Least Squares (high-level)
Norms and inner-products

ROB 501

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- Some matrix facts
- ~~Last time:~~ Least squares (high level)

$$\hat{\alpha} = \underset{\alpha \in \mathbb{R}^2}{\operatorname{argmin}} ||Y - A\alpha||^2 \qquad \hat{\alpha} = (A^T A)^{-1} A^T Y$$

- We will build the proof but we need a few new concepts

Similar matrices

Def: Two square matrices A and B are similar if $\exists$ an invertible matrix P s.t. $B = \underbrace{P A P^{-1}}_{\text{similarity transformation.}}$

Remark: If A and B are similar, then they represent the same linear operator wrt different bases.

Consider A $n \times n$ with complex coefficients, and suppose $\underbrace{\{\lambda_1, \lambda_2, \dots, \lambda_n\}}_{\text{e-values}}$ not necessarily distinct but s.t. $\{v^1, v^2, \dots, v^n\}$ are independent.

$M = [v^1 | v^2 | \dots | v^n]$ $(n \times n)$ what would be $M^{-1}AM$?

Define $\Lambda = \begin{bmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{bmatrix}$

$$AM = [Av^1 | Av^2 | \dots | Av^n]$$
$$= [\lambda_1 v^1 | \lambda_2 v^2 | \dots | \lambda_n v^n]$$
$$= [v^1 | v^2 | \dots | v^n] \begin{bmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{bmatrix} = M\Lambda$$

$\Rightarrow AM = M\Lambda \Rightarrow M^{-1}AM = \Lambda$

Exercise:

1) If A and B are similar, what is the relation of their eigenvalues?

2) Prove $\{v^1, \dots, v^n\}$ linearly indep. $\Longrightarrow M$ is invertible.

3) Find a matrix representation B of the linear operator $L : \mathbb{C}^n \to \mathbb{C}^n$, $L(x) = Ax$ when you use the basis of e-vectors both for the domain and co-domain.

Useful matrix facts

Let $A \in \mathbb{F}^{n \times m}$

Def: $\text{rank}(A) = \#$ of linearly independent columns

Note: # of lin. indep col. = # of lin. indep rows.

$\text{rank}(A) \leq \min(n, m)$

Fact: $\forall A_1, A_2$ w/ app. dimension $(A_1 A_2)^T = A_2^T A_1^T$

Theorem: Let $A \in \mathbb{R}^{n \times m}$. Then,

$$rank(A) = rank(A^T) = rank(A^T A) = rank(AA^T).$$

Also, a matrix M is symmetric, if $M = M^T$ (and $A^T A$ and AA^T are symmetric)

Linear Regression or Least Squares Fit of Functions to Data

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We discuss the process of fitting functions to data, which is usually called *regression*. A typical problem goes as follows. We are data as shown in Table I, which is also plotted in Figure 1. It is clear that the data do NOT lie exactly on a straight line. How can we **approximately** fit a straight line to the data? In particular, how can we do the fit in such a way as to **minimize the error**, in a given sense?

TABLE I
DATA FOR OUR FIRST LINEAR REGRESSION.

