Math 254: Introduction to Linear Algebra

Notes #5.2 — Gram-Schmidt Process and QR Factorization

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Outline

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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
 - \Rightarrow This builds an orthonormal basis (the columns of Q) for the subspace $V=\operatorname{im}(A)$, which gives us the means to compute the orthogonal projection $\operatorname{proj}_V(\vec{x})$ onto V.
- to orthogonally project onto any subspace.



The Gram-Schmidt Orthogonalization Process The \ensuremath{QR} Factorization Observations

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 $\vec{u}_1,\ldots,\vec{u}_m$, then

$$\operatorname{proj}_{V}(\vec{x}) = \vec{x}^{\parallel} = (\vec{u}_{1} \cdot \vec{x})\vec{u}_{1} + \dots + (\vec{u}_{m} \cdot \vec{x})\vec{u}_{m}$$

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

How do you project onto a subspace if/when the given basis is <u>not</u> 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

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

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:

$$\operatorname{proj}_{V}(\vec{x}) = (\vec{v}_{1} \cdot \vec{x})\vec{v}_{1} + (\vec{v}_{2} \cdot \vec{x})\vec{v}_{2} = 5\vec{v}_{1} + 8\vec{v}_{2} = \begin{bmatrix} 13 \\ 21 \end{bmatrix}.$$

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

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





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

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

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



The Gram-Schmidt Orthogonalization Process The QR Factorization

The QR Factorization
Observations

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 $V = \operatorname{span}\left(\vec{v}_1, \dots, \vec{v}_m\right) \subset \mathbb{R}^n$; compute $\operatorname{proj}_V(\vec{x})$:

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

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

and then use the projection formula.

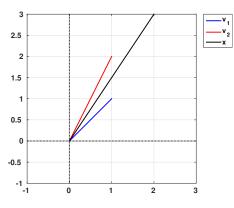


The QR Factorization
Observations

Example: Doing it Right...

Build an Orthonormal Basis

Figure: This is where we start.



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



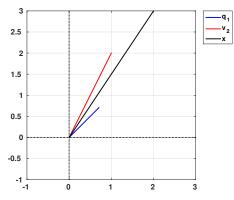
The Gram-Schmidt Orthogonalization Process

The QR Factorization
Observations

Example: Doing it Right...

(i) Rescale the first vector

Figure: Rescale* $\vec{v_1}$ to be norm 1, and call it $\vec{q_1}$.



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



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

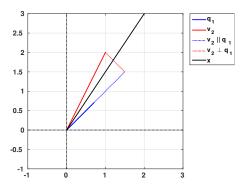
The Gram-Schmidt Orthogonalization Process

The QR Factorization
Observations

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 $\vec{v}_2^{\parallel \mid \vec{q}_1}$, and $\vec{v}_2^{\perp \mid \vec{q}_1}$.



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

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

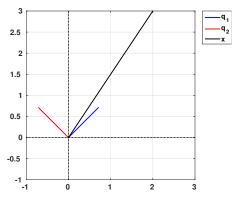


The QR Factorization
Observations

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 $\mathfrak{Q} = \langle \vec{q}_1, \vec{q}_2 \rangle!$



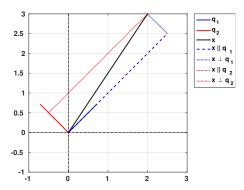
The Gram-Schmidt Orthogonalization Process

The QR Factorization Observations

Example: Doing it Right...

(iv) Project using the new orthonormal basis!

Figure: Finally, we can use the projection formula.



$$\operatorname{proj}_{V}(\vec{x}) = (\vec{q}_{1} \cdot \vec{x})\vec{q}_{1} + (\vec{q}_{2} \cdot \vec{x})\vec{q}_{2} = \frac{5}{\sqrt{2}}\vec{q}_{1} + \frac{1}{\sqrt{2}}\vec{q}_{2}$$

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



Example: Doing it Right...

Coordinates

In the context of [Coordinates (Notes#3.4)], we have

Basis:
$$\mathfrak{Q} = \langle \vec{q}_1, \, \vec{q}_2 \rangle$$

Observations

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



The Gram-Schmidt Orthogonalization Process The QR Factorization

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.

Observations

It is "easy" to see that

$$\underbrace{\begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix}}_{A = \begin{bmatrix} \vec{V}_1 & \vec{V}_2 \end{bmatrix}} = \underbrace{\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}}_{Q = \begin{bmatrix} \vec{q}_1 & \vec{q}_2 \end{bmatrix}} \underbrace{\begin{bmatrix} \sqrt{2} & \frac{3}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} \end{bmatrix}}_{R},$$

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...



Observations

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 $\operatorname{span}(\vec{q}_1) = \operatorname{span}(\vec{v}_1)$.
 - $\vec{q}_2 = \vec{w}_2 / ||\vec{w}_2||$
- 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 $\vec{q}_k = \vec{w}_k / ||\vec{w}_k||$.



