

Math 254: Introduction to Linear Algebra

Notes #5.2 — Gram-Schmidt Process and QR Factorization

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SLOs 5.2

Gram-Schmidt Process and QR Factorization

After this lecture you should know how:

- to perform *The Gram-Schmidt Orthogonalization Process* on a set of vectors, and
- it can be used to compute *The QR-factorization* of a matrix A : $A = QR$
 - ⇒ This builds an orthonormal basis (the columns of Q) for the subspace $V = \text{im}(A)$, which gives us the means to compute the orthogonal projection $\text{proj}_V(\vec{x})$ onto V .
- to orthogonally project onto *any* subspace.

Orthogonal Projection onto a Subspace V

From [NOTES#5.1] we have:

Theorem (Formula for the Orthogonal Projection)

If V is a subspace of \mathbb{R}^n with an orthonormal basis $\vec{u}_1, \dots, \vec{u}_m$, then

$$\text{proj}_V(\vec{x}) = \vec{x}^{\parallel} = (\vec{u}_1 \cdot \vec{x})\vec{u}_1 + \dots + (\vec{u}_m \cdot \vec{x})\vec{u}_m$$

$\forall \vec{x} \in \mathbb{R}^n$.

How do you project onto a subspace if/when the given basis is not orthonormal?!?

It turns out that before we compute the projection, we have to find a new — *orthonormal* — basis...



THIS IS ALL WRONG!!!!



Ponder what happens if we use the formula, but the given basis is **not** orthonormal...

Let's live in \mathbb{R}^2 , let $V = \mathbb{R}^2$, with basis $\mathfrak{B} = (\vec{v}_1, \vec{v}_2)$ defined by

$$\vec{v}_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \vec{v}_2 = \begin{bmatrix} 1 \\ 2 \end{bmatrix}; \quad \text{and } \vec{x} = \begin{bmatrix} 2 \\ 3 \end{bmatrix}; \quad \|\vec{x}\| = \sqrt{13}.$$

Clearly \vec{v}_1 and \vec{v}_2 are linearly independent, and $\vec{x} = 1\vec{v}_1 + 1\vec{v}_2$, but the projection formula goes haywire:

$$\text{proj}_V(\vec{x}) = (\vec{v}_1 \cdot \vec{x})\vec{v}_1 + (\vec{v}_2 \cdot \vec{x})\vec{v}_2 = 5\vec{v}_1 + 8\vec{v}_2 = \begin{bmatrix} 13 \\ 21 \end{bmatrix}.$$

... even if we remember to correct for the non-unit length of $\vec{v}_{1,2}$:

$$\text{proj}_V(\vec{x}) = \frac{(\vec{v}_1 \cdot \vec{x})}{\|\vec{v}_1\|^2} \vec{v}_1 + \frac{(\vec{v}_2 \cdot \vec{x})}{\|\vec{v}_2\|^2} \vec{v}_2 = \frac{5}{2}\vec{v}_1 + \frac{8}{5}\vec{v}_2 = \begin{bmatrix} 4.1 \\ 5.7 \end{bmatrix}.$$

Comments

There are other ways to realize the “projection” went awry:

- This is “life in \mathbb{R}^2 ,” and since

$$\vec{v}_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \vec{v}_2 = \begin{bmatrix} 1 \\ 2 \end{bmatrix},$$

are linearly independent \rightsquigarrow they form a basis for $\mathbb{R}^2 \rightsquigarrow$ any projection of a vector $\vec{w} \in \mathbb{R}^2$ onto the subspace $V = \text{span}(\vec{v}_1, \vec{v}_2) \equiv \mathbb{R}^2$ must be the original vector \vec{w} .

- Even simpler, the famous *Method of the Eyeball* already showed that $\vec{v}_1 + \vec{v}_2 = \vec{x}$:

$$\begin{bmatrix} 1 \\ 1 \end{bmatrix} + \begin{bmatrix} 1 \\ 2 \end{bmatrix} = \begin{bmatrix} 2 \\ 3 \end{bmatrix}.$$

Example: Doing it Right...

Build an Orthonormal Basis

In this case, given a basis of \mathbb{R}^2 , the answer is “obvious.”

Next, we develop (still in \mathbb{R}^2 so we easily can visualize and use our intuition) a method for building an *orthonormal basis* given *any* starting basis.

Once we have the orthonormal basis, we can use the projection formula...

ⓘ The method will work in the general case: Given $\vec{x} \in \mathbb{R}^n$, and $V = \text{span}(\vec{v}_1, \dots, \vec{v}_m) \subset \mathbb{R}^n$; compute $\text{proj}_V(\vec{x})$:

We find an orthonormal basis $\vec{q}_1, \dots, \vec{q}_m$, so that

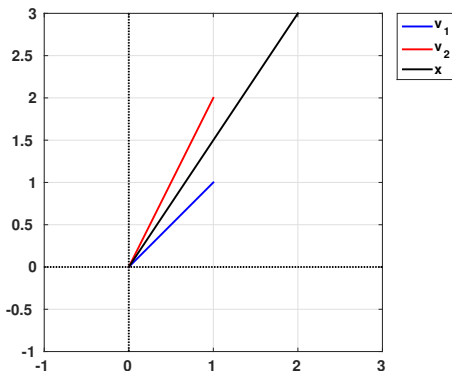
$$V = \text{span}(\vec{v}_1, \dots, \vec{v}_m) = \text{span}(\vec{q}_1, \dots, \vec{q}_m);$$

and then use the projection formula.

Example: Doing it Right...

Build an Orthonormal Basis

Figure: This is where we start.

