Dot product and linear least squares problems

Dot Product

For vectors $u, v \in \mathbb{R}^n$ we define the **dot product**

$$\boxed{u \cdot v = u_1 v_1 + \cdots + u_n v_n}$$

Note that we can also write this as $u^\top v = [u_1, \ldots, u_n] \begin{bmatrix} v_1 \\ \vdots \\ v_n \end{bmatrix} = u_1 v_1 + \cdots + u_n v_n$.

The dot product $u \cdot u = u_1^2 + \cdots + u_n^2$ gives the square of the Euclidean length of the vector, a.k.a. **norm of the vector**:

$$\boxed{\|u\| = (u \cdot u)^{1/2} = \left(u_1^2 + \cdots + u_n^2\right)^{1/2}}$$

Theorem 1 (Cauchy-Schwarz inequality). *For $a, b \in \mathbb{R}^n$ we have*

$$\boxed{|a \cdot b| \leq \|a\| \, \|b\|} \tag{1}$$

Proof. *Step 1* for vectors with $\|a\| = 1$ and $\|b\| = 1$: Then

$$\begin{aligned} 0 \leq (b-a) \cdot (b-a) &= b \cdot b - 2a \cdot b + a \cdot a \\ 2a \cdot b &\leq a \cdot a + b \cdot b = 1 + 1 \end{aligned}$$

Hence $a \cdot b \leq 1$. Using $(b+a)$ instead of $(b-a)$ gives $-2a \cdot b \leq 2$, i.e., $a \cdot b \geq -1$.
Step 2 for general vectors a, b: If $a = \vec{0}$ or $b = \vec{0}$ we see that (1) obviously holds. If both vectors are different from $\vec{0}$ let $u := a/\|a\|$ and $v := b/\|b\|$, then $u \cdot v = \frac{a \cdot b}{\|a\|\|b\|}$. Since $\|u\| = 1$ and $\|v\| = 1$ we get from step 1 that $|u \cdot v| \leq 1$. $\square$

Consider a triangle with the three points $\vec{0}$, a, b. Then the vector from a to b is given by $c = b - a$, and the lengths of the three sides of the triangle are $\|a\|$, $\|b\|$, $\|c\|$.

Let θ denote the **angle between the vectors** a **and** b. Then the *law of cosines* tells us that

$$\|c\|^2 = \|a\|^2 + \|b\|^2 - 2\|a\| \, \|b\| \cos\theta$$

Multiplying out $\|c\|^2 = (b-a) \cdot (b-a)$ gives

$$\|c\|^2 = \|a\|^2 + \|b\|^2 - 2a \cdot b$$

By comparing the last two equations we obtain

$$\boxed{a \cdot b = \|a\| \, \|b\| \cos\theta}$$

If a and b are different from $\vec{0}$ we have

$$\boxed{\cos\theta = \frac{a \cdot b}{\|a\| \, \|b\|}}$$

This tells us **how to compute the angle θ between two vectors:**

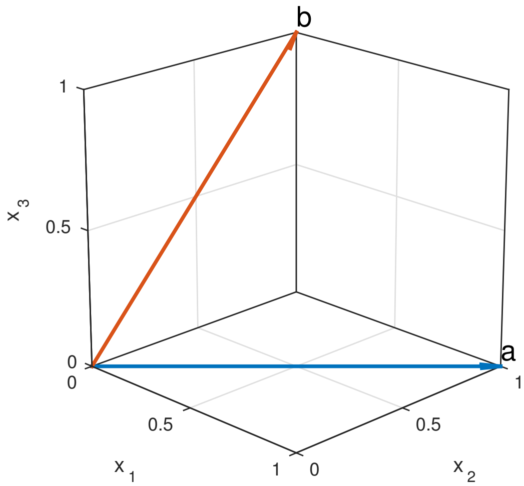
$$q := \frac{a \cdot b}{\|a\| \, \|b\|}, \qquad \theta := \cos^{-1} q$$

Because of (1) we have $-1 \leq q \leq 1$, hence the inverse cosine function gives $0 \leq \theta \leq \pi$:

$$\begin{aligned} q = 1 &\iff \theta = 0, \quad \text{i.e., } a, b \text{ point in the same direction} \\ q = 0 &\iff \theta = \frac{\pi}{2}, \quad \text{i.e., } a, b \text{ are orthogonal} \\ q = -1 &\iff \theta = \pi, \quad \text{i.e. } a, b \text{ point in opposite directions} \end{aligned}$$

Example 1. Find the angle between the vectors $a = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$ and $b = \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix}$: We get

$$q := \frac{a \cdot b}{\|a\| \, \|b\|} = \frac{1}{\sqrt{2}\sqrt{2}} = \frac{1}{2}, \qquad \theta := \cos^{-1} q = \cos^{-1} \frac{1}{2} = \frac{\pi}{3}$$