5.2. Gram-Schmidt and OR Factorization

The QR Factorization

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

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

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

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

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

$$\underbrace{\begin{pmatrix} \vec{v}_1 & \cdots & \vec{v}_n \end{pmatrix}}_{A} = \underbrace{\begin{pmatrix} \vec{q}_1 & \cdots & \vec{q}_n \end{pmatrix}}_{Q} R$$



Interpretations and Relations

With A = QR, we have to following relations:

- $\bullet \ [\vec{x}]_{\mathfrak{Q}} = R[\vec{x}]_{\mathfrak{A}}$
 - Multiplication by *R* moves us from *A*-coordinates to *Q*-coordinates.
- $\bullet \ \vec{x} = Q[\vec{x}]_{\mathfrak{Q}} = QR[\vec{x}]_{\mathfrak{A}}$
 - Multiplying the Q-coordinate vector by Q "builds" the vector \vec{x} .
- $\bullet \ \vec{x} = A[\vec{x}]_{\mathfrak{A}}$
 - Multiplying the A-coordinate vector by A "builds" the (same) vector \vec{x} .

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



The Gram-Schmidt Orthogonalization Process
The QR Factorization
Observations

What's in R?

1 of 3

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

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

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

Note: Subspaces, Orthogonal Complements, and Bases

We are constructing a sequence of subspace-pairs

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

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

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



The Gram-Schmidt Orthogonalization Process The QR Factorization Observations

What's in R?

2 of 3

OK, let's rearrange the previous expression:

$$ec{\mathbf{v}}_k = \underbrace{(ec{q}_1 \cdot ec{\mathbf{v}}_k) ec{q}_1 - (ec{q}_2 \cdot ec{\mathbf{v}}_k) ec{q}_2 - \dots - (ec{q}_{k-1} \cdot ec{\mathbf{v}}_k) ec{q}_{k-1}}_{ec{\mathbf{v}}_k^{\perp}} + \underbrace{ec{\mathbf{w}}_k}_{ec{\mathbf{v}}_k^{\perp}}$$

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:

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

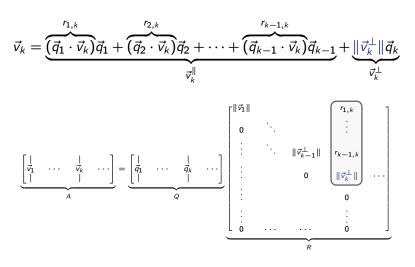
This is the "recipe" for rebuilding the k^{th} column of A using the first k columns of Q. The entries in R are given by

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



What's in R?

3 of 3





Summarizing \rightsquigarrow The QR-factorization

Theorem (QR-Factorization)

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

Further

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

Note that

[QR-factorization] = [Gram-Schmidt] + [Bookkeeping].



The Gram-Schmidt Orthogonalization Process
The QR Factorization
Observations

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

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

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



Suggested Problems 5.2

Available on Learning Glass videos:

5.2 — 3, 7, 13, 31, 32, 33, <u>35</u>, 39



Lecture - Book Roadmap

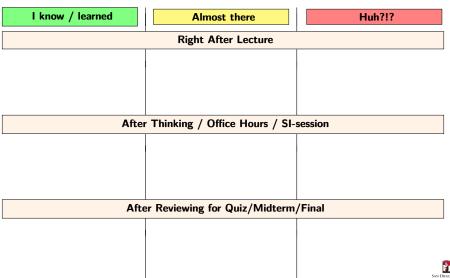
Lecture	Book, [GS5-]
5.1	§4.1, §4.2, § 4.4
5.2	§4.1, §4.2, § 4.4
5.3	§4.1, §4.2, § 4.4



Metacognitive Reflection **Problem Statements 5.2**

Why Orthogonal Projections Matter

Metacognitive Exercise — Thinking About Thinking & Learning





(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

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

and

$$\operatorname{span}\left(\vec{u}_{1},\vec{u}_{2}
ight)=\operatorname{span}\left(egin{bmatrix}1\\2\\3\end{bmatrix},egin{bmatrix}1\\1\\-1\end{bmatrix}
ight),$$



Why Orthogonal Projections Matter → Solving the "Unsolvable"

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

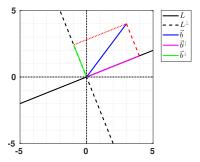
- Known We need orthogonal bases to perform (correct) orthogonal projections to higher dimensional ($n \ge 2$) subspaces.
 - But The previous example (projecting from $\mathbb{R}^2 \to \mathbb{R}^2$) was not very satisfying...
- Mystery Why are orthogonal projections such a big deal? (Bad reasons include:)
 - "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 → 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 → 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 $\vec{b} \in \operatorname{im}(A) = L$.

When $\vec{b} \not\in \operatorname{im}(A)$ we can either

- say "• you guys, I'm going home!" or
- extend the concept of a "solution" to the problem...



