CHAPTERS 3-5

Inner Products and Norms

The most basic inner product is the dot product

$$\vec{v} \cdot \vec{w} = v_1 w_1 + v_2 w_2 + \cdots + v_n w_n$$

On $\mathbb{R}^n$, the dot product obeys:

1) Bilinearity $(c\vec{u} + d\vec{v}) \cdot \vec{w} = c(\vec{u} \cdot \vec{w}) + d(\vec{v} \cdot \vec{w})$

$\vec{u} \cdot (c\vec{v} + d\vec{w}) = c(\vec{u} \cdot \vec{v}) + d(\vec{u} \cdot \vec{w})$

2) Symmetry $\vec{u} \cdot \vec{v} = \vec{v} \cdot \vec{u}$

3) Positivity $\vec{v} \cdot \vec{v} \geq 0$ and $\vec{v} \cdot \vec{v} = 0$ if and only if $\vec{v} = \vec{0}$.

From the dot product we get the 2-norm

$$\|\vec{v}\|_2 = \sqrt{\vec{v} \cdot \vec{v}} = \left(v_1^2 + v_2^2 + \cdots + v_n^2 \right)^{1/2}$$

Other norms:

$$\|\vec{v}\|_p = \left(v_1^p + v_2^p + \cdots + v_n^p \right)^{1/p}$$

Most common cases: $p = 1, 2, \infty$.

$$\|\vec{v}\|_\infty = \max_{1 \leq i \leq n} |v_i|.$$

Other norms and inner product come up naturally throughout mathematics and physics. The text book details this but we will largely avoid any generalizations.

General properties of a norm:

i) Positivity: $\|\vec{v}\| \geq 0$ and $\|\vec{v}\| = 0$ if and only if $\vec{v} = \vec{0}$

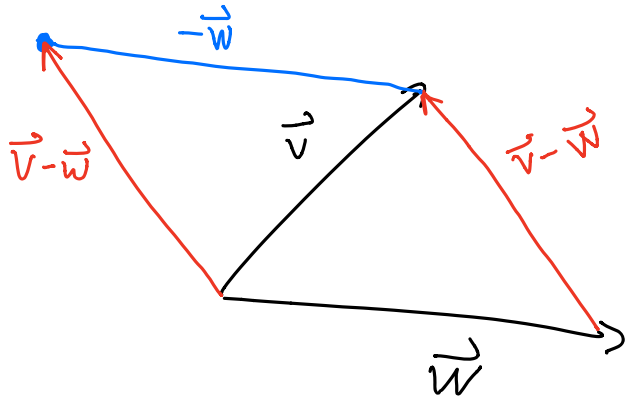
ii) Homogeneity: $\|c\vec{v}\| = |c|\,\|\vec{v}\|$.

iii) Triangle inequality: $\|\vec{v} + \vec{w}\| \leq \|\vec{v}\| + \|\vec{w}\|$.

A norm measures the size of a vector.

$$\|\vec{v} - \vec{w}\|$$

measures the distance:



Matrices also have norms. We will encounter one later in the course.

We have three situations to consider:

$\text{img } A \neq \mathbb{R}^m$
$\ker A = \{\vec{0}\}$

1) Solving $A\vec{x} = \vec{b}$ when there is no solution.

$\ker A \neq \{\vec{0}\}$
$\text{img } A = \mathbb{R}^m$

2) Solving $A\vec{x} = \vec{b}$ when there is no solution.

3) Solving $A\vec{x} = \vec{b}$ when

$$\text{img } A \neq \mathbb{R}^m \text{ and } \ker A \neq \{\vec{0}\}.$$

Some of these statements seem contradictory. But as we will see, we can make sense of them. But there are many ways to make sense of them.

Solving $A\vec{x} = \vec{b}$ when there is no solution

Since we cannot find $\vec{x}$ such that $A\vec{x} = \vec{b}$, we find $\vec{x}$ such that

$$\| A\vec{x} - \vec{b} \|_2$$

is as small as possible.

i.e. $\| A\vec{x} - \vec{b} \|_2 < \| A\vec{y} - \vec{b} \|$ for $\vec{x} \neq \vec{y}$.