We say vectors $a, b \in \mathbb{R}^n$ are orthogonal or $a \perp b$

$$a \perp b \quad \iff \quad a \cdot b = 0$$

We say a vector $a \in \mathbb{R}^n$ is orthogonal on a subspace V of $\mathbb{R}^n$ or $a \perp V$

$$a \perp V \quad \iff \quad a \cdot v = 0 \quad \text{for all } v \in V$$

Orthogonal projection onto a line

Consider a 1-dimensional subspace $V = \operatorname{span}\{v\}$ of $\mathbb{R}^n$ given by a vector $v \in \mathbb{R}^n$. This is a line through the origin. For a given point $b \in \mathbb{R}^n$ we want to find the point $u \in V$ which is closest to the point b:

$$\boxed{\text{Find } u \in V \text{ such that } \|u - b\| \text{ is minimal}}$$

The point u must have the following properties:

- $u \in V$, i.e., $u = cv$ with some unknown $c \in \mathbb{R}$
- $u - b \perp V$, i.e., $v \cdot (u - b) = 0$

By plugging $u = cv$ into the second property we get by multiplying out

$$v \cdot (cv - b) = 0 \quad \iff \quad c(v \cdot v) - (v \cdot b) = 0 \quad \iff \quad c = \frac{v \cdot b}{v \cdot v}$$

Therefore the point u on the line given by v which is closest to the point b is given by

$$u = \frac{v \cdot b}{v \cdot v} v$$

We say that u is the **orthogonal projection of the point b onto the line given by v** and use the notation

$$\boxed{\operatorname{pr}_v b = \frac{v \cdot b}{v \cdot v} v}$$

Orthogonal projection onto a 2-dimensional subspace V

Consider a 2-dimensional subspace $V = \text{span}\left\{v^{(1)}, v^{(2)}\right\}$ of $\mathbb{R}^n$ given by two linearly independent vectors $v^{(1)}, v^{(2)} \in \mathbb{R}^n$. This is a plane through the origin.

For a given point $b \in \mathbb{R}^n$ we want to find the point $u \in V$ which is closest to the point b:

$$\boxed{\text{Find } u \in V \text{ such that } \|u-b\| \text{ is minimal}}$$

The point u must have the following properties:

- $u \in V$, i.e., $u = c_1 v^{(1)} + c_2 v^{(2)}$ with some unknowns $c_1, c_2 \in \mathbb{R}$
- $u - b \perp V$, i.e., $v^{(1)} \cdot (u-b) = 0$ and $v^{(2)} \cdot (u-b) = 0$

By plugging $u = c_1 v^{(1)} + c_2 v^{(2)}$ into the second property we obtain a linear system of two equations for two unknowns which we can then solve.

We can use the $k \times 2$ matrix $A = [v^{(1)}, v^{(2)}]$ to express the two properties:

- $u \in V$, i.e., $u = Ac$ with an unknown vector $c = \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} \in \mathbb{R}^2$
- $u - b \perp V$, i.e., $v^{(1)\top}(u-b) = 0$ and $v^{(2)\top}(u-b) = 0$, i.e., $\begin{bmatrix} v^{(1)\top} \\ v^{(2)\top} \end{bmatrix} (u-b) = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ or

$$A^\top (u-b) = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

By plugging $u = Ac$ into the second property we obtain

$$\boxed{A^\top (Ac - b) = 0}$$

$$\boxed{A^\top A c = A^\top b}$$

These are the so-called **normal equations** (since they express that $u - b$ is orthogonal or normal on the subspace V.

This is **how to find the point $u \in V$ which is closest to b:**

- find the matrix $M := A^\top A \in \mathbb{R}^{2\times 2}$ and the vector $g := A^\top b \in \mathbb{R}^2$
- solve the 2×2 linear system $Mc = g$ for $c \in \mathbb{R}^2$
- let $u := Ac$

Example 2. Consider the plane $V = \text{span}\left\{ \begin{bmatrix} -1 \\ 2 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \right\}$. Find the point $u \in V$ which is closest to $b = \begin{bmatrix} 0 \\ 1 \\ 3 \end{bmatrix}$.