i	x_i	y_i
1	1	4
2	2	8
3	4	10
4	5	12
5	7	18

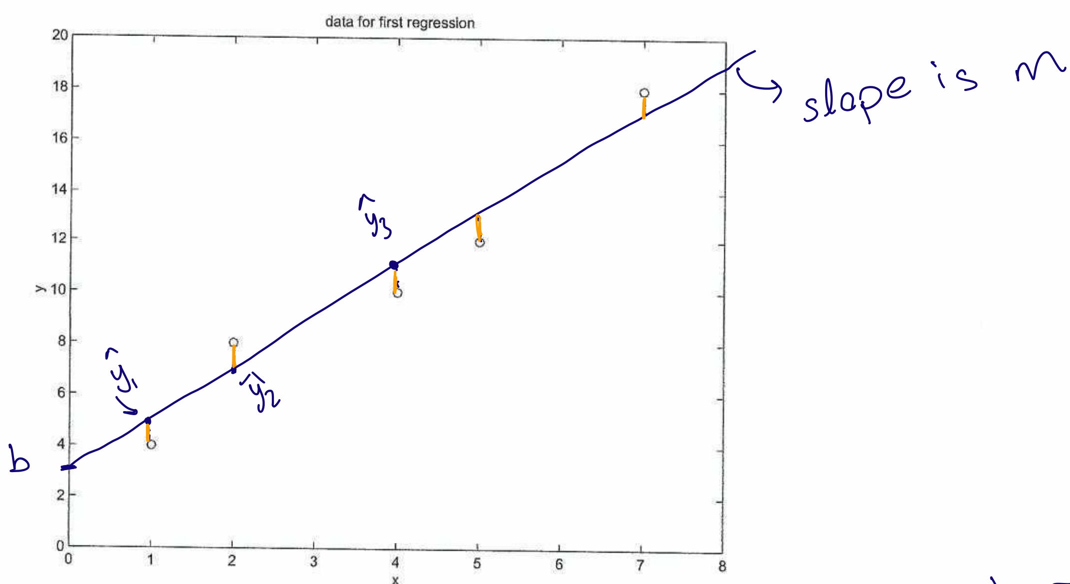


Fig. 1. Plot of data in Table 1.

Let's suppose that we want to fit a linear model

$$y = mx + b.$$

slope and intercept model

For $1 \leq i \leq N$, define

$$\hat{y}_i = mx_i + b,$$

$\hat{y}_i$

where N is the number of data points (five in the case of Table I). Define the i-th error term to be

$$\boxed{\boxed{e_i} = y_i - \hat{y}_i}$$

and the total squared error to be

$$E_{tot} = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2.$$

Note that since $\hat{y}_i$ depends on m and b, so does E_{tot}.

We select the coefficients m and b in the model so as to minimize E_{tot} as a function of m and b. This is called a **Least Squared Error** fit, or a **Least Squares** fit.

Using basic calculus, we choose m and b so that

$$\frac{\partial E_{tot}}{\partial m} = 0$$
$$\frac{\partial E_{tot}}{\partial b} = 0$$

This yields two equations in the two unknowns. Depending on the particular problem , deriving these equations is more or less tedious. One way to do this is to grind out the partial derivatives, and produce the equations for m and b. We will use a more sophisticated but EQUIVALENT method that is MUCH EASIER to use in practice.

Write out the equations $y_i = mx_i + b$, $i = 1, \cdots, N$ in matrix form. That is, note that

$$\underline{y_i = mx_i + b} = \begin{bmatrix} x_i & 1 \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix}$$

Now, do this for $i = 1, \cdots, N$

$$\underbrace{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}}_{Y} = \underbrace{\begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_N & 1 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} m \\ b \end{bmatrix}}_{\alpha}$$

$Y = A\alpha$

$$E = Y - A\alpha = \begin{bmatrix} e_1 \\ \vdots \\ e_N \end{bmatrix}$$

in order to arrive at the **(over determined)** equation $Y = A\alpha$. For our example, the various quantities are

$$Y = \begin{bmatrix} 4 \\ 8 \\ 10 \\ 12 \\ 18 \end{bmatrix} \qquad A = \begin{bmatrix} 1 & 1 \\ 2 & 1 \\ 4 & 1 \\ 5 & 1 \\ 7 & 1 \end{bmatrix} \qquad \alpha = \begin{bmatrix} m \\ b \end{bmatrix}$$

Theorem (to be proven in lecture): If $\det(A^T A) \neq 0$, then the least squares solution to $Y = A\alpha$ is given by

$$\hat{\alpha} = (A^T A)^{-1} A^T Y \rightarrow \text{normal equations}$$

$$\|E\|^2 = E^T E = E_{tot}$$

That is

$$\hat{\alpha} = \underset{\alpha \in \mathbb{R}^2}{\operatorname{argmin}} \; ||\overbrace{Y - A\alpha}^{E}||^2$$

where $|| \cdot ||^2$ is the sum of the squares of the elements of the vector.