Theorem Suppose A is $m \times n$ and A^TA is invertible. 4

For $\vec{x} = (A^TA)^{-1}A\vec{b}$ we have

$$\|A\vec{x} - \vec{b}\|_2 < \|A\vec{y} - b\|_2 \quad \text{for}$$

every $\vec{y} \in \mathbb{R}^n$, $\vec{y} \neq \vec{x}$.

This means that the solution of

$$A^TA\vec{x} = A^T\vec{b}$$ ← Normal equations.

is the unique minimum for $\|A\vec{y} - b\|_2$.

$\vec{x}$ is called the least-squares solution

Proof It suffices to consider

$$\|A\vec{y} - \vec{b}\|_2^2 = (A\vec{y} - \vec{b})^T(A\vec{y} - \vec{b})$$

$$= (\vec{y}^TA^T - \vec{b}^T)(A\vec{y} - \vec{b})$$

$$= \vec{y}^TA^TA\vec{y} - \vec{y}^TA^T\vec{b} - \vec{b}^TA\vec{y} + \vec{b}^T\vec{b} =: F(\vec{y})$$

$$\frac{\partial F}{\partial y_i} \stackrel{?}{=}$$

$$\frac{\partial \vec{y}}{\partial y_i} = \vec{e}_i = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} \leftarrow \text{ith entry.}$$

$$\frac{\partial F}{\partial y_i} = \vec{e}_i^T A^T A\vec{y} + \vec{y} A^T A \vec{e}_i - \vec{b}^T A\vec{e}_i - \vec{e}_i^T A^T \vec{b}$$

$$= 2\vec{e}_i^T \left(A^T A\vec{y} - A^T \vec{b} \right)$$

$$\Longrightarrow \quad \nabla F(\vec{y}) = 2\left(A^T A\vec{y} - A^T \vec{b} \right)$$

The minimum occurs when the gradient is zero:

Solve $\underline{A^T A\vec{y} - A^T \vec{b}}$.

One then needs to show that this critical point is indeed a minimum. ∎

Ex Find the least-squares solution of

$$\begin{pmatrix} 1 & 1 \\ 0 & 1 \\ 1 & 1 \end{pmatrix} \vec{x} = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$$

A $\qquad$ $\vec{b}$

$$A^T A = \begin{pmatrix} 1 & 0 & 1 \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 0 & 1 \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} 2 & 2 \\ 2 & 3 \end{pmatrix}$$

$$A^T \vec{b} = \begin{pmatrix} 1 & 0 & 1 \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} = \begin{matrix} 1 \\ 2 \end{matrix} \qquad \vec{x} = \begin{pmatrix} -\frac{1}{2} \\ 1 \end{pmatrix}$$

Solve $\left(\begin{array}{cc|c} 2 & 2 & 1 \\ 2 & 3 & 2 \end{array}\right) \rightsquigarrow \left(\begin{array}{cc|c} 2 & 2 & 1 \\ 0 & 1 & 1 \end{array}\right)$

Block Matrix Notation

Consider a matrix

$$\left(\begin{array}{ccc|c} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ \hline a_{41} & a_{42} & a_{43} & a_{44} \end{array}\right) \left(\begin{array}{c} x_1 \\ x_2 \\ x_3 \\ \hline x_4 \end{array}\right)$$

$$= \begin{pmatrix} A_{11} & A_{21} \\ A_{12} & A_{22} \end{pmatrix} \begin{pmatrix} \vec{x}_1 \\ \vec{x}_2 \end{pmatrix} = \begin{pmatrix} A_{11}\vec{x}_1 + A_{21}\vec{x}_2 \\ A_{12}\vec{x}_1 + A_{22}\vec{x}_2 \end{pmatrix}$$

$\emptyset$ = block of all zeros.