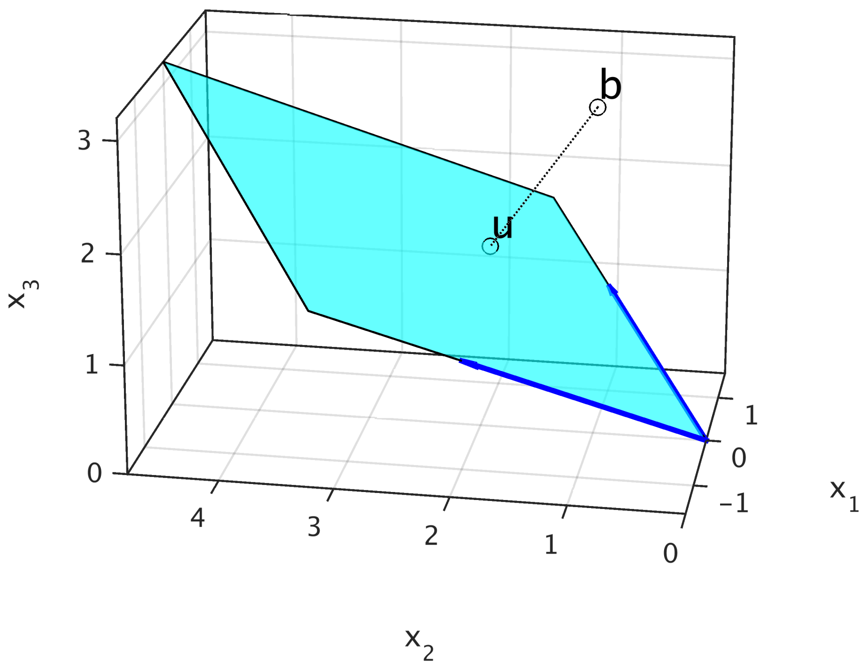
Let $A = \begin{bmatrix} -1 & 1 \\ 2 & 1 \\ 1 & 1 \end{bmatrix}$. Then

$$M = A^\top A = \begin{bmatrix} 6 & 2 \\ 2 & 3 \end{bmatrix}, \qquad g = \begin{bmatrix} 5 \\ 4 \end{bmatrix}$$

Solving the linear system $\begin{bmatrix} 6 & 2 \\ 2 & 3 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} 5 \\ 4 \end{bmatrix}$ gives $c = \begin{bmatrix} \frac{1}{2} \\ 1 \end{bmatrix}$.

Hence the closest point is $u = Ac = \begin{bmatrix} \frac{1}{2} \\ 2 \\ \frac{3}{2} \end{bmatrix}$. We can check that this is correct by finding the difference vector $r = u - b$ and checking $v^{(1)} \cdot r = 0$ and $v^{(2)} \cdot r = 0$: We have

$$r = Ac - b = \begin{bmatrix} \frac{1}{2} \\ 1 \\ -\frac{3}{2} \end{bmatrix} \qquad v^{(1)} \cdot r = \begin{bmatrix} -1 \\ 2 \\ 1 \end{bmatrix} \cdot \begin{bmatrix} \frac{1}{2} \\ 1 \\ -\frac{3}{2} \end{bmatrix} = 0, \qquad v^{(2)} \cdot r = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \cdot \begin{bmatrix} \frac{1}{2} \\ 1 \\ -\frac{3}{2} \end{bmatrix} = 0.$$



Orthogonal projection onto a k-dimensional subspace V a.k.a. "least squares problem"

Consider a k-dimensional subspace $V = \operatorname{span}\left\{v^{(1)}, \ldots, v^{(k)}\right\}$ of $\mathbb{R}^n$ given by k linearly independent vectors $v^{(1)}, \ldots, v^{(k)} \in \mathbb{R}^n$. I.e., the vectors $v^{(1)}, \ldots, v^{(k)}$ form a basis for the subspace V.

For a given point $b \in \mathbb{R}^n$ we want to find the point $u \in V$ which is closest to the point b:

$$\boxed{\text{Find } u \in V \text{ such that } \|u-b\| \text{ is minimal}} \tag{2}$$

Let us define the $n \times k$ matrix $A = \left[v^{(1)}, \ldots, v^{(k)}\right]$.

The point u must have the following properties:

- $u \in V$, i.e., $u = c_1 v^{(1)} + \cdots + c_k v^{(k)} = Ac$ with some unknown vector $c \in \mathbb{R}^k$
- $u - b \perp V$, i.e., $v^{(1)} \cdot (u-b) = 0, \ldots, v^{(k)} \cdot (u-b) = 0$, i.e., $\begin{bmatrix} v^{(1)\top} \\ \vdots \\ v^{(k)\top} \end{bmatrix} (u-b) = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}$ or

$$A^\top (u-b) = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}$$

By plugging $u = Ac$ into the second property we obtain

$$\boxed{A^\top (Ac - b) = 0} \tag{3}$$

$$\boxed{A^\top A c = A^\top b} \tag{4}$$

These are the so-called **normal equations** (since they express that $u-b$ is "orthogonal" or "normal" on the subspace V.)