Remark: This will be a special case of the *Normal Equations*!

Computations in Matlab

```
x=[1     2     4     5     7]'

x =

     1
     2
     4
     5
     7

 Y=[ 4     8     10     12     18]'

Y =

     4
     8
    10
    12
```

```
   18

 A=[x,ones(5,1)]

A =

     1     1
     2     1
     4     1
     5     1
     7     1

 det(A'*A)

ans =

   114

 theta_hat=inv(A'*A)*A'*Y

theta_hat =

    2.1228
    2.3333

 m=theta_hat(1)

m =

    2.1228

 b=theta_hat(2)

b =

    2.3333

 plot(x,Y,'o',x,m*x+b)
 axis([0 8 0 20])
 gtext('y = mx + b')
 xlabel('x')
 ylabel('y')
```

α

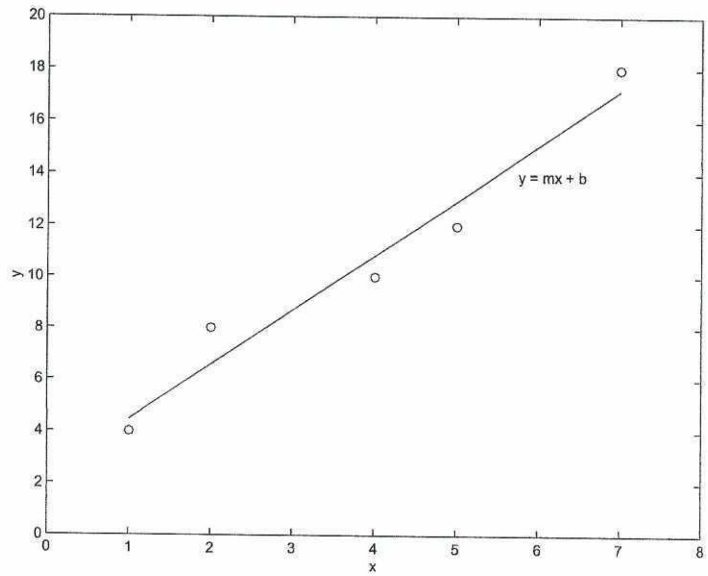


Fig. 2. Plot of data from Table 1 along with the least squares fit.

Now, all of this can be applied for any **model** that depends linearly on its unknown coefficients. For example, consider the data of Table II, which is plotted in Figure 3.

TABLE II

DATA FOR OUR SECOND LINEAR REGRESSION.

i	x_i	y_i
1	0	1.0
2	0.25	1.0
3	0.5	1.5
4	0.75	2.0
5	1.0	3.0
6	1.25	4.25
7	1.5	5.5
8	1.75	7.0
9	2.0	10.0

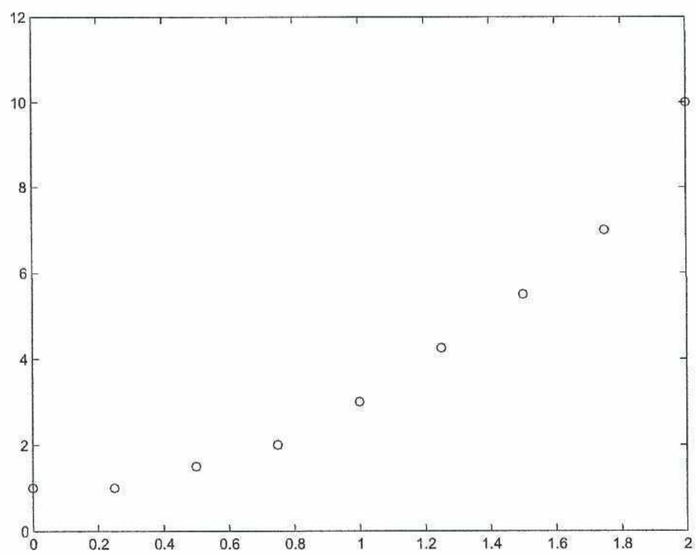


Fig. 3. Plot of data in Table 2.

