Northeastern University, Department of Mathematics

MATH 5110: Applied Linear Algebra and Matrix Analysis. (Fall 2021)

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§11 Least Squares and Data Fitting

Contents

Least Squares Problem
 Approximate Solutions to Inconsistent Systems
 Data Fitting
 Best Approximation for Functions

Review:

1. Inner Product Space (vector space with an inner product)

Example: 1. R (weighteel) dut product

2. C[a,b] . <f, 9>= 5 fwgw dx

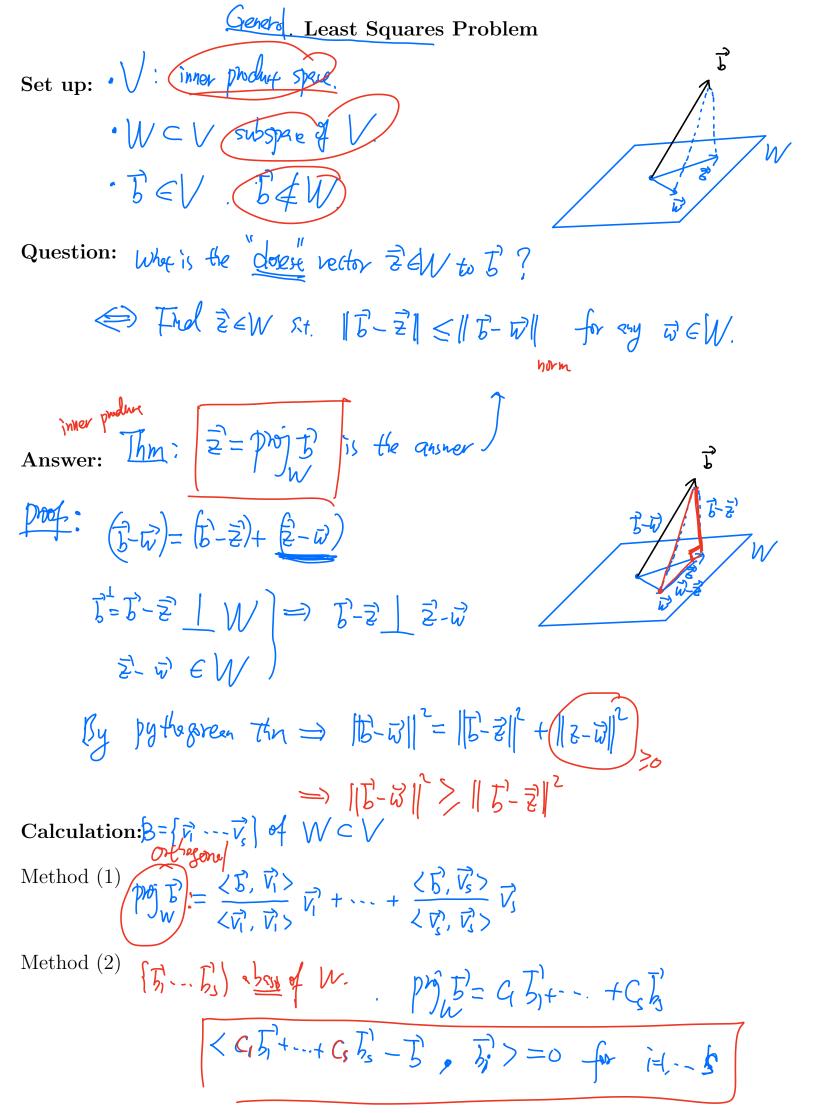
Geometry -> norm
>> angle

 $\begin{array}{c}
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\left(\begin{array}{c}
\overline{V}, \overline{$

3. Find orthogonal basis (Gram-Schmidt process)

A basis (b) --- b) of W --- orthogonal basis vi --- vs) of W.

1. Othern (6-P35) [W projection phys & W



Set up:

Let A be an $n \times m$ matrix.

Let $\vec{b} \in \mathbb{R}^n$.

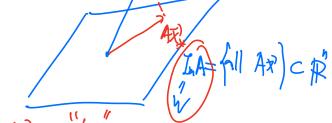
54 im/

Suppose $A\vec{x} = \vec{b}$ has no solution.

