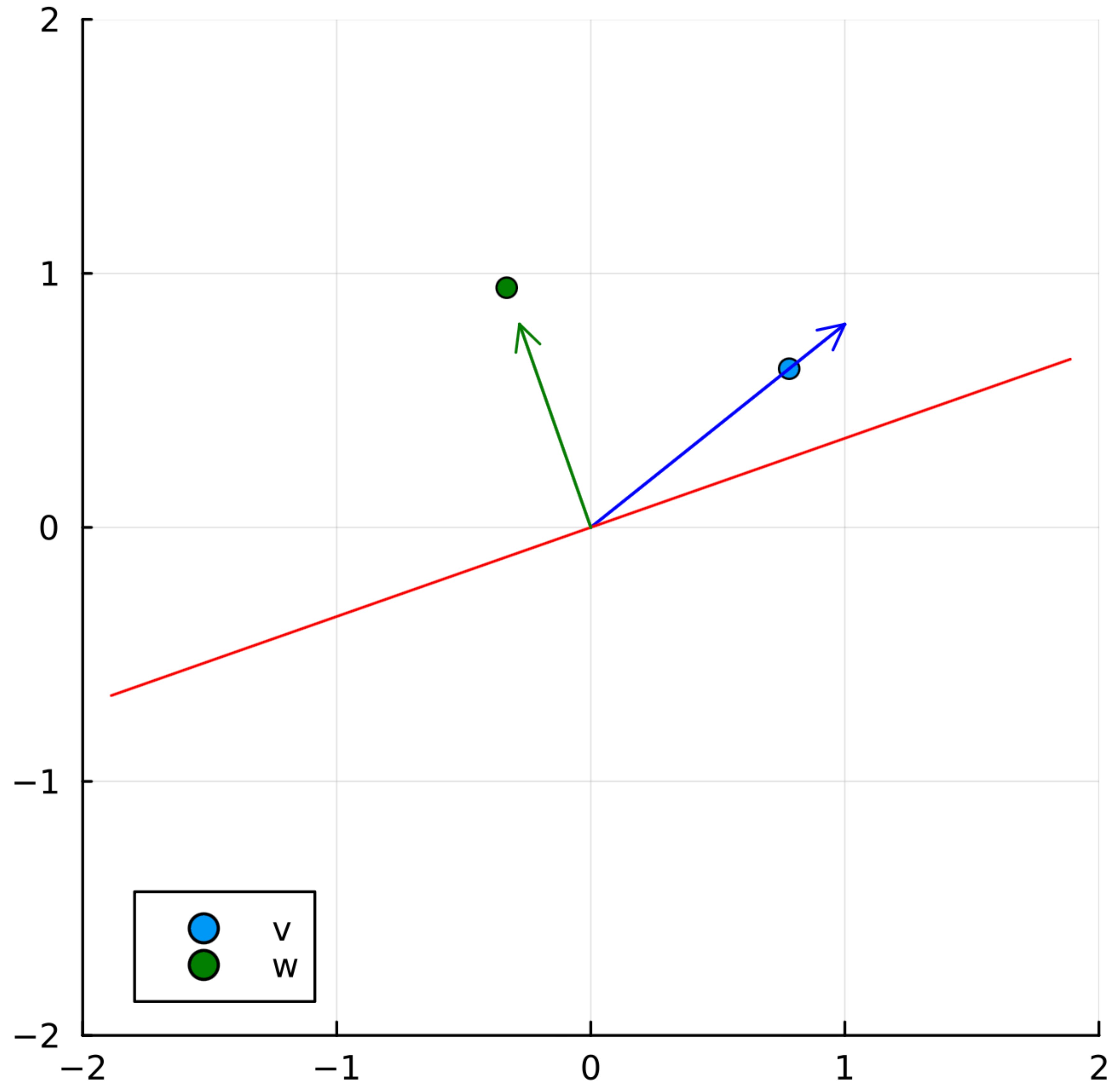
Reflect to the x-axis

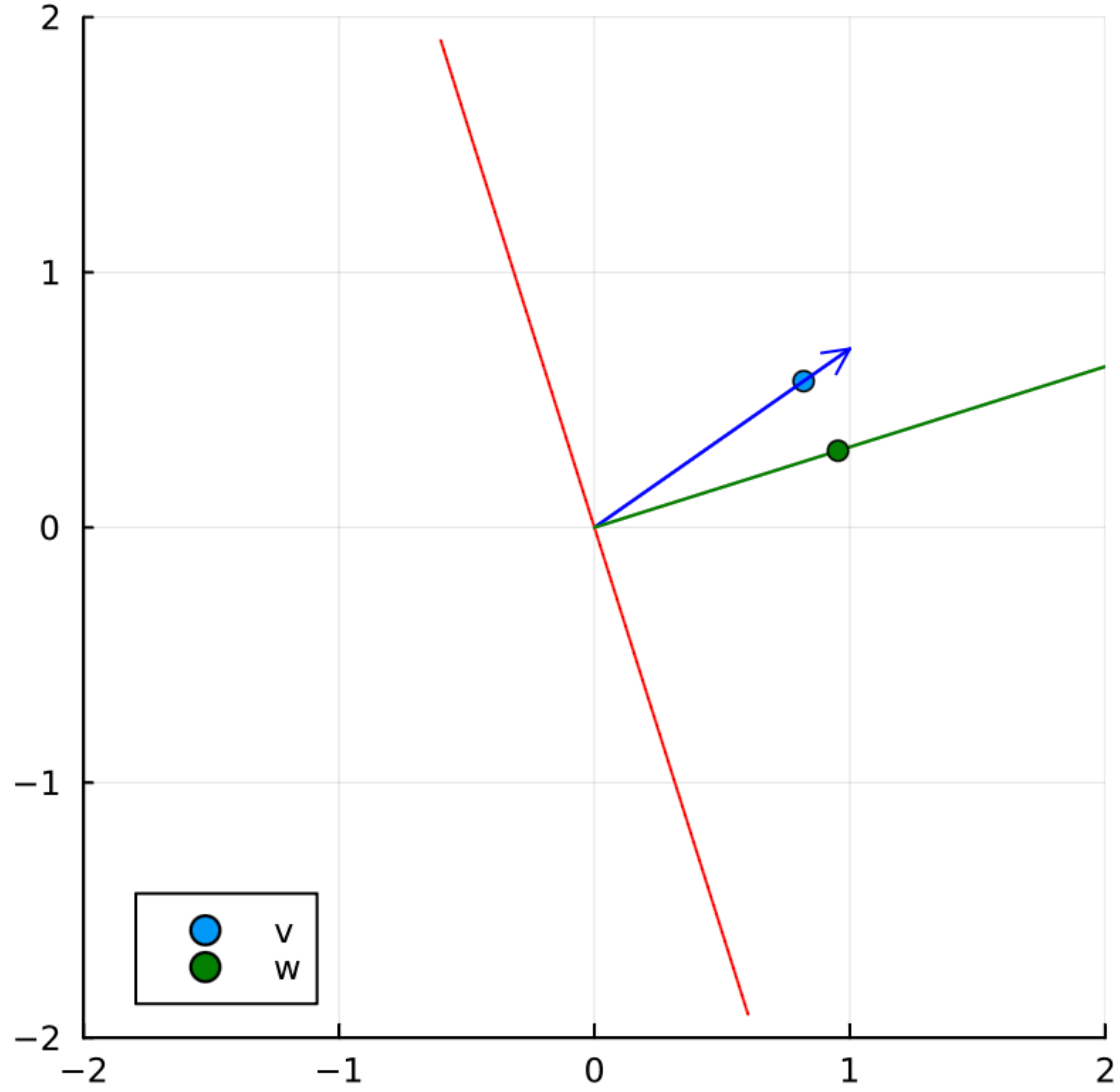




Householder reflections

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* $\boldsymbol{x} \in \mathbb{C}^n$,

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