Let's choose a model of the form

$$\boxed{y = c_0 + c_1 x + c_2 x^2,}$$

where here x^2 does mean x to power 2 (squared). Note that even though the model is nonlinear in x, it is linear in the unknown coefficients c_0, c_1, c_2. This is what is important!!! Just as before, define $\hat{y}_i = c_0 + c_1 x_i + c_2 x_i^2$, the i-th error term to be

$$e_i = y_i - \hat{y}_i$$

and the total squared error to be

$$E_{tot} = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2.$$

To find the coefficients c_0, c_1, c_2 that minimize E_{tot}, we write out the model in matrix form:

$$y_i = c_0 + c_1 x_i + c_2 (x_i)^2 = \begin{bmatrix} 1 & x_i & (x_i)^2 \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \end{bmatrix}.$$

$y = c_0 \sin x + c_1 e^x + c_2 x + c_3$

$y_i = \begin{bmatrix} \sin(x_i) & e^{x_i} & x_i & 1 \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \end{bmatrix}$

Doing this for $i = 1, \cdots, N$ yields

$$\underbrace{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}}_{Y} = \underbrace{\begin{bmatrix} 1 & x_1 & (x_1)^2 \\ 1 & x_2 & (x_2)^2 \\ \vdots & \vdots & \\ 1 & x_N & (x_N)^2 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} c_0 \\ c_1 \\ c_2 \end{bmatrix}}_{\alpha}$$

which gives us the equation $Y = A\alpha$. For our second example, the various quantities are

$$Y = \begin{bmatrix} 1.0 \\ 1.0 \\ 1.5 \\ 2.0 \\ 3.0 \\ 4.25 \\ 5.5 \\ 7.0 \\ 10.0 \end{bmatrix} \qquad A = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0.25 & 0.0625 \\ 1 & 0.5 & 0.25 \\ 1 & 0.75 & 0.5625 \\ 1 & 1.0 & 1.0 \\ 1 & 1.25 & 1.5625 \\ 1 & 1.5 & 2.25 \\ 1 & 1.75 & 3.0625 \\ 1 & 2.0 & 4.0 \end{bmatrix} \qquad \alpha = \begin{bmatrix} c_0 \\ c_1 \\ c_2 \end{bmatrix}$$

Computations in Matlab

```
x=[0:.25:2]';
Y=[ 1 1 1.5 2 3 4.25 5.5 7 10]';
A=[ones(9,1),x,x.^2]

A =

    1.0000         0         0
    1.0000    0.2500    0.0625
    1.0000    0.5000    0.2500
    1.0000    0.7500    0.5625
    1.0000    1.0000    1.0000
    1.0000    1.2500    1.5625
    1.0000    1.5000    2.2500
    1.0000    1.7500    3.0625
    1.0000    2.0000    4.0000

det(A'*A)

ans =

   40.6055

alpha_hat=inv(A'*A)*A'*Y

alpha_hat =

    1.0652
   -0.6258
    2.4545

c0=alpha_hat(1)

c0 =

    1.0652

c1=alpha_hat(2)

c1 =

   -0.6258

c2=alpha_hat(3)
```

```
c2 =

    2.4545

 plot(x,y,'o',x,c0+c1*x+c2*x.^2)
 axis([0 2 0 12])
 gtext('y = c_0+c_1x + c_2 x^2')
 xlabel('x')
 ylabel('y')
 title('Least square fit of a quadratic to data')
```

