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THE LEAST SQUARES PROBLEM

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THE LEAST SQUARES PROBLEM

QR decomposition

Another useful viewpoint is reached by rewriting the equations $Q^T A = R$ as

$$A = QR$$

A is a product QR where Q is orthogonal and R is upper triangular.

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QR decomposition

Example 1 We will use a QR decomposition to solve the system

$$\begin{bmatrix} 1 & 2 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}.$$

First we require Q such that $Q^T \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} * \\ 0 \end{bmatrix}$. with $x_1 = 1$ and $x_2 = 1$ to get $c = \cos\theta = 1/\sqrt{2}$ and $s = \sin\theta = 1/\sqrt{2}$. Then

$$Q = \begin{bmatrix} c & -s \\ s & c \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$$

, and

$$R = Q^T A = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 1 & 3 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 2 & 5 \\ 0 & 1 \end{bmatrix}.$$

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QR decomposition

Solving $Qc = b$, we have

$$c = Q^T b = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 3 \\ 1 \end{bmatrix}.$$

Finally we solve $Rz = c$ by back substitution and get $z_2 = 1$ and $z_1 = -1$.

Exercice Use a QR decomposition to solve the linear system

$$\begin{bmatrix} 2 & 3 \\ 5 & 7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 12 \\ 29 \end{bmatrix}.$$

QR decomposition

We now turn our attention to $n \times n$ matrices. A *plane rotator* is a matrix of the form

$$Q = \begin{array}{cc} \begin{bmatrix} 1 & & & & & & & & & & \\ & \ddots & & & & & & & & & \\ & & 1 & & & & & & & & \\ & & & c & & & & -s & & & \\ & & & & 1 & & & & & & \\ & & & & & \ddots & & & & & \\ & & & & & & 1 & & & & \\ & & & s & & & & c & & & \\ & & & & & & & & 1 & & \\ & & & & & & & & & \ddots & \\ & & & & & & & & & & 1 \end{bmatrix} & \begin{matrix} \\ \\ \\ \leftarrow i \\ \\ \\ \\ \leftarrow j \\ \\ \\ \\ \end{matrix} \\ \begin{matrix} \qquad\qquad\qquad \uparrow \qquad\qquad\qquad\qquad \uparrow \\ \qquad\qquad\qquad i \qquad\qquad\qquad\qquad j \end{matrix} & \end{array}$$

1

$$c = \cos\theta, \qquad s = \sin\theta.$$

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QR decomposition

All of the entries that have not been filled in are zeros. Thus a plane rotator looks like an identity matrix, except that one pair of rows and columns contains a rotator. Plane rotators are used extensively in matrix computations. They are sometimes called *Givens rotators* or *Jacobi rotators*, depending on the context . We will usually drop the adjective “plane” and refer simply to *rotators*.

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QR decomposition

The geometric interpretation of the action of a plane rotator is clear. All vectors lying in the $x_i x_j$ plane are rotated through an angle θ. All vectors orthogonal to the $x_i x_j$ plane are left fixed. A typical vector x is neither in the $x_i x_j$ plane nor orthogonal to it but can be expressed uniquely as a sum $x = p + p^{\perp}$, where p is in the $x_i x_j$ plane, and $p^{\perp}$ is orthogonal to it. The plane rotator rotates p through an angle θ and leaves $p^{\perp}$ fixed.