Q: Ird xx st. Ax is dnest to t

2. Approximate Solutions to Inconsistent Systems

Consider \mathbb{R}^n with any inner product.



[Least-Squares Problem/Solution for $A\vec{x} = \vec{b}$]

Problem: Find the vector(s) $\vec{x}_* \in \mathbb{R}^m$ such that for all $x \in \mathbb{R}^m$,

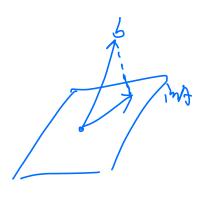
$$||\overrightarrow{A}\overrightarrow{x}_* - \overrightarrow{b}|| \le ||\overrightarrow{A}\overrightarrow{x} - \overrightarrow{b}||$$

Solutions:

Example 1. Find the least-squares solutions for $A\vec{x} = \vec{b}$, where $A = \begin{bmatrix} -1 & 4 \\ -1 & 8 \end{bmatrix}$ and $\begin{bmatrix} 14 \\ -4 \\ 0 \end{bmatrix}$

Step 1:
$$\vec{z} = \vec{D} \cdot \vec{a_1} = \frac{\vec{b} \cdot \vec{a_1}}{\vec{a_1} \cdot \vec{a_1}} \vec{a_1} + \frac{\vec{b} \cdot \vec{a_1}}{\vec{a_1} \cdot \vec{a_1}} \vec{a_2}$$

$$=-6\bar{a}_{1}+\frac{1}{4}\bar{a}_{2}$$



Step2: Solve AX===

$$\begin{bmatrix} -1 & 4 & | & 7 \\ 1 & 8 & | & -4 \\ -1 & 4 & | & 7 \end{bmatrix} \longrightarrow \cdots \longrightarrow rref = \begin{bmatrix} 1 & 0 & | & -6 \\ 0 & 1 & | & 4 \\ 0 & 0 & | & 0 \end{bmatrix}$$

So
$$\vec{x}_* = \begin{bmatrix} -6 \\ /4 \end{bmatrix}$$
 is the least squares solution of $A\vec{x} = \vec{b}$.

In particular, if we consider **dot product** on \mathbb{R}^n , we have the following formula.

Theorem 2. (Normal Equation) The Least-Square solutions of $A\vec{x} = \vec{b}$ coincide with the solutions of of **normal equations**

$$(A^T A)\vec{x} = A^T \vec{b}.$$

· $\overline{\chi}_{\star}$ is a least-spine sol. of $A\overline{\chi}=\overline{b}$



$$\overrightarrow{b} - \overrightarrow{A} \overrightarrow{x}_{*} = \overrightarrow{b}^{\perp} \leftarrow (mA)^{\perp} = (ker(A^{\top}))$$

$$A^{T}(\overline{b}-A\overline{x}_{*})=\overline{o}$$

$$A^TAX_*=A^TJ^T$$

2

More generally, we can also consider weighted dot product on \mathbb{R}^n ,

where W is a positive-definite symmetric matrix.

Example 3. Find the least-squares solutions for $A\vec{x} = \vec{b}$, where $A = \begin{bmatrix} -1 & 4 \\ 1 & 8 \\ -1 & 4 \end{bmatrix}$

$$\vec{b} = \begin{bmatrix} 14 \\ -4 \\ 0 \end{bmatrix}$$

$$A^{T}A = \begin{bmatrix} -1 & 1 & -1 \\ 4 & 8 & 4 \end{bmatrix} \begin{bmatrix} -1 & 4 \\ 1 & 1 \\ -1 & 4 \end{bmatrix} = \begin{bmatrix} 3 & 0 \\ 0 & 96 \end{bmatrix}$$

$$A^{T}B^{T} = \begin{bmatrix} -1 & 1 & -1 \\ 4 & 8 & 4 \end{bmatrix} \begin{bmatrix} 14 \\ -4 \\ 0 \end{bmatrix} = \begin{bmatrix} -18 \\ 24 \end{bmatrix}$$
Solve the normal equation $A^{T}A \overrightarrow{X} = A^{T}B^{T}$