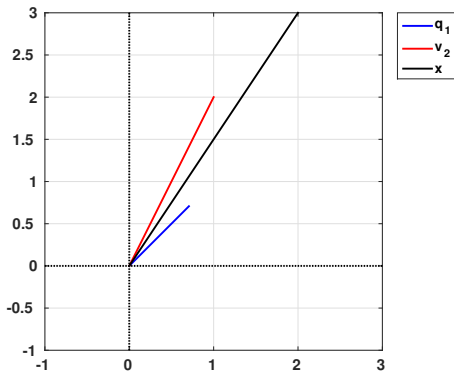


$$\vec{v}_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \vec{v}_2 = \begin{bmatrix} 1 \\ 2 \end{bmatrix}; \quad \text{and } \vec{x} = \begin{bmatrix} 2 \\ 3 \end{bmatrix}.$$

Example: Doing it Right...

(i) Rescale the first vector

Figure: Rescale* \vec{v}_1 to be norm 1, and call it \vec{q}_1 .



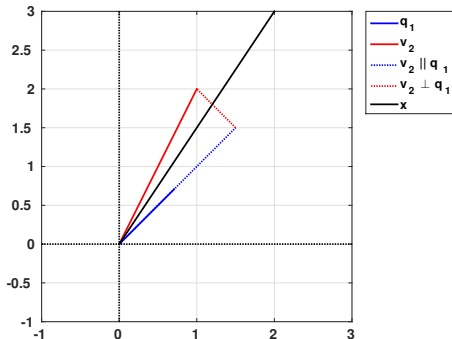
$$\vec{q}_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \vec{v}_2 = \begin{bmatrix} 1 \\ 2 \end{bmatrix}; \quad \text{and } \vec{x} = \begin{bmatrix} 2 \\ 3 \end{bmatrix}.$$

* Divide by the original norm, $\sqrt{2}$.

Example: Doing it Right...

(ii) Split the next vector into \parallel and \perp parts...

Figure: Next, project* \vec{v}_2 onto \vec{q}_1 and get $\vec{v}_2^{\parallel \vec{q}_1}$, and $\vec{v}_2^{\perp \vec{q}_1}$.



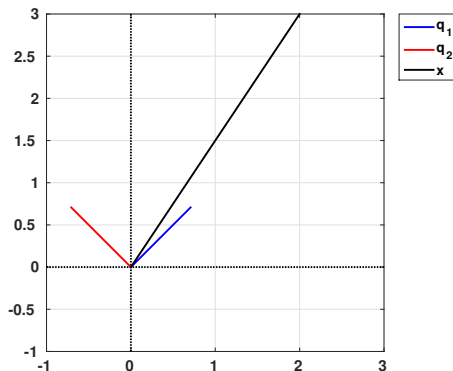
$$\vec{q}_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \vec{v}_2^{\parallel \vec{q}_1} = \begin{bmatrix} 1.5 \\ 1.5 \end{bmatrix}; \quad \vec{v}_2^{\perp \vec{q}_1} = \begin{bmatrix} -0.5 \\ 0.5 \end{bmatrix}; \quad \text{and } \vec{x} = \begin{bmatrix} 2 \\ 3 \end{bmatrix}.$$

$$* \vec{v}_2^{\parallel \vec{q}_1} = (\vec{q}_1 \cdot \vec{v}_2) \vec{q}_1 = \left(\frac{3}{\sqrt{2}}\right) \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{3}{2} \begin{bmatrix} 1 \\ 1 \end{bmatrix}; \quad \vec{v}_2^{\perp \vec{q}_1} = \begin{bmatrix} 1 \\ 2 \end{bmatrix} - \vec{v}_2^{\parallel \vec{q}_1} = \frac{1}{2} \begin{bmatrix} -1 \\ 1 \end{bmatrix}.$$

Example: Doing it Right...

(iii) Rescale the \perp part, discard \parallel part

Figure: Next, throw away $\vec{v}_2^{\parallel \vec{q}_1}$;
rescale $\vec{v}_2^{\perp \vec{q}_1}$ to norm 1, and name
it \vec{q}_2 .



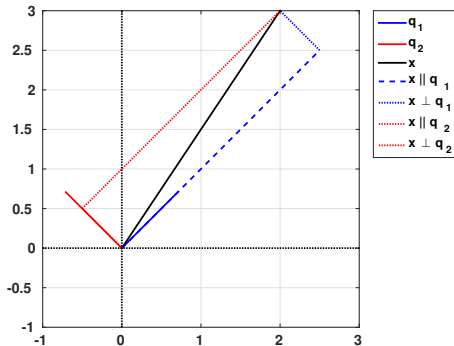
$$\vec{q}_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \vec{q}_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 1 \end{bmatrix}; \quad \text{and } \vec{x} = \begin{bmatrix} 2 \\ 3 \end{bmatrix},$$

Now we have an orthonormal basis $\mathcal{Q} = \langle \vec{q}_1, \vec{q}_2 \rangle$!

Example: Doing it Right...

(iv) Project using the new orthonormal basis!

Figure: Finally, we can use the projection formula.



$$\text{proj}_V(\vec{x}) = (\vec{q}_1 \cdot \vec{x})\vec{q}_1 + (\vec{q}_2 \cdot \vec{x})\vec{q}_2 = \frac{5}{\sqrt{2}}\vec{q}_1 + \frac{1}{\sqrt{2}}\vec{q}_2$$

$$\frac{5}{\sqrt{2}} \left(\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \right) + \frac{1}{\sqrt{2}} \left(\frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 1 \end{bmatrix} \right) = \begin{bmatrix} 2 \\ 3 \end{bmatrix}$$

Example: Doing it Right...

Coordinates

In the context of [COORDINATES (NOTES#3.4)], we have

$$\text{BASIS: } \Omega = \langle \vec{q}_1, \vec{q}_2 \rangle$$

$$\text{COORDINATES: } [\vec{x}]_{\Omega} = \begin{bmatrix} \frac{5}{\sqrt{2}} \\ 1 \\ \frac{1}{\sqrt{2}} \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 5 \\ 1 \\ 1 \end{bmatrix}$$

Milking the Example for More Details...