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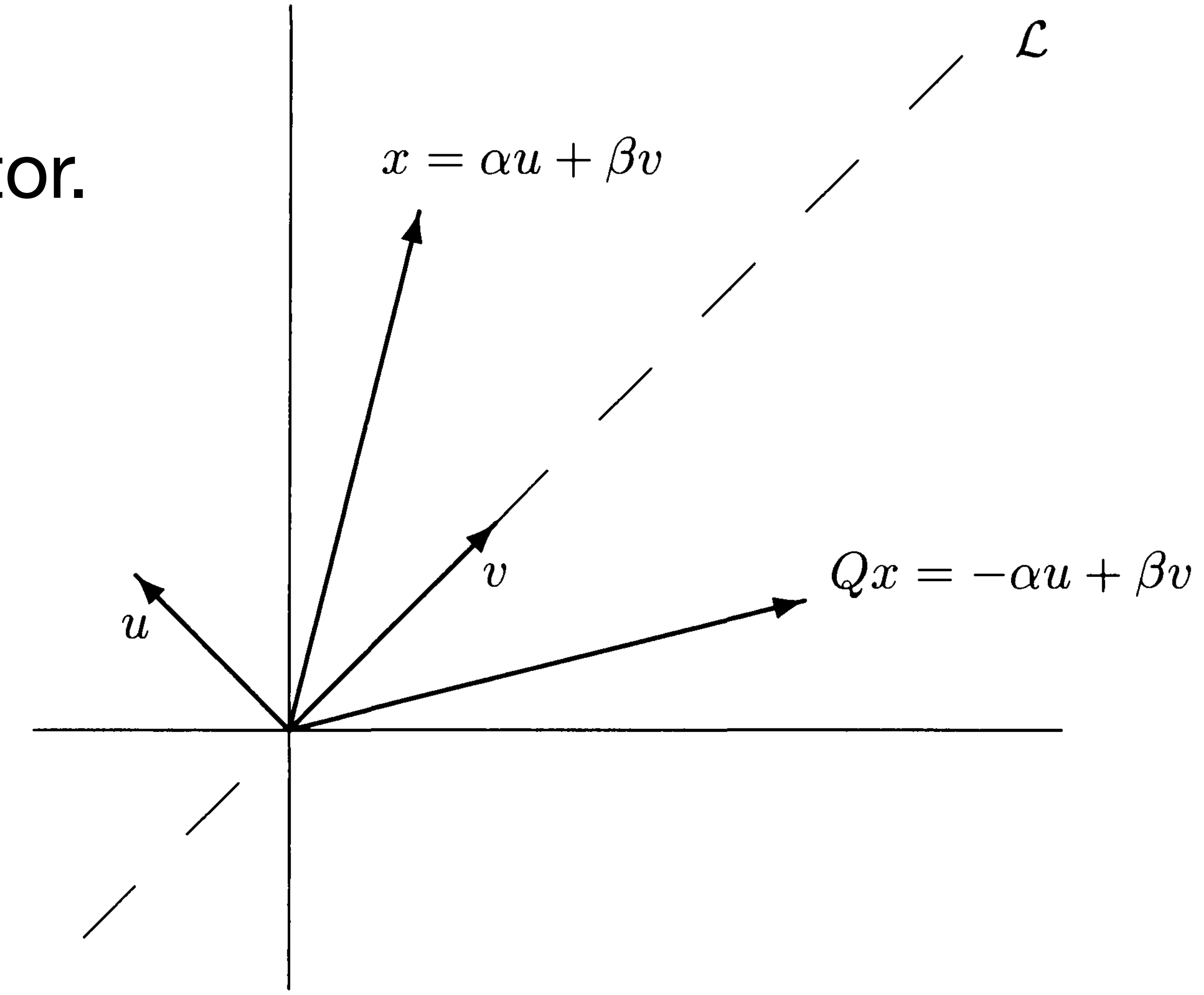
QR decomposition

Theorem *Let $A \in \mathbb{R}^{n \times n}$. Then there exists an orthogonal matrix Q and an upper triangular matrix R such that $A = QR$.*

Reflector

We consider first the case $n = 2$ and $\mathscr{L} \in \mathbb{R}^2$ that passes through the origin

The operator that reflects any vector of $\mathbb{R}^2$ is a linear operator. We can then find its matrix representation.