Orthogonality

- Two vectors $\vec{u}, \vec{v}$ are orthogonal if $\vec{u} \cdot \vec{v} = 0$.

Ex $\vec{u} = \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix}$, $\vec{v} = \begin{pmatrix} 1 \\ 1 \\ 2 \end{pmatrix}$

- A square matrix Q is orthogonal if

$$Q^T Q = I$$

Ex Permutation matrices!

From a computational point of view there is a much better way to solve the normal equations.

Suppose $\underset{m\times n}{A} = \underset{m\times m}{Q} \begin{pmatrix} \hat{R} \\ \emptyset \end{pmatrix}$ $\quad m \geq n$

$\hat{R}$: $n \times n$

$\emptyset$: $(m-n)\times n$ zero matrix

when $Q^T Q = I$ and $\hat{R}_{ii} \neq 0$.

$$A^T A = (R^T \emptyset) Q^T Q \begin{pmatrix} \hat{R} \\ 0 \end{pmatrix}$$

$$= (\hat{R}^T \emptyset) \begin{pmatrix} \hat{R} \\ \emptyset \end{pmatrix}$$

$$= \hat{R}^T \hat{R}.$$

$$A^T \vec{b} = (\hat{R}^T \emptyset) Q^T \vec{b}$$

$$= \hat{R}^T (I \ \emptyset) Q^T \vec{b}$$

$$A^T A \vec{x} = A^T \vec{b}$$

$$\hat{R}^T R x = \hat{R}^T (I \ \emptyset) Q^T \vec{b}$$

$$\boxed{\hat{R} x = (I \ \emptyset) Q^T \vec{b}}$$

Recall: For the LU factorization, we used elementary matrices

$$A = \begin{bmatrix} x & x & x \\ x & x & x \\ x & x & x \end{bmatrix}$$

$$E_1 A = \begin{bmatrix} x & x & x \\ 0 & x & x \\ x & x & x \end{bmatrix}, \quad E_2 E_1 A = \begin{bmatrix} x & x & x \\ 0 & x & x \\ 0 & x & x \end{bmatrix}$$

$$E_3 E_2 E_1 A = \begin{bmatrix} x & x & x \\ 0 & x & x \\ 0 & 0 & x \end{bmatrix}$$

Then it turned out that because each of E_3, E_2, E_1 is special upper triangular,

$$(E_3 E_2 E_1)^{-1} = L$$

is also special upper triangular.

Now for

$$A = \begin{bmatrix} x & x & x \\ x & x & x \\ x & x & x \\ x & x & x \end{bmatrix}$$

we find Q_1, $Q_1 Q_1^T = I$:

$$Q_1 A = \begin{bmatrix} x & x & x \\ 0 & x & x \\ 0 & x & x \\ 0 & x & x \end{bmatrix}$$

$$Q_2 Q_1 A = \begin{bmatrix} x & x & x \\ 0 & x & x \\ 0 & 0 & x \\ 0 & 0 & x \end{bmatrix} \qquad Q_3 Q_2 Q_1 A = \begin{bmatrix} x & x & x \\ 0 & x & x \\ 0 & 0 & x \\ 0 & 0 & 0 \end{bmatrix}$$

$$(Q_3 Q_2 Q_1)^{-1} = (Q_3 Q_2 Q_1)^T$$

The QR factorization

There are many ways to compute the $A = QR$ factorization of a matrix. We will use a method that is closer to row reduction:

Theorem Let $\vec{x} \in \mathbb{R}^n$. Define

$$\vec{w} = \vec{x} + \begin{pmatrix} \text{sign}(x_1)\,\|\vec{x}\|_2 \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

Then $H = I - 2\dfrac{\vec{w}\,\vec{w}^T}{\|w\|_2^2}$ satisfies

- $H^T H = I$
- $H\vec{x} = \begin{pmatrix} -\text{sign}(x_1)\,\|\vec{x}\|_2 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$

$$\text{sign}(x) = \begin{cases} 1 & x \geq 0 \\ -1 & x < 0 \end{cases}$$

This H is called a Householder reflector.