We have performed a *Change of Basis*, in this case for the purpose of making the projection onto the subspace easily (after the change of basis, that is) computable.

It is “easy” to see that

$$\underbrace{\begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix}}_{A = [\vec{v}_1 \quad \vec{v}_2]} = \underbrace{\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}}_{Q = [\vec{q}_1 \quad \vec{q}_2]} \underbrace{\begin{bmatrix} \sqrt{2} & \frac{3}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} \end{bmatrix}}_R,$$

we have $A = QR$, where Q is the new orthonormal basis, and R is an upper triangular matrix.

The entries in the R matrix are — $\sqrt{2}$: the original norm of \vec{v}_1 ; $\frac{3}{\sqrt{2}}$: the dot product $(\vec{q}_1 \cdot \vec{v}_2)$; $\frac{1}{\sqrt{2}}$: the norm of $\vec{v}_2^\perp \vec{q}_1$. Not likely a coincidence...

Let's Ponder Higher Dimensions

When you have more basis vectors $\vec{v}_1, \dots, \vec{v}_n$ needing orthogonalization (to make an orthonormal basis):

Theorem (Gram-Schmidt Process (annotated))

- *Start like we did:*
 - $\vec{q}_1 = \vec{v}_1 / \|\vec{v}_1\|$
 - $\vec{w}_2 = \vec{v}_2 - (\vec{q}_1 \cdot \vec{v}_2)\vec{q}_1$, note that this is a vector in the orthogonal complement of $\text{span}(\vec{q}_1) = \text{span}(\vec{v}_1)$.
 - $\vec{q}_2 = \vec{w}_2 / \|\vec{w}_2\|$
- *Each time we grab a new vector (\vec{v}_k), find a "help vector" \vec{w}_k in the orthogonal complement of the space spanned by the previously computed \vec{q} -vectors:*
 - $\vec{w}_k = \vec{v}_k - (\vec{q}_1 \cdot \vec{v}_k)\vec{q}_1 - (\vec{q}_2 \cdot \vec{v}_k)\vec{q}_2 - \dots - (\vec{q}_{k-1} \cdot \vec{v}_k)\vec{q}_{k-1}$
- *Then $\vec{q}_k = \vec{w}_k / \|\vec{w}_k\|$.*

The QR Factorization

The Gram-Schmidt process computed a change of basis from the old basis (funky-script-A)

$$\mathfrak{A} = (\vec{v}_1, \dots, \vec{v}_n)$$

to a new *orthonormal* basis (funky-script-Q)

$$\mathfrak{Q} = (\vec{q}_1, \dots, \vec{q}_n).$$

We describe the result using the change-of-basis-Matrix R from \mathfrak{A} to \mathfrak{Q} , writing

$$\underbrace{(\vec{v}_1 \quad \cdots \quad \vec{v}_n)}_A = \underbrace{(\vec{q}_1 \quad \cdots \quad \vec{q}_n)}_Q R$$

Interpretations and Relations

With $A = QR$, we have the following relations:

- $[\vec{x}]_{\Omega} = R[\vec{x}]_{\mathcal{A}}$
 - Multiplication by R moves us from A -coordinates to Q -coordinates.
- $\vec{x} = Q[\vec{x}]_{\Omega} = QR[\vec{x}]_{\mathcal{A}}$
 - Multiplying the Q -coordinate vector by Q “builds” the vector \vec{x} .
- $\vec{x} = A[\vec{x}]_{\mathcal{A}}$
 - Multiplying the A -coordinate vector by A “builds” the (same) vector \vec{x} .

The “burning” question is *how do we construct R ?* It turns out we already have all the pieces, we just need some book-keeping.

What's in R ?

1 of 3

If we think back to the k^{th} step, we compute

$$\underbrace{\vec{w}_k}_{\vec{v}_k^\perp} = \vec{v}_k - \underbrace{(\vec{q}_1 \cdot \vec{v}_k)\vec{q}_1 + (\vec{q}_2 \cdot \vec{v}_k)\vec{q}_2 + \cdots + (\vec{q}_{k-1} \cdot \vec{v}_k)\vec{q}_{k-1}}_{\vec{v}_k^\parallel}$$

\vec{v}_k^\perp is orthogonal to $V_{k-1} = \text{span}(\vec{q}_1, \dots, \vec{q}_{k-1}) = \text{span}(\vec{v}_1, \dots, \vec{v}_{k-1})$,
and $\vec{v}_k^\parallel \in \text{span}(\vec{q}_1, \dots, \vec{q}_{k-1})$.

Note: Subspaces, Orthogonal Complements, and Bases

We are constructing a sequence of subspace-pairs

$$V_k \oplus V_k^\perp = \mathbb{R}^n; \quad \dim(V_k) = k, \quad \dim(V_k^\perp) = (n - k); \quad k = 1, \dots, n$$

and orthonormal bases $\Omega_k = (\vec{q}_1, \dots, \vec{q}_k)$ for each of the V_k -spaces; and we have $V_{k-1} \subset V_k$ and $V_k^\perp \subset V_{k-1}^\perp$.

We are explicitly constructing V_k and Ω_k ; whereas we're only concerned with a specific vector $\vec{v}_k^\perp \in V_k^\perp$.



What's in R ?