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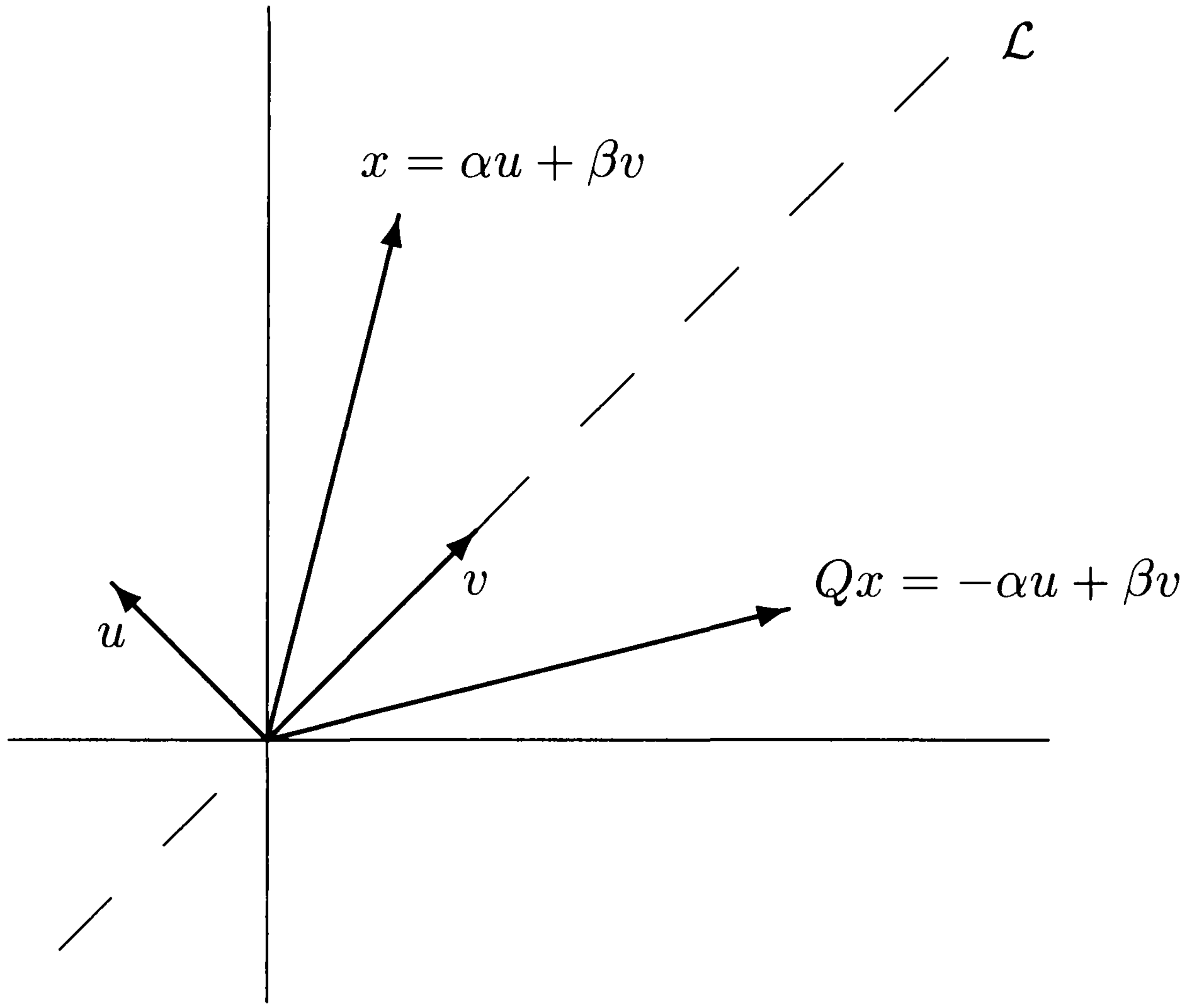
QR decomposition



Let v be a nonzero vector lying in $\mathcal{L}$. Then every vector that lies in $\mathcal{L}$ is a multiple of v. Let u be a nonzero vector orthogonal to $\mathcal{L}$. Then $\{u, v\}$ is a basis of $\mathbb{R}^2$, so every $x \in \mathbb{R}^2$ can be expressed as a linear combination of u and v: $x = \alpha u + \beta v$. The reflection of x through $\mathcal{L}$ is $-\alpha u + \beta v$, so the matrix Q of the reflection must satisfy $Q(\alpha u + \beta v) = -\alpha u + \beta v$ for all α and β. For this it is necessary and sufficient that