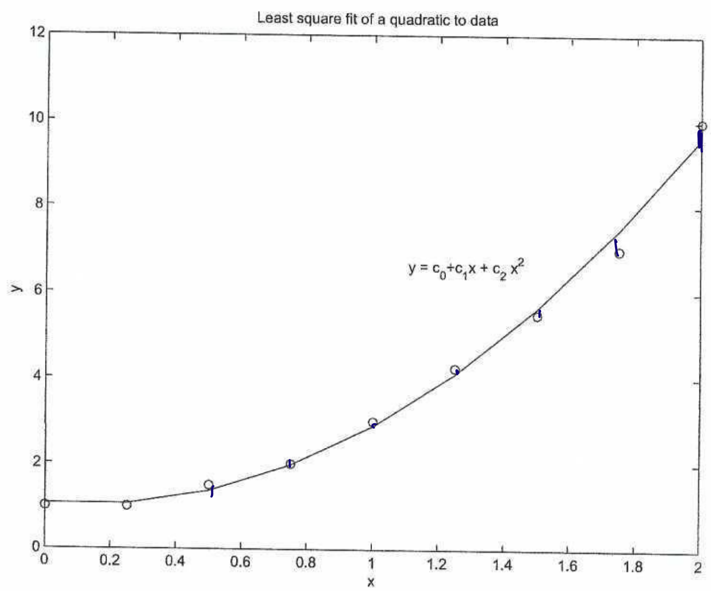


Fig. 4. Plot of data from Table 2 along with the least squares fit of a quadratic function to the data.

Norms

$\mathbb{F} = \mathbb{R}$ or $\mathbb{C}$, $(\mathcal{X}, \mathbb{F})$ is a vector space.

<u>Def:</u> $\|\cdot\| : \mathcal{X} \longrightarrow \mathbb{R}$ is <u>a norm</u> if

a) $\forall x \in \mathcal{X}$, $\|x\| \geq 0$ and $\|x\| = 0 \iff x = 0$

(positive definiteness)

b) [Triangular inequality] $\forall x, y \in \mathcal{X}$

$\|x+y\| \leq \|x\| + \|y\|$

c) [Positive homogeneity] $\forall \alpha \in \mathbb{F}$, $\forall x \in \mathcal{X}$

$\|\alpha \cdot x\| = |\alpha| \cdot \|x\|$

where $|\alpha| = \begin{cases} \text{absolute value if } \alpha \in \mathbb{R} \\ \text{magnitude if } \alpha \in \mathbb{C} \end{cases}$

<u>Examples</u>:

$$x = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$$

1) $\mathcal{F} = \mathbb{R}$ or $\mathbb{C}$, $X = \mathcal{F}^n$

i) $\|x\|_2 := \sqrt{\sum_{i=1}^{n} |x_i|^2}$ (for $\mathcal{F} = \mathbb{R}$, this is known as the Euclidean norm)

ii) $\|x\|_p := \sqrt[p]{\sum_{i=1}^{n} |x_i|^p} = \left(\sum_{i=1}^{n} |x_i|^p\right)^{1/p}$

where $1 \leq p < \infty$ (known as p-norms)

iii) $\|x\|_\infty := \max\limits_{0 \leq i \leq n} |x_i|$ (known as max-norm, sup-norm, or infinity norm)

<u>Def</u>: $(X, \mathcal{F}, \|\cdot\|)$ called normed space if $(X, \mathcal{F})$ is a vector space and $\|\cdot\|$ is a norm.