$$\begin{bmatrix} 3 & 0 & | -18 \\ 0 & 16 & | 24 \end{bmatrix} \longrightarrow \begin{bmatrix} 1 & 0 & | -6 \\ 0 & 1 & | 4 \end{bmatrix}$$

$$\begin{bmatrix} -18 \\ 0 & 16 & | 24 \end{bmatrix} \longrightarrow \begin{bmatrix} 0 & | -6 \\ 0 & 1 & | 4 \end{bmatrix}$$

$$\begin{cases} -18 \\ 0 & 16 & | 24 \end{bmatrix} \xrightarrow{R} \text{ the least-squares solution}$$

(2) The image im(A) is a plane in \mathbb{R}^3 passing the origin. Find the distance from the vector \vec{b} (or the point (14, -4, 0)) to the plane im(A).

The distance is given be the norm of
$$\vec{b}^{\perp} = \vec{b} - \operatorname{proj}_{\operatorname{im}(A)} \vec{b}$$
.

We know that $\operatorname{proj}_{\operatorname{im}(A)} \vec{b} = Ax_* = \begin{bmatrix} -1 & 4 \\ 1 & 8 \\ -1 & 4 \end{bmatrix} \begin{bmatrix} -6 \\ 1/4 \end{bmatrix} = \begin{bmatrix} 7 \\ -4 \\ 7 \end{bmatrix}$.

So,
$$\vec{b}^{\perp} = \begin{bmatrix} 14 \\ -4 \\ 0 \end{bmatrix} - \begin{bmatrix} 7 \\ -4 \\ 7 \end{bmatrix} = \begin{bmatrix} 7 \\ 0 \\ -7 \end{bmatrix}$$
. So the distance is $||\vec{b}^{\perp}|| = 7\sqrt{2}$.

Example 4. Find the least-squares solutions for the system $A\vec{x} = \vec{b}$, where $A = \vec{b}$

$$\begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix} \text{ and } \vec{b} = \begin{bmatrix} 1 \\ 3 \\ 2 \\ 4 \end{bmatrix}$$

Sep. Construct the normal equation
$$A^TA\vec{x}=A^T\vec{b}$$

$$A^{T}A = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 4 & 2 & 2 \\ 2 & 2 & 0 \\ 2 & 0 & 2 \end{bmatrix}$$

$$A^{\mathsf{T}} \mathcal{B} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 3 \\ 1 \\ 4 \end{bmatrix} = \begin{bmatrix} 10 \\ 4 \\ 6 \end{bmatrix}$$

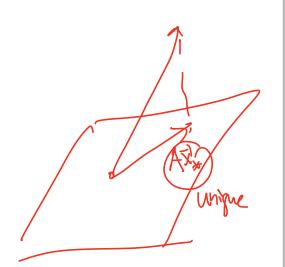
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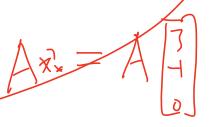
$$\begin{bmatrix} 4 & 2 & 2 & 10 \\ 2 & 2 & 0 & 4 \\ 2 & 0 & 2 & 6 \end{bmatrix} \rightarrow \cdots \rightarrow rref = \begin{bmatrix} 1 & 0 & 1 & 3 \\ 0 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 - x_3 \\ -1 + x_3 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 \\ -1 \\ 0 \end{bmatrix} + \begin{bmatrix} x_1 \\ 1 \\ 1 \end{bmatrix}$$

$$X_1 = 3 - X_3$$

 $X_2 = 1 + X_3$
 X_3 free





Proposition 5. Let A be an $n \times m$ matrix $\ker(A^T A)$ $\ker(A)$ rank A = rank (mxm man nam ATA is invoked & Konk ATA=m Corollary 6. If rank A = h, the normal equation $(A^T A)\vec{x} = A^T \vec{b}$ has a unique solution: $\vec{x} = (A^T A)^{-1} A^T \vec{b}$ QR factorization method Suppose A is $n \times m$ matrix with full column rank. Solve the least squares solution using QR factorization A = QR where Q is an orthogonal matrix $n \times m$ and R is an $m \times m$ upper triangular matrix with rank m. $Q^TQ=I$ 7 = RTQTI AX = QQT

3. Data Fitting

Problem: Fitting a function of a certain type of data. We use the following three example to illustrate this application.