This is **how to find the point $u \in V$ which is closest to b:**

- find the matrix $M := A^\top A \in \mathbb{R}^{k\times k}$ and the vector $g := A^\top b \in \mathbb{R}^k$
- solve the $k\times k$ linear system $Mc = g$ for $c \in \mathbb{R}^k$
- let $u := Ac$

Note that the normal equations (4) always have a unique solution:

Theorem 2. *Assume the matrix $A \in \mathbb{R}^{n\times k}$ with $k \le n$ has linearly independent columns (i.e.,* $\operatorname{rank} A = k$*). Then the matrix $M = A^\top A$ is nonsingular.*

Proof. We have to show that $Mc = \vec{0}$ implies $c = \vec{0}$.
Assume we have $c \in \mathbb{R}^k$ such that $Mc = \vec{0}$. Then we can multiply from the left with $c^\top$ and get with $y := Ac$

$$0 = c^\top Mc = c^\top A^\top Ac = y^\top y = \|y\|^2$$

as $y^\top = c^\top A^\top$. Since $\|y\| = 0$ we have $y = Ac = \vec{0}$. This means that we have a linear combination of the columns of A which gives the zero vector. Since by assumption the columns of A are linearly independent we must have $c = \vec{0}$. □

So solving the normal equations gives us a unique $c \in \mathbb{R}^n$. We then get by $u = Ac$ a point on the subspace V. We now want to formally prove that this point $u \in V$ is really the unique answer to our minimization problem (2).

Theorem 3. *Assume the matrix $A \in \mathbb{R}^{n\times k}$ with $k \le n$ has linearly independent columns (i.e.,* $\operatorname{rank} A = k$*). Then for any given $b \in \mathbb{R}^n$ the minimization problem*

$$\text{find } c \in \mathbb{R}^k \text{ such that } \|Ac - b\| \text{ is minimal} \tag{5}$$

has a unique solution which is obtained by solving the normal equations $A^\top Ac = A^\top b$.

Proof. Let $c \in \mathbb{R}^k$ be the unique solution of the normal equations. Consider now $\tilde{c} = c + d$ where $d \in \mathbb{R}^k$ is nonzero. We then have

$$\begin{aligned} \|A\tilde{c} - b\|^2 = \|Ac - b + Ad\|^2 &= \Big((Ac - b) + Ad\Big)\cdot\Big((Ac - b) + Ad\Big) \\ &= (Ac - b)\cdot(Ac - b) + 2(Ad)\cdot(Ac - b) + (Ad)\cdot(Ad) \end{aligned}$$

We have for the middle term $(Ad)\cdot(Ac - b) = (Ad)^\top(Ac - b) = d^\top A^\top(Ac - b) = 0$ by the normal equations (3). Hence

$$\|A\tilde{c} - b\|^2 = \|Ac - b\|^2 + \|Ad\|^2$$

Since $d \neq \vec{0}$ we have $Ad \neq \vec{0}$ since the columns of A are linearly independent, and hence $\|Ad\| > 0$. This means that for any vector $\tilde{c}$ different from c we get $\|A\tilde{c} - b\| > \|Ac - b\|$, i.e., the vector c from the normal equations is the unique solution of (5). □

Least squares problem with orthogonal basis

For a least squares problem we are given n linearly independent vectors $a^{(1)}, \ldots, a^{(n)} \in \mathbb{R}^m$ which form a basis for the subspace $V = \operatorname{span}\{a^{(1)}, \ldots, a^{(n)}\}$. For a given right hand side vector $b \in \mathbb{R}^m$ we want to find $u \in V$ such that $\|u - b\|$ is minimal. We can write $u = c_1 a^{(1)} + \cdots + c_n a^{(n)} = Ac$ with the matrix $A = \left[a^{(1)}, \ldots, a^{(n)}\right] \in \mathbb{R}^{m\times n}$. Hence we want to find $c \in \mathbb{R}^n$ such that $\|Ac - b\|$ is minimal.

Solving this problem is much simpler if we have an **orthogonal basis for the subspace** V: Assume we have vectors $p^{(1)}, \ldots, p^{(n)}$ such that

- $\operatorname{span}\left\{p^{(1)}, \ldots, p^{(n)}\right\} = V$
- the vectors are orthogonal on each other: $p^{(i)} \cdot p^{(j)} = 0$ for $i \neq j$

We can then write $u = d_1 p^{(1)} + \cdots + d_n p^{(n)} = Pd$ with the matrix $P = [p^{(1)}, \ldots, p^{(n)}] \in \mathbb{R}^{m \times n}$. Hence we want to find $d \in \mathbb{R}^n$ such that $\|Pd - b\|$ is minimal. The normal equations for this problem give

$$(P^\top P)d = P^\top b \tag{6}$$

where the matrix

$$P^\top P = \begin{bmatrix} p^{(1)\top} \\ \vdots \\ p^{(n)\top} \end{bmatrix} \left[p^{(1)}, \ldots, p^{(n)} \right] = \begin{bmatrix} p^{(1)} \cdot p^{(1)} & \cdots & p^{(1)} \cdot p^{(n)} \\ \vdots & & \vdots \\ p^{(n)} \cdot p^{(1)} & \cdots & p^{(n)} \cdot p^{(n)} \end{bmatrix} = \begin{bmatrix} p^{(1)} \cdot p^{(1)} & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & p^{(n)} \cdot p^{(n)} \end{bmatrix}$$

is now diagonal since $p^{(i)} \cdot p^{(j)} = 0$ for $i \neq j$. Therefore the normal equations (6) are actually decoupled

$$\left(p^{(1)} \cdot p^{(1)} \right) d_1 = p^{(1)} \cdot b$$
$$\vdots$$
$$\left(p^{(n)} \cdot p^{(n)} \right) d_n = p^{(n)} \cdot b$$

and have the solution

$$d_i = \frac{p^{(i)} \cdot b}{p^{(i)} \cdot p^{(i)}} \qquad \text{for } i = 1, \ldots, n$$

Gram-Schmidt orthogonalization

We still need a method to construct from a given basis $a^{(1)}, \ldots, a^{(n)}$ an orthogonal basis $p^{(1)}, \ldots, p^{(n)}$.