2 of 3

OK, let's rearrange the previous expression:

$$\vec{v}_k = \underbrace{(\vec{q}_1 \cdot \vec{v}_k)\vec{q}_1 - (\vec{q}_2 \cdot \vec{v}_k)\vec{q}_2 - \cdots - (\vec{q}_{k-1} \cdot \vec{v}_k)\vec{q}_{k-1}}_{\vec{v}_k^{\parallel}} + \underbrace{\vec{w}_k}_{\vec{v}_k^{\perp}}$$

The next thing we do is normalize \vec{v}_k^{\perp} to be norm 1, and name it \vec{q}_k ; which means we can write the relation above:

$$\vec{v}_k = \underbrace{(\vec{q}_1 \cdot \vec{v}_k)\vec{q}_1 + (\vec{q}_2 \cdot \vec{v}_k)\vec{q}_2 + \cdots + (\vec{q}_{k-1} \cdot \vec{v}_k)\vec{q}_{k-1}}_{\vec{v}_k^{\parallel}} + \underbrace{\|\vec{v}_k^{\perp}\| \vec{q}_k}_{\vec{v}_k^{\perp}}$$

This is the “recipe” for rebuilding the k^{th} column of A using the first k columns of Q . The entries in R are given by

- $r_{\ell,k} = (\vec{q}_\ell \cdot \vec{v}_k)$, $\ell < k$; ($r_{\ell,k} = 0$, $\ell > k$), and
- $r_{k,k} = \|\vec{v}_k^{\perp}\|$.

Summarizing \rightsquigarrow The QR-factorization

Theorem (QR-Factorization)

Consider an $(n \times m)$ matrix A , with linearly independent columns, $\vec{v}_1, \dots, \vec{v}_m \in \mathbb{R}^n$. Then there exists an $(n \times m)$ matrix Q whose columns $\vec{q}_1, \dots, \vec{q}_m \in \mathbb{R}^n$ are orthonormal, and an upper triangular matrix R with positive diagonal entries such that $A = QR$. This representation is unique.

Further

- $r_{11} = \|\vec{v}_1\|$,
- $r_{kk} = \|\vec{v}_k^\perp \text{span}(\vec{q}_1, \dots, \vec{q}_{k-1})\|$, $k \in \{2, \dots, m\}$, and
- $r_{\ell,k} = (\vec{q}_\ell \cdot \vec{v}_k)$, $\ell \in \{1, \dots, k-1\}$.

Note that

$$[QR\text{-factorization}] = [\text{Gram-Schmidt}] + [\text{Bookkeeping}].$$

Observations $A = [\vec{v}_1 \cdots \vec{v}_m] = QR$, $A \in \mathbb{R}^{n \times m}$

- Note that $\text{span}(\vec{q}_1, \dots, \vec{q}_k) = \text{span}(\vec{v}_1, \dots, \vec{v}_k)$, $k = 1, \dots, m$
(that's the point — we are building an orthonormal set of vectors, describing the same subspaces spanned the columns of the matrix A)
- Let $V_k = \text{span}(\vec{q}_1, \dots, \vec{q}_k) \equiv \text{span}(\vec{v}_1, \dots, \vec{v}_k)$; these subspaces are “nested”:

$$V_0 \subset V_1 \subset \cdots \subset V_k,$$

$$\dim(V_0) \leq \dim(V_1) \leq \cdots \leq \dim(V_k),$$

(the maximal dimension is limited by the number of linearly independent vectors in $\{\vec{v}_1, \dots, \vec{v}_k\}$)

- #ProjectionFestival**

$$\text{proj}_{V_k}(\vec{x}) = (\vec{x} \cdot \vec{q}_1)\vec{q}_1 + \cdots + (\vec{x} \cdot \vec{q}_k)\vec{q}_k$$

Suggested Problems 5.2

Available on Learning Glass videos:

5.2 — 3, 7, 13, 31, 32, 33, 35, 39

Lecture – Book Roadmap

Lecture	Book, [GS5–]
5.1	§4.1, §4.2, §4.4
5.2	§4.1, §4.2, §4.4
5.3	§4.1, §4.2, §4.4

Metacognitive Exercise — Thinking About Thinking & Learning

I know / learned	Almost there	Huh?!?
Right After Lecture		
After Thinking / Office Hours / SI-session		
After Reviewing for Quiz/Midterm/Final		

(5.2.3), (5.2.7)

(5.2.3) Perform the Gram-Schmidt process on the sequence of vectors given:

$$\vec{v}_1 = \begin{bmatrix} 4 \\ 0 \\ 3 \end{bmatrix}, \quad \vec{v}_2 = \begin{bmatrix} 25 \\ 0 \\ -25 \end{bmatrix}.$$

(5.2.7) Perform the Gram-Schmidt process on the sequence of vectors given:

$$\vec{v}_1 = \begin{bmatrix} 2 \\ 2 \\ 1 \end{bmatrix}, \quad \vec{v}_2 = \begin{bmatrix} -2 \\ 1 \\ 2 \end{bmatrix}, \quad \vec{v}_3 = \begin{bmatrix} 18 \\ 0 \\ 0 \end{bmatrix}.$$

(5.2.13), (5.2.31)

(5.2.13) Perform the Gram-Schmidt process on the sequence of vectors given:

$$\vec{v}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \quad \vec{v}_2 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}, \quad \vec{v}_3 = \begin{bmatrix} 0 \\ 2 \\ 1 \\ -1 \end{bmatrix}.$$

(5.2.31) Perform the Gram-Schmidt process on the following basis of \mathbb{R}^3 :

$$\vec{v}_1 = \begin{bmatrix} a \\ 0 \\ 0 \end{bmatrix}, \quad \vec{v}_2 = \begin{bmatrix} b \\ c \\ 0 \end{bmatrix}, \quad \vec{v}_3 = \begin{bmatrix} d \\ e \\ f \end{bmatrix}.$$

(5.2.33), (5.2.35)

(5.2.33) Find an orthonormal basis for the kernel of the matrix

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

(5.2.35) Find an orthonormal basis for the image of the matrix

$$A = \begin{bmatrix} 1 & 2 & 1 \\ 2 & 1 & 1 \\ 2 & -2 & 0 \end{bmatrix}.$$

(5.2.39)

(5.2.39) Find an orthonormal basis $\langle \vec{u}_1, \vec{u}_2, \vec{u}_3 \rangle$ of \mathbb{R}^3 , such that

$$\text{span}(\vec{u}_1) = \text{span} \left(\begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \right),$$

and

$$\text{span}(\vec{u}_1, \vec{u}_2) = \text{span} \left(\begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix} \right),$$

Why Orthogonal Projections Matter \rightsquigarrow Solving the “Unsolvable”

Experience shows that at this point, most students tend to be a bit lost...