Example 7. Find a cubic polynomial $f(t) = c_0 + c_1t + c_2t^2 + c_3t^3$ whose graph passes through the points (0,5), (1,3), (-1,13), (2,1)

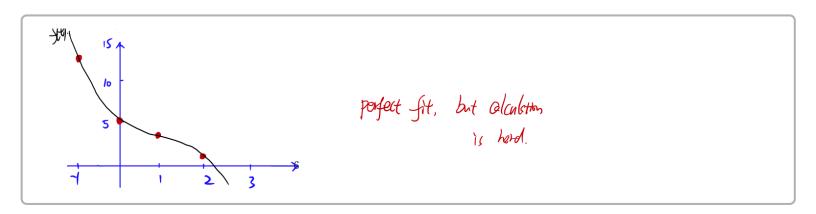
Solution:

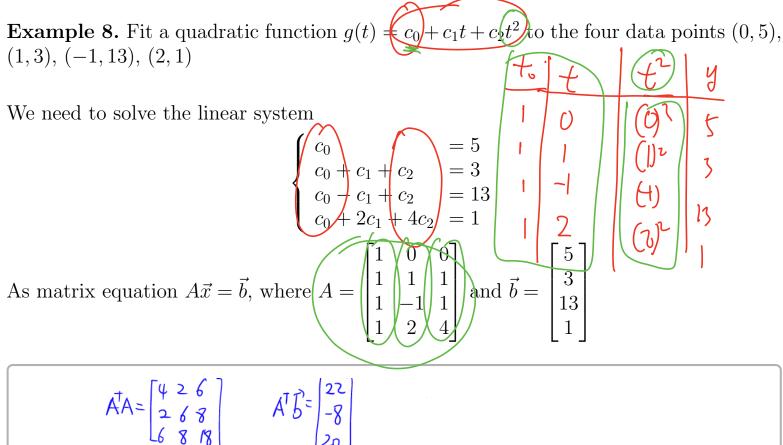
We need to solve the linear system $\begin{cases} c_0 = 5 \\ c_0 + c_1 + c_2 + c_3 = 3 \\ c_0 - c_1 + c_2 - c_3 = 13 \\ c_0 + 2c_1 + 4c_2 + 8c_3 = 1 \end{cases}$

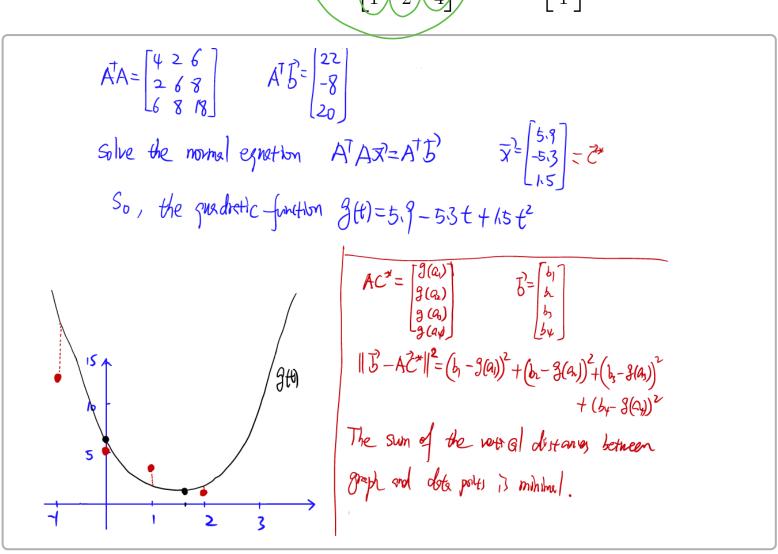
$$[A|\vec{b}] = \begin{bmatrix} 1 & 0 & 0 & 0 & 5 \\ 1 & 1 & 1 & 1 & 3 \\ 1 & -1 & 1 & -1 & 13 \\ 1 & 2 & 4 & 8 & 1 \end{bmatrix} \to \cdots \to \mathbf{rref}[A|\vec{b}] = \begin{bmatrix} 1 & 0 & 0 & 0 & 5 \\ 0 & 1 & 0 & 0 & -4 \\ 0 & 0 & 1 & 0 & 3 \\ 0 & 0 & 0 & 1 & -1 \end{bmatrix}$$