We also use $H(\vec{x})$ to refer to this matrix

Define $H(\alpha) = I \qquad \alpha \in \mathbb{R}$.

Important: Consider a vector $\begin{pmatrix} a \\ x_1 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} a \\ \vec{x} \end{pmatrix}$

$$\begin{pmatrix} 1 & 0 \\ 0 & H(\vec{x}) \end{pmatrix} \begin{pmatrix} a \\ \vec{x} \end{pmatrix} = \begin{pmatrix} a \\ \|\vec{x}\|_2 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} I & 0 \\ 0 & H(\vec{x}) \end{pmatrix} \begin{pmatrix} \vec{a} \\ \vec{x} \end{pmatrix} = \begin{pmatrix} \vec{a} \\ \|\vec{x}\|_2 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

Algorithm (QR factorization)

Input: An $m \times n$ matrix A

Output: An $m \times m$ matrix Q, an $m \times n$ matrix R

Step 1: Initialize $Q = I$, $R = A$

Step 2: For $j = 1, 2, \ldots, n$ do steps 3-5

Step 3:

Set $H_0 = H(R(j{:}end, j))$

Step 4:

Set $R(j{:}end, j{:}end) = H_0 R(j{:}end, j{:}end)$

Step 5:

Set $Q(:, j{:}end) = Q(:, j{:}end) H_0^T$

Output (Q, R).

As we will see in the next coding project, the details of coding this make it look a bit different.

How the algorithm actually proceeds:

$$A = R = \begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \\ x & x & x \end{pmatrix} \to \begin{pmatrix} x & x & x \\ 0 & x & x \\ 0 & x & x \\ 0 & x & x \end{pmatrix} \to \begin{pmatrix} x & x & x \\ 0 & x & x \\ 0 & 0 & x \\ 0 & 0 & x \end{pmatrix}$$

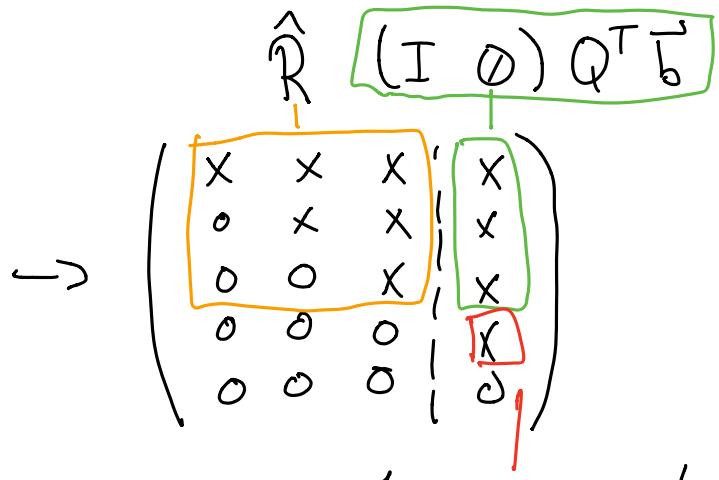
$$\to \begin{pmatrix} x & x & x \\ 0 & x & x \\ 0 & 0 & x \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} \hat{R} \\ 0 \end{pmatrix}$$

How to use the QR algorithm to effectively solve the normal equations

$$\begin{pmatrix} A \end{pmatrix} \vec{x} = \begin{pmatrix} \vec{b} \end{pmatrix}$$

$$\left(\begin{array}{c|c} A & \vec{b} \end{array}\right) = \left(\begin{array}{ccc|c} x & x & x & x \\ x & x & x & x \\ x & x & x & x \\ x & x & x & x \\ x & x & x & x \end{array}\right) \to \left(\begin{array}{ccc|c} x & x & x & x \\ 0 & x & x & x \\ 0 & x & x & x \\ 0 & x & x & x \\ 0 & x & x & x \end{array}\right)$$

$$\to \left(\begin{array}{ccc|c} x & x & x & x \\ 0 & x & x & x \\ 0 & 0 & x & x \\ 0 & 0 & x & x \\ 0 & 0 & x & x \end{array}\right) \to \left(\begin{array}{ccc|c} x & x & x & x \\ 0 & x & x & x \\ 0 & 0 & x & x \\ 0 & 0 & 0 & x \\ 0 & 0 & 0 & x \end{array}\right)$$



The absolute value of this entry gives $\|A\vec{x} - b\|_2$ where $A^TA\vec{x} = A^T\vec{b}$.