Known We need orthogonal bases to perform (correct) orthogonal projections to higher dimensional ($n \geq 2$) subspaces.

But The previous example (projecting from $\mathbb{R}^2 \rightarrow \mathbb{R}^2$) was not very satisfying...

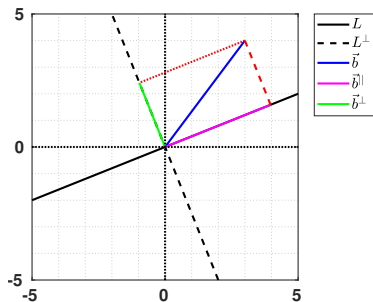
Mystery Why are orthogonal projections such a big deal? (Bad reasons include:)

- “The professor said so.” (multiple times)
- “It’ll be on the test.”

The goal of the next example is to give some idea as to why orthogonal projections can be useful... while re-visiting and connecting several “old” ideas.

Why Orthogonal Projections Matter \rightsquigarrow Solving the “Unsolvable”

Recall our old cartoon of orthogonal projections:



where $\vec{w} \in \mathbb{R}^n$, $L = \{ k\vec{w}, k \in \mathbb{R} \}$ is the (line) subspace of \mathbb{R}^n .

Important Note:

\vec{b}^\parallel is the point (in the subspace L) which is closest to \vec{b} .

Why Orthogonal Projections Matter \rightsquigarrow Solving the “Unsolvable”

Now, let

$$A = \begin{bmatrix} | \\ \vec{w} \\ | \end{bmatrix} \in \mathbb{R}^{n \times 1},$$

then we are interested in solving the linear system $A\vec{x} = \vec{b}$, where $\vec{x} \in \mathbb{R}^1$ (for now), and $\vec{b} \in \mathbb{R}^n$.

The system has a solution **if and only if** $\vec{b} \in \text{im}(A) = L$.

When $\vec{b} \notin \text{im}(A)$ we can either

- say “🔑 *you guys, I’m going home!*” 🧑, or
- extend the concept of a “solution” to the problem...

Why Orthogonal Projections Matter \rightsquigarrow Solving the “Unsolvable”

Since this is not a South Park episode, we decide to extend the concept of what it means to “solve” this problem:

We decide to look for a value \vec{x}^* which makes the **residual***

$$r(\vec{x}) = \|A\vec{x} - \vec{b}\|$$

as small as possible.

In our example, that value is $\vec{x}^* = \left(\frac{\vec{b} \cdot \vec{w}}{\vec{w} \cdot \vec{w}} \right)$, which makes $A\vec{x}^* = \vec{b}^{\parallel}$, and $r(\vec{x}^*) = \|\vec{b}^{\perp}\| = \|\vec{b} - \vec{b}^{\parallel}\| = \|\vec{b}^{\perp}\|$.

It is true in general that the shortest distance between \vec{b} and a subspace L , is $\vec{b}^{\perp} = \vec{b} - \text{proj}_L(\vec{b})$.

* think of $r(\vec{x})$ as a measure of how far we are from solving the linear system in the “traditional” sense.

Why Orthogonal Projections Matter \rightsquigarrow Solving the “Unsolvable”

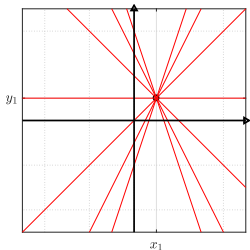
Next we consider a slightly different category of problems: fitting a straight line $y = a + bx$ to some number of given points in the x - y -plane, $\{(x_k, y_k)\}_{k=1}^n$.

Case ($n = 1$, a single point): In this case we have infinitely many solutions. In our notation the solutions are given by

$$\underbrace{\begin{bmatrix} 1 & x_1 \end{bmatrix}}_A \begin{bmatrix} a \\ b \end{bmatrix} = [y_1]$$

which gives

$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} y_1 \\ 0 \end{bmatrix} + s \begin{bmatrix} -x_1 \\ 1 \end{bmatrix}$$



Why Orthogonal Projections Matter \rightsquigarrow Solving the “Unsolvable”

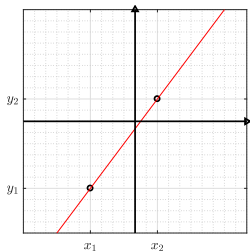
Case ($n = 2$, two distinct points): In this case we have a unique solution. In our notation the solutions are given by

$$\underbrace{\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \end{bmatrix}}_A \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

which gives

$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \end{bmatrix}^{-1} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

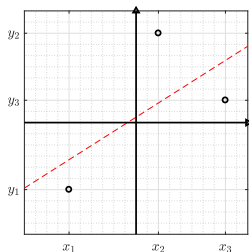
where the inverse is guaranteed to exist when $x_1 \neq x_2$.



Why Orthogonal Projections Matter \rightsquigarrow Solving the “Unsolvable”

Case ($n = 3$, three distinct points): In this case we have no solution. In our notation the solutions would be given by

$$\underbrace{\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \end{bmatrix}}_A \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$



which gives

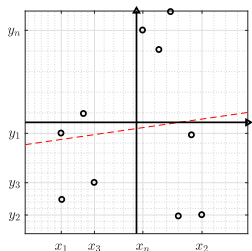
$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \text{MAGIC} \\ \text{MATRIX} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \quad ???$$

There is no solution, unless the 3 points are on a common line...