Given n linearly independent vectors $a^{(1)}, \ldots, a^{(n)} \in \mathbb{R}^m$ we want to find vectors $p^{(1)}, \ldots, p^{(n)}$ such that

- $\operatorname{span}\left\{ p^{(1)}, \ldots, p^{(n)} \right\} = \operatorname{span}\left\{ a^{(1)}, \ldots, a^{(n)} \right\}$
- the vectors are orthogonal on each other: $p^{(i)} \cdot p^{(j)} = 0$ for $i \neq j$

Step 1: $\boxed{p^{(1)} := a^{(1)}}$

Step 2: $\boxed{p^{(2)} := a^{(2)} - s_{12} p^{(1)}}$ where we choose s_{12} such that $p^{(1)} \cdot p^{(2)} = 0$:

$$p^{(1)} \cdot a^{(2)} - s_{12} p^{(1)} \cdot p^{(1)} = 0 \qquad \Longleftrightarrow \qquad \boxed{s_{12} = \frac{p^{(1)} \cdot a^{(2)}}{p^{(1)} \cdot p^{(1)}}}$$

Step 3: $\boxed{p^{(3)} := a^{(3)} - s_{13} p^{(1)} - s_{23} p^{(2)}}$ where we choose s_{13}, s_{23} such that

- $p^{(1)} \cdot p^{(3)} = 0$, i.e., $p^{(1)} \cdot a^{(3)} - s_{13} p^{(1)} \cdot p^{(1)} - s_{23} \underbrace{p^{(1)} \cdot p^{(2)}}_{0} = 0$, hence $\boxed{s_{13} = \frac{p^{(1)} \cdot a^{(3)}}{p^{(1)} \cdot p^{(1)}}}$
- $p^{(2)} \cdot p^{(3)} = 0$, i.e., $p^{(2)} \cdot a^{(3)} - s_{13} \underbrace{p^{(2)} \cdot p^{(1)}}_{0} - s_{23} p^{(2)} \cdot p^{(2)} = 0$, hence $\boxed{s_{23} = \frac{p^{(2)} \cdot a^{(3)}}{p^{(2)} \cdot p^{(1)}}}$

$\vdots$

Step n: $\boxed{p^{(n)} := a^{(n)} - s_{1n} p^{(1)} - \cdots - s_{n-1,n} p^{(n-1)}}$ where we choose $s_{1n}, \ldots, s_{n-1,n}$ such that $p^{(j)} \cdot p^{(n)} = 0$ for $j = 1, \ldots, n-1$ which yields

$$\boxed{s_{jn} = \frac{p^{(j)} \cdot p^{(n)}}{p^{(j)} \cdot p^{(j)}} \quad \text{for } j = 1, \ldots, n-1}$$

Example: We are given the vectors $a^{(1)} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$, $a^{(2)} = \begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \end{bmatrix}$, $a^{(3)} = \begin{bmatrix} 0 \\ 1 \\ 4 \\ 9 \end{bmatrix}$. Use Gram-Schmidt orthogonalization to find an orthogonal basis $p^{(1)}, p^{(2)}, p^{(3)}$ for the subspace $V = \operatorname{span}\left\{a^{(1)}, a^{(2)}, a^{(3)}\right\}$.

Step 1: $\boxed{p^{(1)} := a^{(1)}} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$

Step 2: $\boxed{p^{(2)} := a^{(2)} - \frac{p^{(1)} \cdot a^{(2)}}{p^{(1)} \cdot p^{(1)}} p^{(1)}} = \begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \end{bmatrix} - \frac{6}{4} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} -\frac{3}{2} \\ -\frac{1}{2} \\ \frac{1}{2} \\ \frac{3}{2} \end{bmatrix}$

Step 3: $\boxed{p^{(3)} := a^{(3)} - \frac{p^{(1)} \cdot a^{(3)}}{p^{(1)} \cdot p^{(1)}} p^{(1)} - \frac{p^{(2)} \cdot a^{(3)}}{p^{(2)} \cdot p^{(2)}} p^{(2)}} = \begin{bmatrix} 0 \\ 1 \\ 4 \\ 9 \end{bmatrix} - \frac{14}{4} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} - \frac{15}{5} \begin{bmatrix} -\frac{3}{2} \\ -\frac{1}{2} \\ \frac{1}{2} \\ \frac{3}{2} \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \\ -1 \\ 1 \end{bmatrix}$