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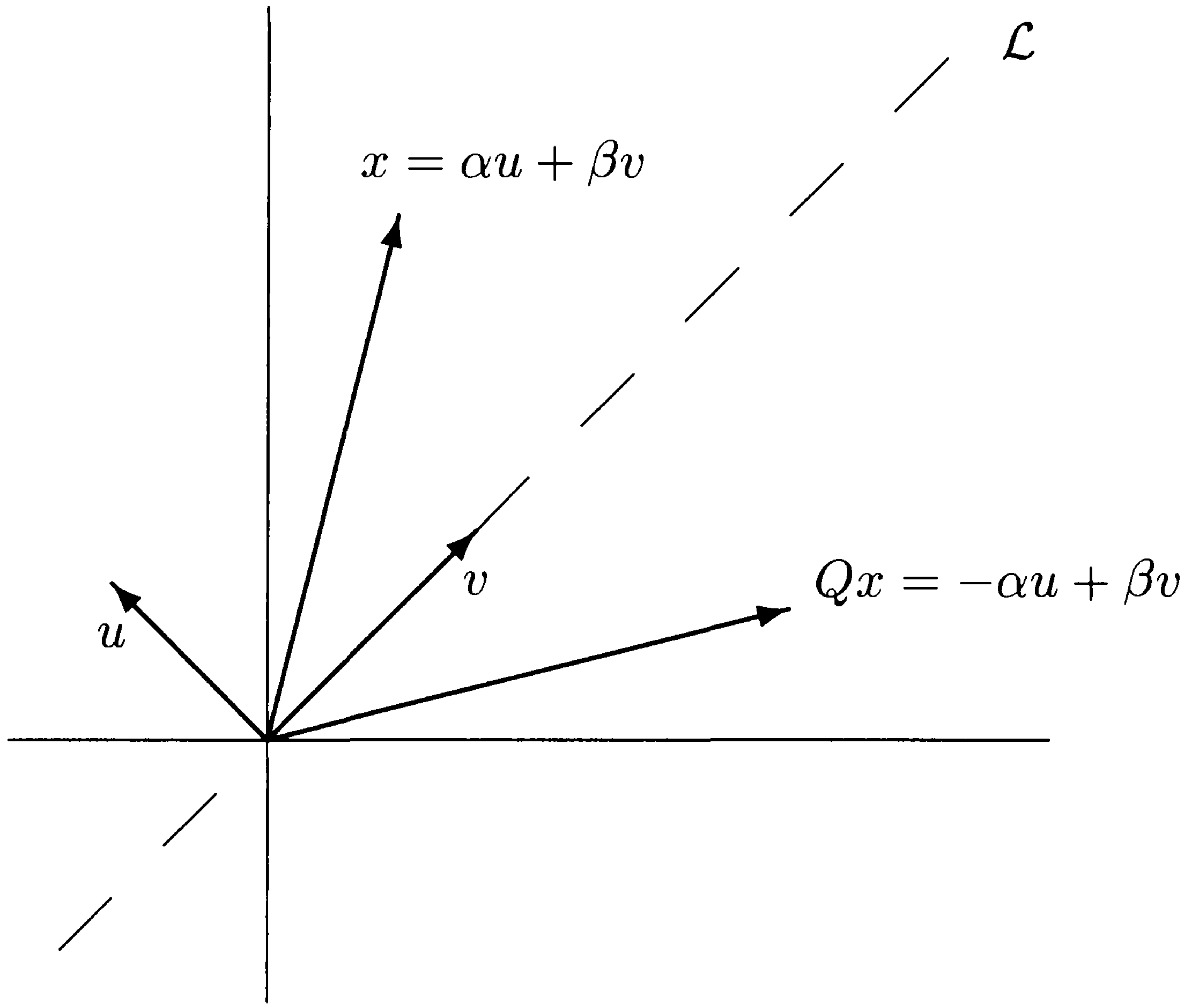
QR decomposition

Reflector



For this it is necessary and sufficient that

$$Qu = -u \qquad \text{and} \qquad Qv = v.$$

We can assume that u is chosen to be a unite vector: $||u||_2 = 1$

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Reflector

Let consider the matrix P, with no special property such that $P = uu^T$

We have $Pu = (uu^T)u = u(u^T u) = u\|u\|_2^2 = u$

and $Pv = (uu^T)v = u(u^T v) = 0$, because u and v are orthogonal.

Let
$$Q = I - 2P$$

Then
$$Qu = u - 2Pu = -u$$

, and
$$Qv = v - 2Pv = v.$$

The matrix $Q \in \mathbb{R}^{2\times 2}$ that reflects vectors through the $\mathscr{L}$.