Why Orthogonal Projections Matter \rightsquigarrow Solving the “Unsolvable”**Case ($n = \text{large}$, many (distinct) points):**

In this case we have no solution. In our notation the solutions would be given by

$$\underbrace{\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}}_{A \in \mathbb{R}^{n \times 2}} \begin{bmatrix} a \\ b \end{bmatrix} = \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}}_{\vec{y} \in \mathbb{R}^n}$$



which gives

$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \text{MAGIC} \\ \text{MATRIX} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \quad ???$$

There is no solution, unless the ALL points are on a common line...

Why Orthogonal Projections Matter \rightsquigarrow Solving the “Unsolvable”

Staying in the general $n = \text{large}$ case, with

$$\underbrace{\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}}_{A \in \mathbb{R}^{n \times 2}} \begin{bmatrix} a \\ b \end{bmatrix} = \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}}_{\vec{y} \in \mathbb{R}^n}$$

In our linear algebra language, we “know” that $P = \text{im}(A)$ is a 2-dimensional subspace of \mathbb{R}^n (the two columns are different, unless all the x_k s coincide)...

and, of course, we only have a solution if/when \vec{y} can be written as a linear combination of the columns of $A \Leftrightarrow “\vec{y} \in \text{im}(A).”$

Why Orthogonal Projections Matter \rightsquigarrow Solving the “Unsolvable”

Now, if we are looking for a best-extended-concept-of-solution candidate; we compute $\text{proj}_P(\vec{y}) \equiv \vec{y}^{\parallel}$, and the system

$$\underbrace{\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}}_{A \in \mathbb{R}^{n \times 2}} \underbrace{\begin{bmatrix} a \\ b \end{bmatrix}}_{\vec{c}} = \text{proj}_P(\vec{y})$$

does have a unique solution, call it \vec{c}^* ; and the residual

$$r(\vec{c}^*) = \|A\vec{c}^* - \vec{y}\| = \|\vec{y}^{\parallel} - \vec{y}\| = \|\vec{y}^{\perp}\|$$

is minimized.

Why Orthogonal Projections Matter \rightsquigarrow Solving the “Unsolvable”

We have defined a new type of “solution” for inconsistent non-square (matrix) problems.

The way we have discussed it, the best name would be a

- “Minimum Residual Solution”

However, the most common mathematical name is the

- “Least Squares Solution”

In many applications (related to statistics), the most common name is the

- “Linear Regression Solution”

$$V = \{x_1 + x_2 + x_3 + x_4 = 0\} \subset \mathbb{R}^4$$

What is your problem?!?

Find an orthonormal basis for the subspace

$$V = \{x_1 + x_2 + x_3 + x_4 = 0\} \subset \mathbb{R}^4,$$

then project the vectors

$$\vec{y}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \quad \text{and} \quad \vec{y}_2 = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix}$$

onto V .

$$V = \{x_1 + x_2 + x_3 + x_4 = 0\} \subset \mathbb{R}^4$$

- First, we need a basis for V ; finding $\ker\left(\begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix}\right)$ will do the trick.
- Since $A = \begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix}$ already is in rref, we can identify the solutions to $\vec{A}\vec{x} = 0$:

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = s \begin{bmatrix} -1 \\ 1 \\ 0 \\ 0 \end{bmatrix} + t \begin{bmatrix} -1 \\ 0 \\ 1 \\ 0 \end{bmatrix} + u \begin{bmatrix} -1 \\ 0 \\ 0 \\ 1 \end{bmatrix},$$

so our basis is

$$B_V = (\vec{v}_1, \vec{v}_2, \vec{v}_3) = \left(\begin{bmatrix} -1 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} -1 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} -1 \\ 0 \\ 0 \\ 1 \end{bmatrix} \right); \quad A = \begin{bmatrix} -1 & -1 & -1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix}$$

as an added bonus we will compute the QR -factorization of A .

$$V = \{x_1 + x_2 + x_3 + x_4 = 0\} \subset \mathbb{R}^4$$

- $\|\vec{v}_1\| = \sqrt{(-1)^2 + 1^2 + 0^2 + 0^2} = \sqrt{2}$

- $\vec{q}_1 = \frac{1}{\|\vec{v}_1\|} \vec{v}_1$

$$Q = \begin{bmatrix} -1/\sqrt{2} & \times & \times \\ 1/\sqrt{2} & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \end{bmatrix}, \quad R = \begin{bmatrix} \sqrt{2} & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \end{bmatrix}$$

- We move on to \vec{v}_2 ...

$$V = \{x_1 + x_2 + x_3 + x_4 = 0\} \subset \mathbb{R}^4$$

$$\bullet \vec{q}_1 \cdot \vec{v}_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 1 \\ 0 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} -1 \\ 0 \\ 1 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} ((-1)^2 + 1 \times 0 + 0 \times 1 + 0 \times 0) = \frac{1}{\sqrt{2}}$$

$$\bullet \vec{v}_2^\perp = \vec{v}_2 - (\vec{q}_1 \cdot \vec{v}_2) \vec{q}_1 = \begin{bmatrix} -1 \\ 0 \\ 1 \\ 0 \end{bmatrix} - \left(\frac{1}{\sqrt{2}}\right) \left(\frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 1 \\ 0 \\ 0 \end{bmatrix}\right) = \frac{1}{2} \begin{bmatrix} -1 \\ -1 \\ 2 \\ 0 \end{bmatrix}$$

$$\bullet \|\vec{v}_2^\perp\| = \frac{1}{2} \sqrt{1 + 1 + 4 + 0} = \frac{\sqrt{6}}{2}$$

$$\bullet \vec{q}_2 = \frac{1}{\|\vec{v}_2^\perp\|} \vec{v}_2^\perp = \frac{1}{\sqrt{6}} \begin{bmatrix} -1 \\ -1 \\ 2 \\ 0 \end{bmatrix}$$