Why Orthogonal Projections Matter ~ 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 $\vec{x}^* = \begin{pmatrix} \vec{b} \cdot \vec{w} \\ \vec{w} \cdot \vec{w} \end{pmatrix}$, which makes $A\vec{x}^* = \vec{b}^{\parallel}$, and $r(\vec{x}^*) = \|\vec{b}^{\parallel} - \vec{b}\| = \|-\vec{b}^{\perp}\| = \|\vec{b}^{\perp}\|$. It is true in general that the shortest distance between \vec{b} and a

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

^{*} think of is as a measure of how far we are from solving the linear system in the "traditional" sense.

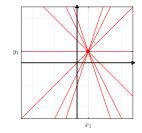


Why Orthogonal Projections Matter --> Solving the "Unsolvable"

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

$$\underbrace{\begin{bmatrix} \mathbf{1} \\ x_1 \end{bmatrix}}_{A} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} y_1 \end{bmatrix}$$



which gives

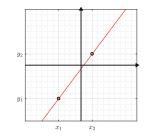
$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} y_1 \\ 0 \end{bmatrix} + s \begin{bmatrix} -x_1 \\ 1 \end{bmatrix}$$



Why Orthogonal Projections Matter ~ 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

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

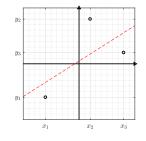
where the inverse is guaranteed to exist when $x_1 \neq x_2$.



Why Orthogonal Projections Matter - 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

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

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

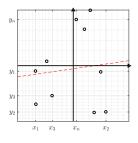


Why Orthogonal Projections Matter ~ Solving the "Unsolvable"

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

$$\begin{bmatrix}
1 & x_1 \\
1 & x_2 \\
\vdots & \vdots \\
1 & x_n
\end{bmatrix}
\begin{bmatrix}
a \\
b
\end{bmatrix} =
\begin{bmatrix}
y_1 \\
y_2 \\
\vdots \\
y_n
\end{bmatrix}$$

$$\overrightarrow{y} \in \mathbb{R}^n$$



which gives

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

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



Why Orthogonal Projections Matter ~ Solving the "Unsolvable"

Staying in the general n = 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 $P = \operatorname{im}(A)$ 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 $A \Leftrightarrow "\vec{y} \in \operatorname{im}(A)$."



Metacognitive Reflection Problem Statements 5.2 Why Orthogonal Projections Matter

Why Orthogonal Projections Matter → Solving the "Unsolvable"

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

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

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

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

is minimized.



Why Orthogonal Projections Matter → 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"



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

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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.



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

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- First, we need a basis for V; finding $ker(\begin{bmatrix} 1 & 1 & 1 \end{bmatrix})$ will do the trick.
- Since $A = \begin{bmatrix} 1 & 1 & 1 \end{bmatrix}$ 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

$$B_V = (\vec{v_1}, \vec{v_2}, \vec{v_3}) = \begin{pmatrix} \begin{bmatrix} -1\\1\\0\\0\end{bmatrix}, \begin{bmatrix} -1\\0\\1\\0\end{bmatrix}, \begin{bmatrix} -1\\0\\0\\1\end{bmatrix} \end{pmatrix}; \quad A = \begin{bmatrix} -1&-1&-1\\1&0&0\\0&1&0\\0&1&1 \end{bmatrix}$$

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



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

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

$$\bullet \quad \vec{q}_1 = \frac{1}{\parallel \vec{v}_1 \parallel} \vec{v}_1$$

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

• We move on to \vec{v}_2 ...



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

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

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

•

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



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

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

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



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

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

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

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

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



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

Projections!

$$\vec{y_1} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

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

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

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

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



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

Projections!

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

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

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

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



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What is your problem?!?

Given A, find an orthonormal basis for im(A), and the QR-factorization QR = A:

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

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

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



$$\vec{v}_2 :: \quad \vec{v}_2^{\perp} = \vec{v}_2 - (\vec{q}_1 \cdot \vec{v}_2) \, \vec{q}_1 = \begin{bmatrix} 2 \\ 1 \\ -2 \end{bmatrix} - \underbrace{\left(\frac{1}{3} \begin{bmatrix} 2 \\ 1 \\ -2 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}\right)}_{0} \left(\frac{1}{3} \begin{bmatrix} 2 \\ 1 \\ -2 \end{bmatrix}\right) = \begin{bmatrix} 2 \\ 1 \\ -2 \end{bmatrix}.$$

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

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



$$\vec{q}_{3}^{\perp} = \vec{v}_{3} - (\vec{q}_{1} \cdot \vec{v}_{3}) \vec{q}_{1} - (\vec{q}_{2} \cdot \vec{v}_{3}) \vec{q}_{2}
= \begin{bmatrix} 1\\1\\0 \end{bmatrix} - \underbrace{\begin{pmatrix} 1\\3\\2\\2 \end{bmatrix} \cdot \begin{bmatrix} 1\\1\\0 \end{bmatrix} \end{pmatrix} \begin{pmatrix} 1\\3\\2\\2 \end{bmatrix} - \underbrace{\begin{pmatrix} 1\\3$$



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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 $\operatorname{im}(A) = \operatorname{span}(\vec{v}_1, \vec{v}_2) = \operatorname{span}(\vec{q}_1, \vec{q}_2)$
- We have 2 options for the *QR*-factorization:

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

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.