Def: For $x, y \in \mathcal{X}$, the *distance* from x to y is $d(x,y) := \|x-y\|$

$d: \mathcal{X} \times \mathcal{X} \to \mathbb{R}$

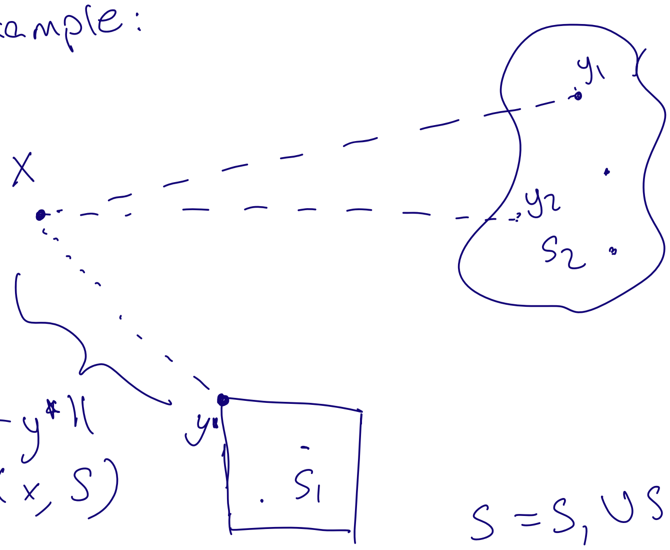
$$= \|y-x\| = d(y,x)$$

$\downarrow$ pos. homogeneity

Def: *Distance to a set*: Let $S \subset \mathcal{X}$, $x \in \mathcal{X}$

$$d(x, S) := \inf_{y \in S} d(x,y) = \inf_{y \in S} \|x-y\|$$

Pictorial example:



$\|x-y^*\| = d(x, S)$

$S = S_1 \cup S_2$

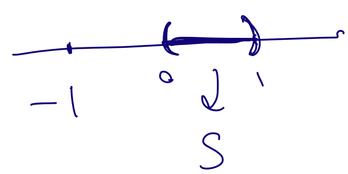
EX:

$\mathcal{X} = \mathbb{R}$

$S = (0, 1)$

$x_1 = -1$

$d(x_1, S) = d(-1, S) = 1$



$x_2 = 0.5$

$d(x_2, S) = d(0.5, S) = 0$

$d(x, S)$ is easy to compute when S is subspace.

<u>Notation</u>: $y^* = \underbrace{\operatorname{argmin}}_{y^* \in S}_{y \in S} \|x-y\|$ means minimum distance exists and attained by the point $y^* \in S$ and y^* is unique.

Uniqueness

$\Rightarrow \|x - y^*\| = \inf_{y \in S} \|x-y\|$

Ex: $S = [0,1]$, $x = -1$ $\Bigg\}$ $y^* = 0 \in S$ and unique

$0 = \operatorname{argmin}_{\underline{y \in S}} \|x-y\|$

Ex: $S = [0,1] \cup [-3,-2]$, $x = -1$ $\Bigg\}$ $\{-2, 0\} \in \operatorname{argmin}_{y \in S} \|x-y\|$

y^* is not unique

Ex: If S is a subspace, $y^* \in S$ always exists and is unique! (will come back to this)

OFFICE HOURS

$S \longrightarrow Q$

$\{s^1, \ldots, s^n\} \quad \{q^1, \ldots, q^n\}$

$P_{S \to Q}$

$$[x]_Q = P_{S \to Q} [x]_S$$

$$\left[[x_1]_Q \,\middle|\, [x_2]_Q \right] = P_{S \to Q} \left[[x_1]_S \,\middle|\, [x_2]_S \right]$$