•

$$Q = \begin{bmatrix} -1/\sqrt{2} & -1/\sqrt{6} & \times \\ 1/\sqrt{2} & -1/\sqrt{6} & \times \\ 0 & 2/\sqrt{6} & \times \\ 0 & 0 & \times \end{bmatrix}, \quad R = \begin{bmatrix} \sqrt{2} & 1/\sqrt{2} & \times \\ 0 & \sqrt{6}/2 & \times \\ 0 & 0 & \times \end{bmatrix}$$

$$V = \{x_1 + x_2 + x_3 + x_4 = 0\} \subset \mathbb{R}^4$$

$$\bullet \vec{q}_1 \cdot \vec{v}_3 = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 1 \\ 0 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} -1 \\ 0 \\ 0 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}} ((-1)^2 + 1 \times 0 + 0 \times 1 + 0 \times 0) = \frac{1}{\sqrt{2}}$$

$$\bullet \vec{q}_2 \cdot \vec{v}_3 = \frac{1}{\sqrt{6}} \begin{bmatrix} -1 \\ -1 \\ 2 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} -1 \\ 0 \\ 0 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{6}} ((-1)^2 + (-1) \times 0 + 0 \times 1 + 0 \times 1) = \frac{1}{\sqrt{6}}$$

•

$$Q = \begin{bmatrix} -1/\sqrt{2} & -1/\sqrt{6} & \times \\ 1/\sqrt{2} & -1/\sqrt{6} & \times \\ 0 & 2/\sqrt{6} & \times \\ 0 & 0 & \times \end{bmatrix}, \quad R = \begin{bmatrix} \sqrt{2} & 1/\sqrt{2} & 1/\sqrt{2} \\ 0 & \sqrt{6}/2 & 1/\sqrt{6} \\ 0 & 0 & \times \end{bmatrix}$$

$$V = \{x_1 + x_2 + x_3 + x_4 = 0\} \subset \mathbb{R}^4$$

$$\bullet \vec{v}_3^\perp = \vec{v}_3 - (\vec{q}_1 \cdot \vec{v}_3)\vec{q}_1 - (\vec{q}_2 \cdot \vec{v}_3)\vec{q}_2:$$

$$\begin{bmatrix} -1 \\ 0 \\ 0 \\ 1 \end{bmatrix} - \left(\frac{1}{\sqrt{2}}\right) \left(\frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 1 \\ 0 \\ 0 \end{bmatrix}\right) - \left(\frac{1}{\sqrt{6}}\right) \left(\frac{1}{\sqrt{6}} \begin{bmatrix} -1 \\ -1 \\ 2 \\ 0 \end{bmatrix}\right) = \frac{1}{3} \begin{bmatrix} -1 \\ -1 \\ -1 \\ 3 \end{bmatrix}$$

$$\bullet \|\vec{v}_3^\perp\| = \frac{1}{3}\sqrt{1+1+1+9} = \frac{\sqrt{12}}{3}$$

$$\bullet \vec{q}_3 = \frac{1}{\|\vec{v}_3^\perp\|} \vec{v}_3^\perp = \frac{1}{\sqrt{12}} \begin{bmatrix} -1 \\ -1 \\ -1 \\ 3 \end{bmatrix}$$

•

$$Q = \begin{bmatrix} -1/\sqrt{2} & -1/\sqrt{6} & -1/\sqrt{12} \\ 1/\sqrt{2} & -1/\sqrt{6} & -1/\sqrt{12} \\ 0 & 2/\sqrt{6} & -1/\sqrt{12} \\ 0 & 0 & 3/\sqrt{12} \end{bmatrix}, \quad R = \begin{bmatrix} \sqrt{2} & 1/\sqrt{2} & 1/\sqrt{2} \\ 0 & \sqrt{6}/2 & 1/\sqrt{6} \\ 0 & 0 & \sqrt{12}/3 \end{bmatrix}$$

$$V = \{x_1 + x_2 + x_3 + x_4 = 0\} \subset \mathbb{R}^4$$

Projections!

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$$\bullet \vec{y}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

$$\bullet \vec{q}_1 \cdot \vec{y}_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 1 \\ 0 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}} (-1 + 1 + 0 + 0) = 0$$

$$\bullet \vec{q}_2 \cdot \vec{y}_1 = \frac{1}{\sqrt{6}} \begin{bmatrix} -1 \\ -1 \\ 2 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{6}} (-1 - 1 + 2 + 0) = 0$$

$$\bullet \vec{q}_3 \cdot \vec{y}_1 = \frac{1}{\sqrt{12}} \begin{bmatrix} -1 \\ -1 \\ -1 \\ 3 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{12}} (-1 - 1 - 1 + 3) = 0$$

$$\bullet \text{proj}_V(\vec{y}_1) = \vec{0}$$

- \bullet Of course! We constructed $B_V = (\vec{v}_1, \vec{v}_2, \vec{v}_3)$ by finding all vectors orthogonal to \vec{y}_1 ((Solving $[1 \ 1 \ 1 \ 1]\vec{x} = 0$))

$$V = \{x_1 + x_2 + x_3 + x_4 = 0\} \subset \mathbb{R}^4$$

Projections!

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$$\bullet \vec{y}_2 = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix}$$

$$\bullet \vec{q}_1 \cdot \vec{y}_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 1 \\ 0 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix} = \frac{1}{\sqrt{2}} (-1 + 2 + 0 + 0) = \frac{1}{\sqrt{2}}$$

$$\bullet \vec{q}_2 \cdot \vec{y}_2 = \frac{1}{\sqrt{6}} \begin{bmatrix} -1 \\ -1 \\ 2 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix} = \frac{1}{\sqrt{6}} (-1 - 2 + 6 + 0) = \frac{3}{\sqrt{6}}$$

$$\bullet \vec{q}_3 \cdot \vec{y}_2 = \frac{1}{\sqrt{12}} \begin{bmatrix} -1 \\ -1 \\ -1 \\ 3 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix} = \frac{1}{\sqrt{12}} (-1 - 2 - 3 + 12) = \frac{6}{\sqrt{12}}$$

$$\bullet \text{proj}_V(\vec{y}_2) = \frac{1}{2} \begin{bmatrix} -1 \\ 1 \\ 0 \\ 0 \end{bmatrix} + \frac{3}{6} \begin{bmatrix} -1 \\ 2 \\ 0 \end{bmatrix} + \frac{6}{12} \begin{bmatrix} -1 \\ -1 \\ 3 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} -3 \\ -1 \\ 1 \\ 3 \end{bmatrix}$$

5.2.35 and Beyond

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What is your problem?!?