To summarize: Suppose A is $m \times n$, $m > n$. Form $(A\,|\,b)$, reduce to upper triangular form using the Householder algorithm.

Take the first n rows and solve using backward substitution.

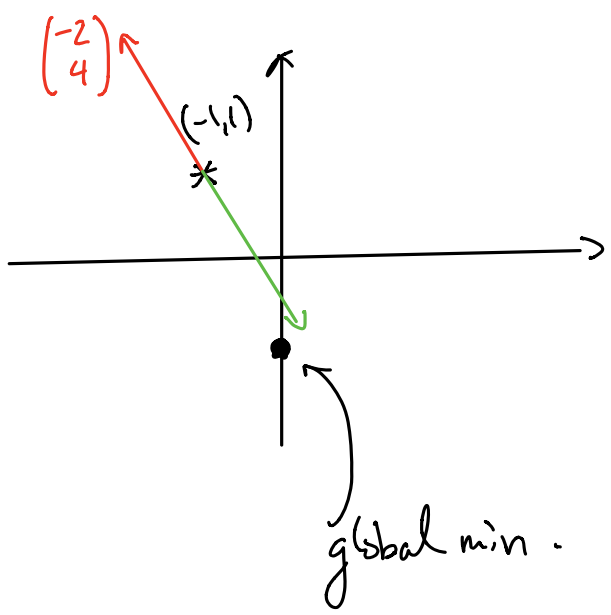
Gradient descent for the normal equations

Consider

$$f : \mathbb{R}^2 \to \mathbb{R}, \text{ say } f(x,y) = x^2 + (y+1)^2.$$

The global minimum for f occurs at $(x,y) = (0,-1)$.

If we are standing at a point $(-1,1)$. How do we figure out what direction to move in?



$$\nabla f(x,y) = \begin{pmatrix} 2x \\ 2(y+1) \end{pmatrix}$$

$$\nabla f(-1,1) = \begin{pmatrix} -2 \\ 4 \end{pmatrix}$$

↑ direction of greatest increase

So, you want to take a step in the direction opposite that of the gradient. But how big of a step? That's the hard part...

Our goal: Minimize $F(\vec{y}) = \| A\vec{y} - \vec{b} \|_2^2$

$$\nabla F(\vec{y}) = 2\left(A^T A\vec{y} - A^T\vec{b}\right)$$

$\vec{y}_0$ initial guess.

$$\vec{y}_{k+1} = \vec{y}_k - h_k\left(A^T A\vec{y}_k - A^T\vec{b}\right)$$

$h_k = ?$

Choose:

$$h_k = \frac{\left(A^T\vec{b} - A^T A\vec{y}_k\right)^T\left(A^T\vec{b} - A^T A\vec{y}_k\right)}{\left(AA^T\vec{b} - AA^T A\vec{y}_k\right)^T\left(AA^T\vec{b} - AA^T A\vec{y}_k\right)}$$

This looks complicated, so break it down:

define $\vec{r}_k = A^T A \vec{y}_k - A^T \vec{b}$

$$h_k = \frac{\vec{r}_k^T \vec{r}_k}{(A\vec{r}_k)^T (A\vec{r}_k)}$$

$$\vec{y}_{k+1} = \vec{y}_k - h_k \vec{r}_k$$

You could choose $h_k = h > 0$ small, but this is, in general, much slower. For problems outside of least-squares such as those from machine learning, an optimal choice of h_k is elusive.