Note that we have

$$\begin{aligned} a^{(1)} &= p^{(1)} \\ a^{(2)} &= p^{(2)} + \frac{6}{4} p^{(1)} \\ a^{(3)} &= p^{(3)} + \frac{14}{4} p^{(1)} + \frac{15}{5} p^{(2)} \end{aligned}$$

which we can write as

$$\left[a^{(1)}, a^{(2)}, a^{(3)}\right] = \left[p^{(1)}, p^{(2)}, p^{(3)}\right] \begin{bmatrix} 1 & \frac{6}{4} & \frac{14}{4} \\ 0 & 1 & \frac{15}{5} \\ 0 & 0 & 1 \end{bmatrix}$$

$$\underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 4 \\ 1 & 3 & 9 \end{bmatrix}}_{A} = \underbrace{\begin{bmatrix} 1 & -1.5 & 1 \\ 1 & -0.5 & -1 \\ 1 & 0.5 & -1 \\ 1 & 1.5 & 1 \end{bmatrix}}_{P} \underbrace{\begin{bmatrix} 1 & 1.5 & 3.5 \\ 0 & 1 & 3 \\ 0 & 0 & 1 \end{bmatrix}}_{S}$$

In the general case we have

$$\begin{aligned} a^{(1)} &= p^{(1)} \\ a^{(2)} &= p^{(2)} + s_{12} p^{(1)} \\ a^{(3)} &= p^{(3)} + s_{13} p^{(1)} + s_{13} p^{(2)} \\ &\vdots \\ a^{(n)} &= p^{(n)} + s_{1n} p^{(1)} + \cdots + s_{n-1,n} p^{(n-1)} \end{aligned}$$

which we can write as

$$\left[a^{(1)}, a^{(2)}, \ldots, a^{(n)}\right] = \left[p^{(1)}, p^{(2)}, \ldots, p^{(n)}\right] \begin{bmatrix} 1 & s_{12} & \cdots & s_{1n} \\ 0 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & s_{n-1,n} \\ 0 & \cdots & 0 & 1 \end{bmatrix}$$

Therefore we obtain a decomposition $A = PS$ where

- $P \in \mathbb{R}^{m\times n}$ has orthogonal columns
- $S \in \mathbb{R}^{n\times n}$ is upper triangular, with 1 on the diagonal.

Note that the vectors $p^{(1)},\dots,p^{(n)}$ are different from $\vec{0}$:

Assume, e.g., that $p^{(3)} = a^{(3)} - s_{13}p^{(1)} - s_{23}p^{(2)} = \vec{0}$, then $a^{(3)} = s_{13}p^{(1)} + s_{23}p^{(2)}$ is in span $\{p^{(1)},p^{(2)}\} = \text{span}\{a^{(1)},a^{(2)}\}$. This is a contradiction to the assumption that $a^{(1)},a^{(2)},a^{(3)}$ are linearly independent.

Solving the least squares problem $\|Ac-b\| = \min$ using orthogonalization

We are given $A \in \mathbb{R}^{m\times n}$ with linearly independent columns, $b \in \mathbb{R}^n$. We want to find $c \in \mathbb{R}^n$ such that $\|Ac-b\| = \min$.

From the Gram-Schmidt method we get $A = PS$, hence we want to find c such that

$$\|P\underbrace{Sc}_{d} - b\| = \min$$

This gives the following method for solving the least squares problem:

- use Gram-Schmidt to find decomposition $A = PS$
- solve $\|Pd-b\| = \min$: $d_i := \dfrac{p^{(i)}\cdot b}{p^{(i)}\cdot p^{(i)}}$ for $i = 1,\dots,n$
- solve $Sc = d$ by back substitution

Example: Solve the least squares problem $\|Ac-b\| = \min$ for $A = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 4 \\ 1 & 3 & 9 \end{bmatrix}$, $b = \begin{bmatrix} 0 \\ 1 \\ 4 \\ 7 \end{bmatrix}$.

- Gram-Schmidt gives $A = \underbrace{\begin{bmatrix} 1 & -1.5 & 1 \\ 1 & -0.5 & -1 \\ 1 & 0.5 & -1 \\ 1 & 1.5 & 1 \end{bmatrix}}_{P} \underbrace{\begin{bmatrix} 1 & 1.5 & 3.5 \\ 0 & 1 & 3 \\ 0 & 0 & 1 \end{bmatrix}}_{S}$ (see above)
- $d_1 = \dfrac{p^{(1)}\cdot b}{p^{(1)}\cdot p^{(1)}} = \dfrac{12}{4} = 3$, $d_2 = \dfrac{p^{(2)}\cdot b}{p^{(2)}\cdot p^{(2)}} = \dfrac{12}{5} = 2.4$, $d_3 = \dfrac{p^{(3)}\cdot b}{p^{(3)}\cdot p^{(3)}} = \dfrac{2}{4} = 0.5$
- solving $\begin{bmatrix} 1 & 1.5 & 3.5 \\ 0 & 1 & 3 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} 3 \\ 2.4 \\ 0.5 \end{bmatrix}$ by back substitution gives $c_3 = 0.5$, $c_2 = 0.9$, $c_1 = -1.1$

Hence the solution of our least squares problem is the vector $c = \begin{bmatrix} -1.1 \\ 0.9 \\ 0.5 \end{bmatrix}$.