Reflector

Theorem 1 *Let* $u \in \mathbb{R}^n$ *with* $\|u\|_2 = 1$, *and define* $P \in \mathbb{R}^{n \times n}$ *by* $P = uu^T$. *Then*

(a) $Pu = u$.

(b) $Pv = 0$ *if* $\langle u, v \rangle = 0$.

(c) $P^2 = P$.

(d) $P^T = P$.

Proof: try yourself

Remark A matrix satisfying $P^2 = P$ is called a *projector* or *idempotent*. A projector that is also symmetric ($P^T = P$) is called an *orthoprojector*. The matrix $P = uu^T$ has rank 1, since its range consists of multiples of u. Thus the properties of P can be summarized by saying that P is a rank-1 orthoprojector. $\square$

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Theorem 2 *Let* $u \in \mathbb{R}^n$ *with* $\|u\|_2 = 1$*, and define* $Q \in \mathbb{R}^{n\times n}$ *by* $Q = I - 2uu^T$*. Then*

(a) $Qu = -u$.

(b) $Qv = v$ *if* $\langle u, v\rangle = 0$.

(c) $Q = Q^T$ *(*Q *is symmetric).*

(d) $Q^T = Q^{-1}$ *(*Q *is orthogonal).*

(e) $Q^{-1} = Q$ *(*Q *is an involution).*

Proposition 3 *Let* u *be a nonzero vector in* $\mathbb{R}^n$*, and define* $\gamma = 2/\|u\|_2^2$ *and* $Q = I - \gamma uu^T$*. Then* Q *is a reflector satisfying*

(a) $Qu = -u$.

(b) $Qv = v$ *if* $\langle u, v\rangle = 0$.

Proof. Let $\hat{u} = u/\|u\|_2$. Then $\|\hat{u}\| = 1$, and it is a simple matter to check that $Q = I - 2\hat{u}\hat{u}^T$. Properties (a) and (b) follow easily. $\square$

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Proposition 4 *Let u be a nonzero vector in $\mathbb{R}^n$, and define $\gamma = 2/\|u\|_2^2$ and $Q = I - \gamma uu^T$. Then Q is a reflector satisfying*

(a) $Qu = -u$.

(b) $Qv = v$ *if* $\langle u, v \rangle = 0$.

Proof. Let $\hat{u} = u/\|u\|_2$. Then $\|\hat{u}\| = 1$, and it is a simple matter to check that $Q = I - 2\hat{u}\hat{u}^T$. Properties (a) and (b) follow easily. $\square$

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Theorem 5 *Let x, $y \in \mathbb{R}^n$ with $x \neq y$ but $\|x\|_2 = \|y\|_2$. Then there is a unique reflector Q such that $Qx = y$.*