Solving $A\vec{x}=\vec{b}$ when there are infinitely many solutions

Suppose: A is $m \times n$ $\quad m < n$

$\operatorname{im} A = \mathbb{R}^m$

$m<n$ implies $\ker A \neq \{\vec{0}\}$

By assumption, $A\vec{x}=\vec{b}$ has infinitely many solutions.

Pick one solution $\vec{x}_p$. Now let $\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_k$ be a basis for the kernel of A.

$$A(\vec{x}_p + c_1\vec{x}_1 + c_2\vec{x}_2 + \cdots + c_k\vec{x}_k) = \vec{b}$$

for <u>any</u> choice of $c_1, c_2, \ldots, c_k$. For example,

$$\begin{cases} c_1 = 1{,}000{,}000{,}000 \\ c_2 = c_3 = \cdots = c_k. \end{cases}$$ works.

It seems unlikely that this is a relevant solution.

One approach: Among all possible solutions of $A\vec{x} = \vec{b}$ find the one with the smallest 2-norm.

[We won't solve this, but it is not difficult ∎]

Our first solution:

Find the minimum of

$$\|A\vec{y} - \vec{b}\|_2^2 + \|\vec{y}\|_2^2$$

over all choices of $\vec{y} \in \mathbb{R}^n$. This is different than the above question.

I claim that this a problem we already know how to solve:

$$\left\| \begin{pmatrix} I \\ A \end{pmatrix} \vec{y} - \begin{pmatrix} 0 \\ \vec{b} \end{pmatrix} \right\|_2^2 = \|\vec{y}\|_2^2 + \|A\vec{y} - \vec{b}\|_2^2$$

Replace A with $\begin{pmatrix} I \\ A \end{pmatrix}$ and $\vec{b}$ with $\begin{pmatrix} 0 \\ \vec{b} \end{pmatrix}$ and solve the normal equations!

But we need not solve this:

$$\|A\vec{y} - \vec{b}\|_2^2 + \gamma \|\vec{y}\|_2^2 \qquad \gamma \geq 0.$$

Effects of γ:

If we want to prioritize $A\vec{x} \approx \vec{b}$ and we care less about how large $\|\vec{x}\|_2$ is, we choose γ small, say $\gamma \approx 10^{-16}$

If we care less about how close $A\vec{x}$ is to $\vec{b}$ but more about

So, we need to find the minimum of

$$\left\| \begin{bmatrix} \sqrt{\gamma} I \\ A \end{bmatrix} \vec{y} - \begin{bmatrix} \vec{0} \\ \vec{b} \end{bmatrix} \right\|_2 !$$

Application Suppose your rock company produces

20 tons of road base (RB)
10 tons of sand (S)
10 tons of gravel (G)

each day. You have 4 categories of jobs and you are wondering if you can increase production by 50%. But you don't want to restructure the company too much...

Equipment estimate: As a simplification, you

Truck : 1 hour → $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ RB / S / G

Shovel A : 1 hour → $\begin{pmatrix} 0 \\ 2 \\ 1 \end{pmatrix}$

Mixer : 1 hour → $\begin{pmatrix} 1 \\ -1/2 \\ -1/2 \end{pmatrix}$

Shovel B : 1 hour → $\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$

$$A = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 2 & -1/2 & 1 \\ 1 & 1 & -1/2 & 1 \end{pmatrix}$$

Currently, $A\vec{x} = \begin{pmatrix} 20 \\ 10 \\ 10 \end{pmatrix}$

We want $A\vec{x}_{new} = \begin{pmatrix} 30 \\ 15 \\ 15 \end{pmatrix}$

$$A(\vec{x}_{new} - \vec{x}) = \begin{pmatrix} 10 \\ 5 \\ 5 \end{pmatrix} = \vec{b}$$

One approach

$$\text{minimize}\left(\|A\vec{y} - \vec{b}\|_2 + \|\vec{y}\|_2 \right)$$

↑ keeps change small!