Note: If you want to solve a least squares problem by hand with pencil and paper, it is usually easier to use the normal equations. But for numerical computation on a computer using orthogonalization is usually more efficient and more accurate.

Finding an ortho*normal* basis $q^{(1)},\dots,q^{(n)}$: the QR decomposition

The Gram-Schmidt method gives an orthogonal basis $p^{(1)},\dots,p^{(n)}$ for $V = \text{span}\{a^{(1)},\dots,a^{(n)}\}$

Often it is convenient to have a so-called ortho*normal* basis $q^{(1)},\dots,q^{(n)}$ where the basis vectors have length 1: Define

$$q^{(j)} = \frac{1}{\|p^{(j)}\|}p^{(j)} \qquad \text{for } j = 1,\dots,n$$

then we have

- $\operatorname{span}\left\{q^{(1)},\ldots,q^{(n)}\right\}=V$
- $q^{(j)}\cdot q^{(k)}=\begin{cases}1 & \text{for } j=k\\ 0 & \text{otherwise}\end{cases}$

This means that the matrix $Q=[q^{(1)},\ldots,q^{(n)}]$ satisfies $Q^\top Q=I$ where I is the $n\times n$ identity matrix.

Since $p^{(j)}=\left\|p^{(j)}\right\|q^{(j)}$ we have

$$\begin{aligned}
a^{(1)} &= \underbrace{\left\|p^{(1)}\right\|q^{(1)}}_{r_{11}}\\
a^{(2)} &= \underbrace{\left\|p^{(2)}\right\|q^{(2)}}_{r_{22}}+\underbrace{s_{12}\left\|p^{(1)}\right\|}_{r_{12}}p^{(1)}\\
&\ \vdots\\
a^{(n)} &= \underbrace{\left\|p^{(n)}\right\|q^{(n)}}_{r_{nn}}+\underbrace{s_{1n}\left\|p^{(1)}\right\|}_{r_{1n}}p^{(1)}+\cdots+\underbrace{s_{n-1,n}\left\|p^{(n-1)}\right\|}_{r_{n-1,n}}q^{(n-1)}
\end{aligned}$$

which we can write as

$$\begin{aligned}
\left[a^{(1)},a^{(2)},\ldots,a^{(n)}\right] &= \left[q^{(1)},q^{(2)},\ldots,q^{(n)}\right]\begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n}\\ 0 & r_{22} & \ddots & \vdots\\ \vdots & \ddots & \ddots & r_{n-1,n}\\ 0 & \cdots & 0 & r_{nn}\end{bmatrix}\\
A &= QR
\end{aligned}$$

where the $n\times n$ matrix R is given by

$$\begin{bmatrix}\text{row 1 of } R\\ \vdots\\ \text{row } n \text{of } R\end{bmatrix}=\begin{bmatrix}\left\|p^{(1)}\right\|(\text{row 1 of } R)\\ \vdots\\ \left\|p^{(n)}\right\|(\text{row } n \text{of } R)\end{bmatrix}$$

We obtain the so-called **QR decomposition** $A=QR$ where

- the matrix $Q\in\mathbb{R}^{m\times n}$ has orthonormal columns, $\operatorname{range}Q=\operatorname{range}A$
- the matrix $R\in\mathbb{R}^{n\times n}$ is upper triangular, with nonzero diagonal elements

Example: In our example we have $p^{(1)}\cdot p^{(1)}=4$, $p^{(2)}\cdot p^{(2)}=5$, $p^{(3)}\cdot p^{(3)}=4$, hence

$$q^{(1)}=\frac{1}{2}p^{(1)}=\begin{bmatrix}.5\\.5\\.5\\.5\end{bmatrix},\qquad q^{(2)}=\frac{1}{\sqrt{5}}p^{(2)}=\frac{1}{\sqrt{5}}\begin{bmatrix}-1.5\\-.5\\.5\\1.5\end{bmatrix},\qquad q^{(3)}=\frac{1}{2}p^{(3)}=\begin{bmatrix}.5\\-.5\\-.5\\.5\end{bmatrix}$$

and we obtain the QR decomposition

$$\begin{bmatrix}1&0&0\\1&1&1\\1&2&4\\1&3&9\end{bmatrix}=\begin{bmatrix}.5 & -1.5/\sqrt{5} & .5\\ .5 & -.5/\sqrt{5} & -.5\\ .5 & .5/\sqrt{5} & -.5\\ .5 & 1.5/\sqrt{5} & .5\end{bmatrix}\begin{bmatrix}2&3&7\\0&\sqrt{5}&3\sqrt{5}\\0&0&2\end{bmatrix}$$