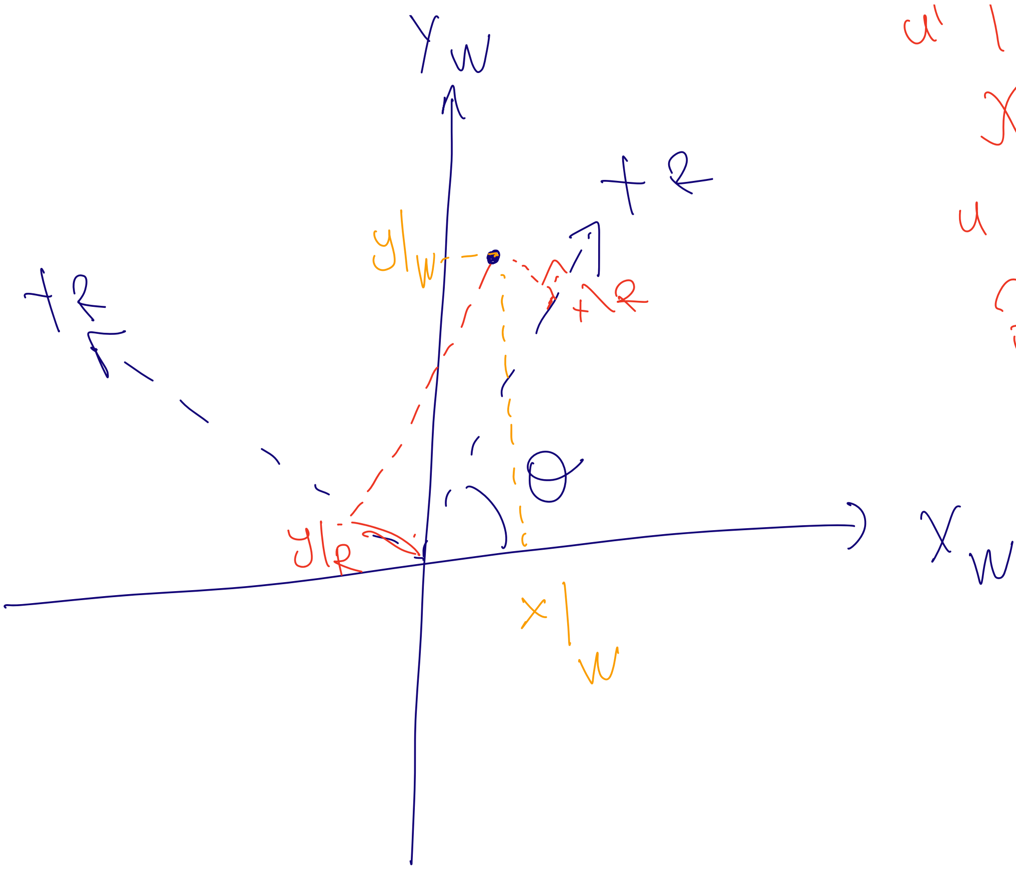
$$P_{i(S \to Q)} = [s^i]_Q$$

$$[s^i]_S = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \rightarrow i\text{th location}$$

$$P_{S \to Q} [s^i]_S = P_i = [s^i]_Q$$

$$\mathbb{F}^n \xrightarrow{\tilde{A}} \mathbb{F}^m$$

$A \qquad\qquad \uparrow \; v'$



$$\begin{tikzcd} X \arrow[r, "L"] \arrow[d, "u"] & Y \arrow[d, "v"] \\ F^n \arrow[r, "A"] \arrow[u, bend left, "u^{-1}"] & F^m \end{tikzcd}$$

$$\lambda_1 v^1 = \underbrace{\alpha_1}_{= \lambda_1} v^1 + \underbrace{\alpha_2}_{= 0} v^2 + \cdots \underbrace{\alpha_n}_{= 0} v^n$$

$$[\lambda_1 v^1]_V =$$

$L : X \to Y$ where $\dim(X) = n$ and $\dim(Y) = m$ then mat. rep. of L is $A \in F^{m \times n}$

$x_1 = 0, 0, 0, 0, 0 \ldots$ —

$x_2 = 1, 1, 1 \ldots$ — — —

$d(x_1, x_2) = \|x_1 - x_2\|_{\ell_1} = \infty$

$\|x\|_{\ell_1} = \sum_{i=1}^{\infty} |x_i|$

$\|x\|_{\ell_\infty} = \sup_i |x_i|$

$d(x_1, x_2) = \|x_1 - x_2\|_{\ell_\infty}$

$= 1$