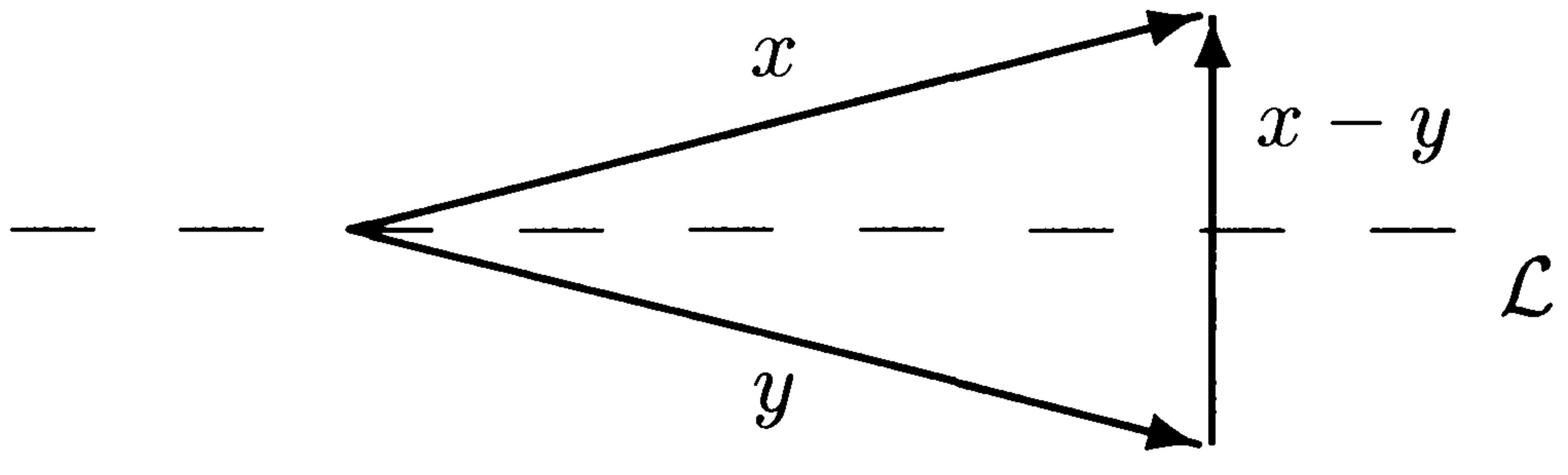
Proof

We must find u such that

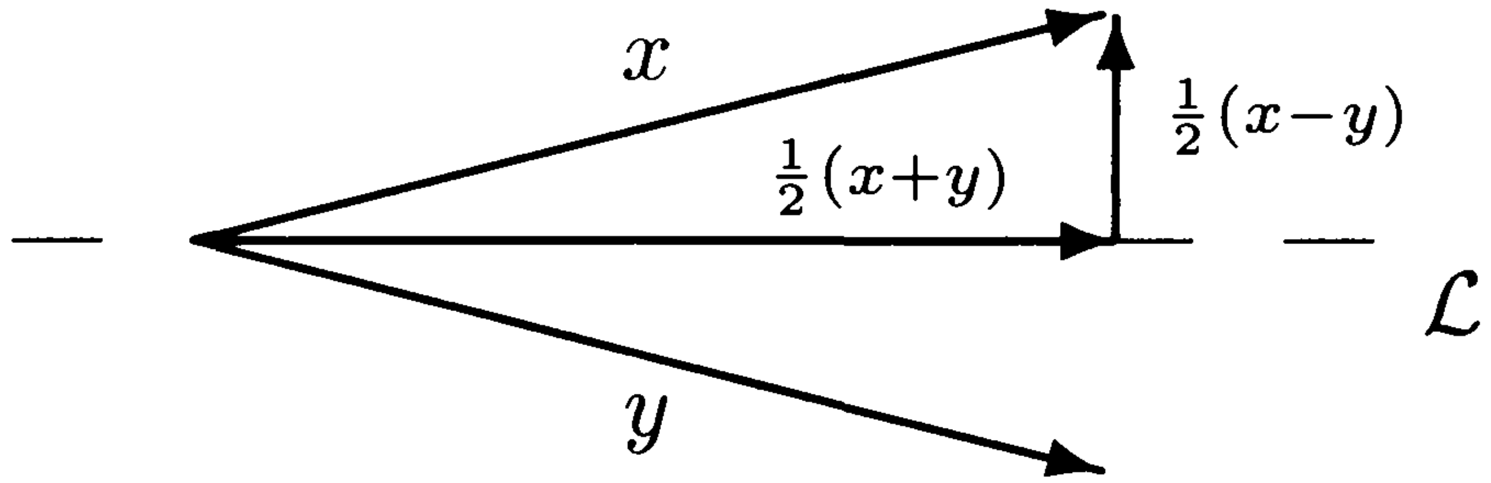
$(I - \gamma u u^T)x = y$, where $\gamma = 2/\|u\|_2^2$.

We consider the line that bisect the angle between x and y

The reflexion of x through this line is y



(a)



Thus we require a vector u that is orthogonal to $\mathcal{L}$. It appears that $u = x - y$, or any multiple thereof, is the right choice.