In Matlab we can find the QR decomposition using **`[Q,R]=qr(A,0)`**

This works for **symbolic matrices**

```
>> A = sym([1 1 1 1; 0 1 2 3; 0 1 4 9])';
>> [Q,R] = qr(A,0)
Q =
[ 1/2, -(3*5^(1/2))/10,  1/2]
[ 1/2,     -5^(1/2)/10, -1/2]
[ 1/2,      5^(1/2)/10, -1/2]
[ 1/2,  (3*5^(1/2))/10,  1/2]
R =
[ 2,       3,         7]
[ 0, 5^(1/2), 3*5^(1/2)]
[ 0,       0,         2]
```

and it works for **numerical matrices**

```
>> A = [1 1 1 1; 0 1 2 3; 0 1 4 9]';
>> [Q,R] = qr(A,0)
Q =
   -0.5000    0.6708    0.5000
   -0.5000    0.2236   -0.5000
   -0.5000   -0.2236   -0.5000
   -0.5000   -0.6708    0.5000
R =
   -2.0000   -3.0000   -7.0000
         0   -2.2361   -6.7082
         0         0    2.0000
```

Note that for numerical matrices Matlab returned the basis $-q^{(1)}, -q^{(2)}, q^{(3)}$ (which is also an orthonormal basis) and hence rows 1 and 2 of the matrix R is (-1) times our previous matrix R.

If we want to find an orthonormal basis for range$A$ and an orthonormal basis for the orthogonal complement $(\text{range} A)^\perp = \text{null} A^\top$ we can use the command **`[Qh,Rh]=qr(A)`** : It returns matrices $\hat{Q} \in \mathbb{R}^{m\times m}$ and $\hat{R} \in \mathbb{R}^{m\times n}$ with

$$\hat{Q} = \begin{bmatrix} \overbrace{q^{(1)},\dots,q^{(n)}}^{\text{basis for range}A}, \overbrace{q^{(n+1)},\dots,q^{(m)}}^{\text{basis for }(\text{range}A)^\perp} \\ \\ \end{bmatrix}, \qquad \hat{R} = \begin{bmatrix} & R & \\ 0 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & 0 \end{bmatrix} \begin{matrix} \\ \left.\begin{matrix} \\ \\ \\ \end{matrix}\right\} m-n \text{rows of zeros} \end{matrix}$$

```
>> A = [1 1 1 1; 0 1 2 3; 0 1 4 9]';
>> [Qh,Rh] = qr(A)
Qh =
   -0.5000    0.6708    0.5000    0.2236
   -0.5000    0.2236   -0.5000   -0.6708
   -0.5000   -0.2236   -0.5000    0.6708
   -0.5000   -0.6708    0.5000   -0.2236
Rh =
   -2.0000   -3.0000   -7.0000
         0   -2.2361   -6.7082
         0         0    2.0000
         0         0         0
```

But in most cases we only need an orthonormal basis for range$A$ and we should use `[Q,R]=qr(A,0)` (which Matlab calls the "economy size" decomposition).

Solving the least squares problem $\|Ac-b\| = \min$ using the QR decomposition

If we use an orthonormal basis $q^{(1)},\ldots,q^{(n)}$ for $\operatorname{span}\{a^{(1)},\ldots,a^{(n)}\}$ we have $Q^\top Q = I$. The solution of $\|Qd-b\| = \min$ is therefore given by the normal equations $(Q^\top Q)d = Q^\top b$, i.e., we obtain $d = Q^\top b$.

This gives the following method for solving the least squares problem:

- find the QR decomposition $A = QR$
- let $d = Q^\top b$
- solve $Rc = d$ by back substitution

In Matlab we can do this as follows:

```
[Q,R] = qr(A,0);
d = Q'*b;
c = R\d;
```

In our example we have

```
>> A = [1 1 1 1; 0 1 2 3; 0 1 4 9]'; b = [0;1;4;7];
>> [Q,R] = qr(A,0);
>> d = Q'*b;
>> c = R\d
c =
   -0.1000
    0.9000
    0.5000
```

This works for both numerical and symbolic matrices.

For a numerical matrix A we can use the shortcut `c=A\y` which actually uses the QR decomposition to find the solution of $\|Ac-b\| = \min$

```
>> A = [1 1 1 1; 0 1 2 3; 0 1 4 9]'; b = [0;1;4;7];
>> c = A\b
c =
   -0.1000
    0.9000
    0.5000
```

Warning: This shortcut does **not** work for symbolic matrices:

```
>> A = sym([1 1 1 1; 0 1 2 3; 0 1 4 9])'; b = sym([0;1;4;7]);
>> c = A\b
Warning: The system is inconsistent. Solution does not exist.
c =
 Inf
 Inf
 Inf
```