So, the linear system has the unique solution $\begin{vmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \end{vmatrix} = \begin{vmatrix} 5 \\ -4 \\ 3 \\ -1 \end{vmatrix}$ So, the cubic polynomial is

 $f(t) = 5 - 4t + 3t^2 - t^3.$







Example 9. Fit a linear function $h(t) = c_0 + c_1 t$ to the four data points (0,5), (1,3), (-1,13), (2,1)

We need to solve the linear system

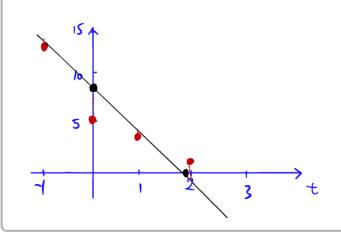
$$\begin{cases}
c_0 &= 5 \\
c_0 + c_1 &= 3 \\
c_0 - c_1 &= 13 \\
c_0 + 2c_1 &= 1
\end{cases}$$

As matrix equation $A\vec{x} = \vec{b}$, where $A = \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & -1 \\ 1 & 2 \end{bmatrix}$ and $\vec{b} = \begin{bmatrix} 5 \\ 3 \\ 13 \\ 1 \end{bmatrix}$

$$AA = \begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & -1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 1 & -1 \\ 2 & 1 & -1 & 2 \end{bmatrix} = \begin{bmatrix} 4 & 2 \\ 2 & 6 \end{bmatrix}$$

$$AB = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & -1 & 2 \end{bmatrix} \begin{bmatrix} 5 \\ 7 \\ 7 \end{bmatrix} = \begin{bmatrix} 22 \\ -8 \end{bmatrix}$$

So the linear function is h(t)=7.4 -3.8t

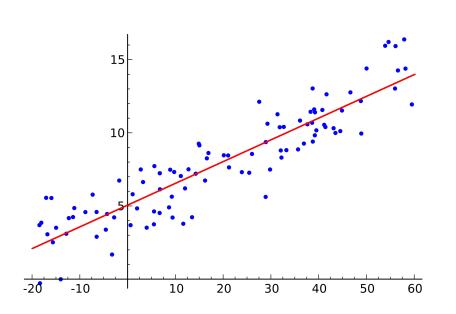


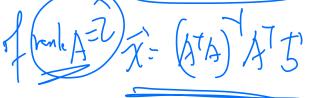
Remark: More generally, we can consider N-points (a_1,b_1) , (a_2,b_1) ; ..., (a_n,b_n) .

• Find a linear function $h(t) = G_0 + G_1 + G_2$ Sits the data by the least synames.

More generally, the following question is very standard in statistics.

Example 10. Consider the data with n points $(a_1, b_1), (a_2, b_2), \ldots, (a_n, b_n)$. Find a linear function $h(t) = c_0 + c_1 t$ fits the data by the least squares. (Suppose $a_1 \neq a_2$)







We need to solve the least-squares problem for
$$A\vec{x} = \vec{b}$$
, for $A = \begin{bmatrix} 1 & a_1 \\ 1 & a_2 \\ \vdots \\ 1 & a_n \end{bmatrix}$ and $\vec{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$

$$A^{T}A = \begin{bmatrix} 1 & a_{1} \\ 1 & a_{2} \\ \vdots \\ 1 & a_{n} \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & 1 \\ a_{1} & a_{2} & \cdots & a_{n} \end{bmatrix} = \begin{bmatrix} n & \sum_{i=1}^{n} a_{i} \\ \sum_{i=1}^{n} a_{i} & \sum_{i=1}^{n} a_{i}^{2} \end{bmatrix}$$

$$A^{T}b = \begin{bmatrix} 1 & a_1 \\ 1 & a_2 \\ \vdots \\ 1 & a_n \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} b_i \\ \sum_{i=1}^{n} a_i a_i \end{bmatrix}$$

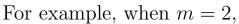
Since $a_1 \neq a_2$, we know that rank A = 2.