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Let $u = x - y$, $\gamma = 2/\| u \|_2^2$, and $Q = I - \gamma uu^T$. To prove that $Qx = y$ we first decompose x into a sum:

$$x = \frac{1}{2}(x - y) + \frac{1}{2}(x + y).$$

By part (a) of Proposition 2 $Q(x - y) = y - x$. Part (b) of Figure 3.4 suggests that $x + y$ is orthogonal to u. To check that this is so, we simply compute the inner

$$\begin{aligned} \langle x + y, x - y \rangle &= \langle x, x \rangle + \langle y, x \rangle - \langle x, y \rangle - \langle y, y \rangle \\ &= \| x \|_2^2 + 0 - \| y \|_2^2 = 0, \end{aligned}$$

because $\| x \|_2 = \| y \|_2$. It follows by part (b) of Proposition 2(b) that $Q(x + y) = x + y$. Finally

$$\begin{aligned} Qx &= \frac{1}{2}Q(x - y) + \frac{1}{2}Q(x + y) \\ &= \frac{1}{2}(y - x) + \frac{1}{2}(x + y) = y. \end{aligned}$$

It follows easily from this theorem that reflectors can be used to create zeros in vectors and matrices.

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Corollary 1 *Let $x \in \mathbb{R}^n$ be any nonzero vector. Then there exists a reflector Q such that*

$$Q \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} * \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

Proof. Let $y = [-\tau, \ 0, \ \ldots, \ 0]^T$, where $\tau = \pm\|x\|_2$. By choosing the sign appropriately we can guarantee that $x \neq y$. Clearly $\|x\|_2 = \|y\|_2$. Thus by Theorem 5 there is a reflector Q such that $Qx = y$. □

Let us take a look at the construction suggested in this proof. The reflector is $Q = I - \gamma u u^T$, where

$$u = x - y = \begin{bmatrix} \tau + x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

SOLUTION TO LEAST SQUARES PROBLEM
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and $\gamma = 2/\|u\|_2^2$. Any multiple of this u will generate the same reflector. It turns out to be convenient to normalize u so that its first entry is 1. Thus we will take

$$u = (x - y)/(\tau + x_1) = \begin{bmatrix} 1 \\ x_2/(\tau + x_1) \\ \vdots \\ x_n/(\tau + x_1) \end{bmatrix}$$

We require that $\tau = \pm\|x\|_2$. In theory both sign can work but in practice we choose to be of the same sign as x_1 .

SOLUTION TO LEAST SQUARES PROBLEM
Reflector

Example: Let see how we can Reflectors to create zeros in a vector

Given a vector $x = \begin{pmatrix} 4 \\ 3 \end{pmatrix}$, we want to reflect x to align it with the x-axis. We want to transform x into $y = \begin{pmatrix} \|x\| \\ 0 \end{pmatrix}$, where $\|x\|$ is the Euclidean norm.

Step 1: Compute the reflection vector $\boldsymbol{u}$

First, compute the norm of x:

$$\|x\| = \sqrt{4^2 + 3^2} = \sqrt{16 + 9} = 5$$

Define the vector $e_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ (a standard basis vector). The reflection vector $\boldsymbol{u}$ is computed as:

$$\boldsymbol{u} = x - \|x\|e_1 = \begin{pmatrix} 4 \\ 3 \end{pmatrix} - 5\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} -1 \\ 3 \end{pmatrix}$$

SOLUTION TO LEAST SQUARES PROBLEM
Reflector

Step 2: Normalize $\boldsymbol{u}$

Now, normalize $\boldsymbol{u}$:

$$\boldsymbol{u} = \frac{1}{\sqrt{(-1)^2 + 3^2}} \begin{pmatrix} -1 \\ 3 \end{pmatrix} = \frac{1}{\sqrt{1+9}} \begin{pmatrix} -1 \\ 3 \end{pmatrix} = \frac{1}{\sqrt{10}} \begin{pmatrix} -1 \\ 3 \end{pmatrix}$$

Step 3: Compute the Householder matrix $Q = I - \gamma u u^T$ with $\gamma = 2/\|u\|^2$

Now, we can compute the Householder matrix:

$$Q = I - \gamma u u^T = I - 2\frac{u u^T}{\|u\|^2} = I - 2\frac{u u^T}{u^T u}$$

Here, I is the identity matrix:

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad vv^T = \begin{pmatrix} -1 \\ 3 \end{pmatrix} \begin{pmatrix} -1 & 3 \end{pmatrix} = \begin{pmatrix} 1 & -3 \\ -3 & 9 \end{pmatrix}$$

Thus:

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$$Q = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - 2\frac{1}{10}\begin{pmatrix} 1 & -3 \\ -3 & 9 \end{pmatrix}$$

$$Q = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \frac{1}{5}\begin{pmatrix} 1 & -3 \\ -3 & 9 \end{pmatrix} = \begin{pmatrix} 1 - \frac{1}{5} & \frac{3}{5} \\ \frac{3}{5} & 1 - \frac{9}{5} \end{pmatrix}$$

$$Q = \begin{pmatrix} \frac{4}{5} & \frac{3}{5} \\ \frac{3}{5} & -\frac{4}{5} \end{pmatrix}$$

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Step 4: Apply the transformation

Now, apply the Householder matrix to the vector x:

$$Qx = \begin{pmatrix} \frac{4}{5} & \frac{3}{5} \\ \frac{3}{5} & -\frac{4}{5} \end{pmatrix} \begin{pmatrix} 4 \\ 3 \end{pmatrix} = \begin{pmatrix} \frac{4}{5} \cdot 4 + \frac{3}{5} \cdot 3 \\ \frac{3}{5} \cdot 4 + -\frac{4}{5} \cdot 3 \end{pmatrix}$$

$$Qx = \begin{pmatrix} \frac{16}{5} + \frac{9}{5} \\ \frac{12}{5} - \frac{12}{5} \end{pmatrix} = \begin{pmatrix} \frac{30}{5} \\ \frac{-15}{5} \end{pmatrix} = \begin{pmatrix} 5 \\ 0 \end{pmatrix}$$

Thus, the vector has been successfully reflected, transforming $x = \begin{pmatrix} 4 \\ 3 \end{pmatrix}$ into $\begin{pmatrix} 6 \\ 0 \end{pmatrix}$.

SOLUTION TO LEAST SQUARES PROBLEM
Reflector

Example Consider the vector $x = \begin{bmatrix} 2 \\ -1 \\ 2 \end{bmatrix}$

Step 1: compute $\|x\|_2$

$$\|x\| = \sqrt{2^2 + (-1)^2 + 2^2} = \sqrt{4 + 1 + 4} = \sqrt{9} = 3$$

Step 2: Step 2: Define e_1: $e_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$

Step 3: compute v: We choose $v = x + \text{sign}(x_1)\|x\|e_1$. Here $\text{sign}(x_1) = +1$ since $x_1 = 2$, so:

$$v = \begin{bmatrix} 2 \\ -1 \\ 2 \end{bmatrix} + 3\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 5 \\ -1 \\ 2 \end{bmatrix}$$

SOLUTION TO LEAST SQUARES PROBLEM
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Step 4: normalise v to obtient u

The normalised vector u is:

$$u = \frac{v}{\|v\|} = \frac{1}{\sqrt{5^2 + (-1)^2 + 2^2}} \begin{bmatrix} 5 \\ -1 \\ 2 \end{bmatrix} = \frac{1}{\sqrt{30}} \begin{bmatrix} 5 \\ -1 \\ 2 \end{bmatrix}$$

Step 5 form the Householder transformation, Q, sometimes written H

$$Q = I - 2uu^T$$

Where, $$uu^T = \frac{1}{30} \begin{bmatrix} 5 \\ -1 \\ 2 \end{bmatrix} [5 \quad -1 \quad 2] = \frac{1}{30} \begin{bmatrix} 25 & -5 & 10 \\ -5 & 1 & -2 \\ 10 & -2 & 4 \end{bmatrix}$$

SOLUTION TO LEAST SQUARES PROBLEM
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$$Q = I - 2 \cdot \frac{1}{30}\begin{bmatrix} 25 & -5 & 10 \\ -5 & 1 & -2 \\ 10 & -2 & 4 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \begin{bmatrix} \frac{5}{3} & -\frac{1}{3} & \frac{1}{3} \\ -\frac{1}{3} & \frac{1}{15} & -\frac{1}{15} \\ \frac{1}{3} & -\frac{1}{15} & \frac{2}{15} \end{bmatrix} = \begin{bmatrix} -\frac{5}{3} & \frac{1}{3} & -\frac{1}{3} \\ \frac{1}{3} & \frac{14}{15} & \frac{1}{15} \\ -\frac{1}{3} & \frac{1}{15} & \frac{13}{15} \end{bmatrix}$$

Step 6: Apply Q to x,

$$Qx = \begin{bmatrix} -3 \\ 0 \\ 0 \end{bmatrix}$$