Given A , find an orthonormal basis for $\text{im}(A)$, and the QR -factorization $QR = A$:

$$A = \begin{bmatrix} 1 & 2 & 1 \\ 2 & 1 & 1 \\ 2 & -2 & 0 \end{bmatrix}, \quad Q = \begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}, \quad R = \begin{bmatrix} \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot \\ 0 & 0 & \cdot \end{bmatrix}$$

$$\vec{v}_1 :: \|\vec{v}_1\| = \sqrt{1^2 + 2^2 + 2^2} = \sqrt{9} = 3; \quad \vec{q}_1 = \frac{\vec{v}_1}{\|\vec{v}_1\|} = \frac{1}{3} \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}$$

$$Q = \begin{bmatrix} 1/3 & \cdot & \cdot \\ 2/3 & \cdot & \cdot \\ 2/3 & \cdot & \cdot \end{bmatrix}, \quad R = \begin{bmatrix} 3 & \cdot & \cdot \\ 0 & \cdot & \cdot \\ 0 & 0 & \cdot \end{bmatrix}$$

5.2.35 and Beyond

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$$\vec{v}_2^\perp :: \vec{v}_2^\perp = \vec{v}_2 - (\vec{q}_1 \cdot \vec{v}_2) \vec{q}_1 = \begin{bmatrix} 2 \\ 1 \\ -2 \end{bmatrix} - \underbrace{\left(\frac{1}{3} \begin{bmatrix} 2 \\ 1 \\ -2 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} \right)}_0 \left(\frac{1}{3} \begin{bmatrix} 2 \\ 1 \\ -2 \end{bmatrix} \right) = \begin{bmatrix} 2 \\ 1 \\ -2 \end{bmatrix}.$$

$$\|\vec{v}_2^\perp\| = \sqrt{2^2 + 1^2 + (-2)^2} = \sqrt{9} = 3, \quad \vec{q}_2 = \frac{\vec{v}_2^\perp}{\|\vec{v}_2^\perp\|} = \frac{1}{3} \begin{bmatrix} 2 \\ 1 \\ -2 \end{bmatrix}$$

$$Q = \begin{bmatrix} 1/3 & 2/3 & \cdot \\ 2/3 & 1/3 & \cdot \\ 2/3 & -2/3 & \cdot \end{bmatrix}, \quad R = \begin{bmatrix} 3 & 0 & \cdot \\ 0 & 3 & \cdot \\ 0 & 0 & \cdot \end{bmatrix}$$

5.2.35 and Beyond

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$$\begin{aligned} \vec{v}_3^\perp &= \vec{v}_3 - (\vec{q}_1 \cdot \vec{v}_3) \vec{q}_1 - (\vec{q}_2 \cdot \vec{v}_3) \vec{q}_2 \\ &= \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} - \underbrace{\left(\frac{1}{3} \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \right)}_1 \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} - \underbrace{\left(\frac{1}{3} \begin{bmatrix} 2 \\ 1 \\ -2 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \right)}_1 \begin{bmatrix} 2 \\ 1 \\ -2 \end{bmatrix} \\ &= \frac{1}{3} \begin{bmatrix} 3 \\ 3 \\ 0 \end{bmatrix} - \frac{1}{3} \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} - \frac{1}{3} \begin{bmatrix} 2 \\ 1 \\ -2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \end{aligned}$$

$$\|\vec{v}_3^\perp\| = 0, \quad \vec{q}_q = \frac{\vec{v}_3^\perp}{\|\vec{v}_3^\perp\|} = \begin{bmatrix} ? \\ ? \\ ? \end{bmatrix}$$

$$Q = \begin{bmatrix} 1/3 & 2/3 & ? \\ 2/3 & 1/3 & ? \\ 2/3 & -2/3 & ? \end{bmatrix},$$

$$R = \begin{bmatrix} 3 & 0 & 1 \\ 0 & 3 & 1 \\ 0 & 0 & 0 \end{bmatrix}$$

5.2.35 and Beyond

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- $\vec{v}_3^\perp = 0$ means that \vec{v}_3 is a linear combination of \vec{v}_1 and \vec{v}_2 .
- Therefore $\text{im}(A) = \text{span}(\vec{v}_1, \vec{v}_2) = \text{span}(\vec{q}_1, \vec{q}_2)$
- We have 2 options for the QR -factorization:

$$A = \underbrace{\begin{bmatrix} 1/3 & 2/3 \\ 2/3 & 1/3 \\ 2/3 & -2/3 \end{bmatrix} \begin{bmatrix} 3 & 0 & 1 \\ 0 & 3 & 1 \end{bmatrix}}_{\text{"Economy Size" } QR\text{-factorization}}, \text{ or } \underbrace{\begin{bmatrix} 1/3 & 2/3 & 2/3 \\ 2/3 & 1/3 & -2/3 \\ 2/3 & -2/3 & 1/3 \end{bmatrix} \begin{bmatrix} 3 & 0 & 1 \\ 0 & 3 & 1 \\ 0 & 0 & 0 \end{bmatrix}}_{\text{"Full" } QR\text{-factorization}}.$$

Note that in the second version, we have added a third orthonormal vector to the Q -matrix, and a row of zeros to the R -matrix.