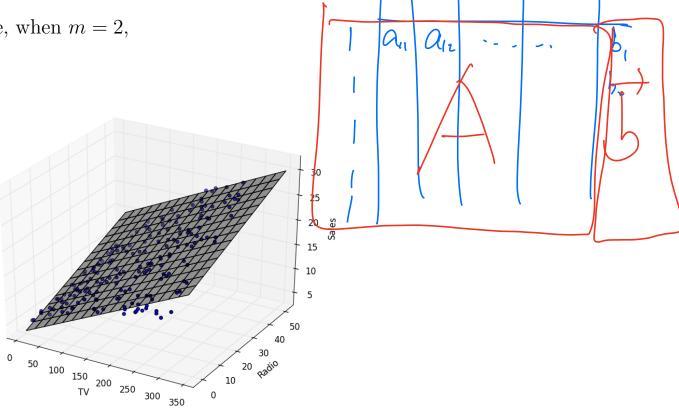
The normal equation $A^T A \vec{x} \neq A^T \vec{b}$ has a unique solution

$$\vec{x}_* = (A^T A)^{-1} A^T \vec{b} = \underbrace{\frac{1}{n \sum_{i=1}^n a_i^2 - (\sum_{i=1}^n a_i)^2} \begin{bmatrix} \sum_{i=1}^n a_i^2 - \sum_{i=1}^n a_i \\ -\sum_{i=1}^n a_i \end{bmatrix} \begin{bmatrix} \sum_{i=1}^n b_i \\ \sum_{i=1}^n a_i a_i \end{bmatrix}}_{n \sum_{i=1}^n a_i^2 - (\sum_{i=1}^n a_i)^2} \begin{bmatrix} (\sum_{i=1}^n a_i^2)(\sum_{i=1}^n b_i) - (\sum_{i=1}^n a_i)(\sum_{i=1}^n a_i a_i) \\ -(\sum_{i=1}^n a_i)(\sum_{i=1}^n b_i) + n \sum_{i=1}^n a_i a_i \end{bmatrix}}$$

Example 11. Consider the data with m inputs and 1 output:

 $(a_{11}, a_{12}, ..., a_{1m}) b_1$, $(a_{21}, a_{22}, ..., a_{2m}, b_2), ..., (a_{n1}, a_{n2}, ..., a_{nm}) b_n$. Find a linear function $h(t_1, t_2, ..., t_n) = c_0 + c_1 t_1 + c_2 t_2 + \cdots + c_n t_n$ fits the data by the least squares.





We need to solve the least-squares problem for
$$A\vec{x} = \vec{b}$$
, for $A = \begin{bmatrix} 1 & a_{11} & a_{12} & \dots & a_{1m} \\ 1 & a_{21} & a_{22} & \dots & a_{2m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & a_{n1} & a_{n2} & \dots & a_{nm} \end{bmatrix}$

and
$$\vec{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

Example 12. Consider the data with m inputs and s outputs:

$$(a_{11}, a_{12}, ..., a_{1m}, b_{11}, ..., b_{1s}), (a_{21}, a_{22}, ..., a_{2m}, b_{21}, ..., b_{2s}), ..., (a_{n1}, a_{n2}, ..., a_{nm}, b_{n1}, ..., b_{ns}).$$

Find a linear function $H(\vec{t}) = \vec{c}_0 + C\vec{t}$ fits the data by the least squares.

4. Best Approximation for Functions

Set up:

Let V be the vector space of continuous functions. e.g. $f(x) = e^x \in V$ Consider the inner product on V: $f(x) = e^x \in V$ $f(x) = e^x \in V$

Let W be the subspace of polynomials of degree $\leq n$.

Consider a function $f(x) \in V$. (e.g., $f(x) = e^x$)

Question:

Find the best degree n polynomial approximation of f(x):

Example: