

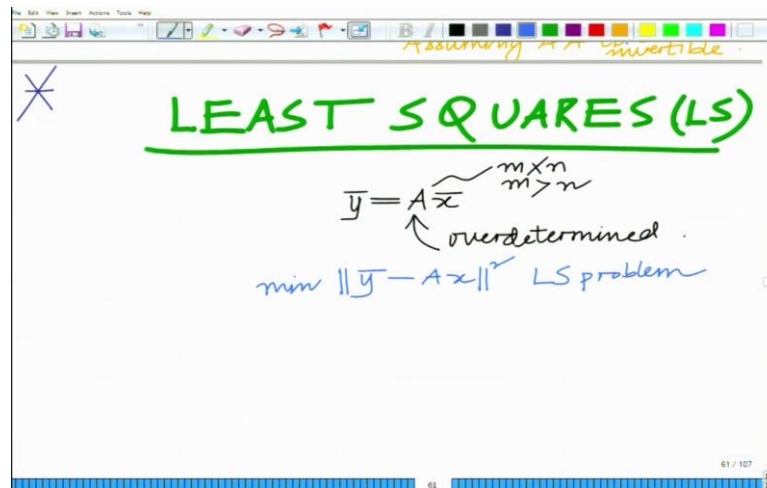
Applied Optimization for Wireless, Machine Learning, Big Data
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Lecture – 42
Geometric Intuition for Least Squares

Keywords: *Least Squares*

Hello, welcome to another module in this massive of online course. So we are looking at the least squares optimization problem and we also derived the least squares solution.

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So when we have an over determined system of equations $\bar{y} = A \bar{x}$ we minimize the norm that is $\min \|\bar{y} - A \bar{x}\|^2$ and this is termed as the least squares problem. The solution to this is $x = (A^T A)^{-1} A^T \bar{y}$.

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$\bar{y} = A\bar{x}$ $m > n$
 \uparrow overdetermined
 $\min \|y - Ax\|^2$ LS problem
 $\hat{x} = (A^T A)^{-1} A^T y$
 Consider $(A^T A)^{-1} A^T$
 $\begin{matrix} n \times m & m \times n & n \times m \\ \hline & n \times n & \end{matrix}$

Now, consider the matrix $(A^T A)^{-1} A^T$, we can see that the size of this matrix is $n \times m$.

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$\frac{(A^T A)^{-1} A^T}{n \times m}$
 $A \leftarrow \begin{matrix} m > n \\ \Rightarrow A \text{ is NOT invertible} \\ \text{Tall matrix} \end{matrix}$
 $\begin{bmatrix} A \end{bmatrix}$

So this has more columns than rows and for $m > n$ this implies that A is not invertible. Now, we are considering a scenario in which the number of rows is much greater than the number of columns, so this is also known as a tall matrix.

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A screenshot of a presentation slide showing a handwritten derivation. At the top, a matrix A is represented by a vertical rectangle with the label "Tall matrix" and an arrow pointing to it. Below this, the equation $(A^T A)^{-1} \cdot A^T \times A$ is written in yellow. This is followed by an equals sign and the expression $(A^T A)^{-1} \cdot (A^T A) = I$, also in yellow. A purple arrow points from the text "is behaving as inverse of A" to the expression $(A^T A)^{-1} \cdot (A^T A)$. The slide has a toolbar at the top and a footer showing "62 / 107".

$$(A^T A)^{-1} \cdot A^T \times A = (A^T A)^{-1} \cdot (A^T A) = I$$

is behaving as inverse of A

If you look at $(A^T A)^{-1} A^T$ and you take its product with A we get an identity matrix. So it is as if $(A^T A)^{-1} A^T$ is acting as an inverse of A when multiplied on the left because A is not invertible when $m > n$ but it is behaving as an inverse and this is therefore known as the pseudo inverse of A .

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A screenshot of a presentation slide. At the top, the equation $(A^T A)^{-1} A^T = \text{Pseudo-inverse of } A$ is written in green. A purple arrow points from the text "Left-inverse of A" to the expression $(A^T A)^{-1} A^T$. Below this, the word "INTUITION:" is written in black and underlined. The slide has a toolbar at the top and a footer showing "63 / 107".

$$(A^T A)^{-1} A^T = \text{Pseudo-inverse of } A$$

Left-inverse of A

INTUITION:

So this is a left inverse because it is only true when you multiply it on the left.

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INITIATION:

$\bar{y} = A\bar{x}$ No solution

$\Rightarrow \bar{y} - A\bar{x} = \bar{e}$

Approximation Error

$\bar{y} - \begin{bmatrix} a_1 & a_2 & \dots & a_n \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$

We have the least squares problem $\bar{y} = A\bar{x}$ and we know that there does not exist any solution. So this implies that no matter what \bar{x} you choose, it will not satisfy $\bar{y} = A\bar{x}$ which means $\bar{y} - A\bar{x} = \bar{e}$ and will always be non-zero. So this is the approximation error and this is represented as shown in slide.

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$\bar{y} - \begin{bmatrix} a_1 & a_2 & \dots & a_n \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$

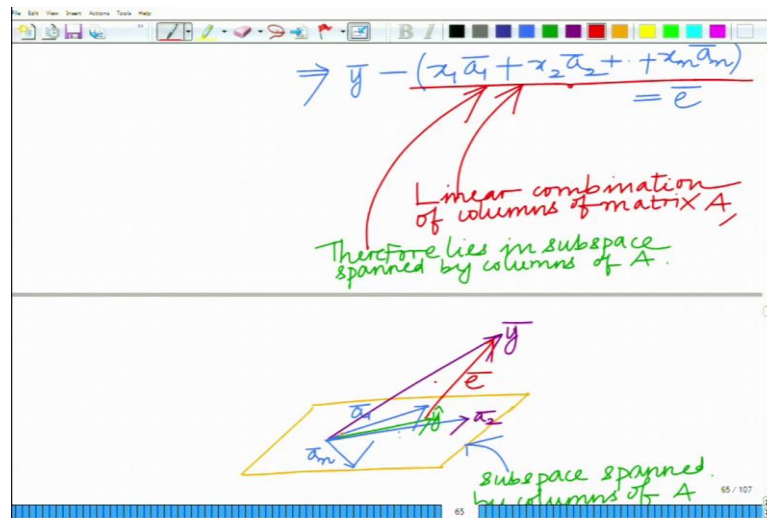
n columns of matrix A .

$\Rightarrow \bar{y} - (x_1 a_1 + x_2 a_2 + \dots + x_n a_n) = \bar{e}$

Linear combination of columns of matrix A .

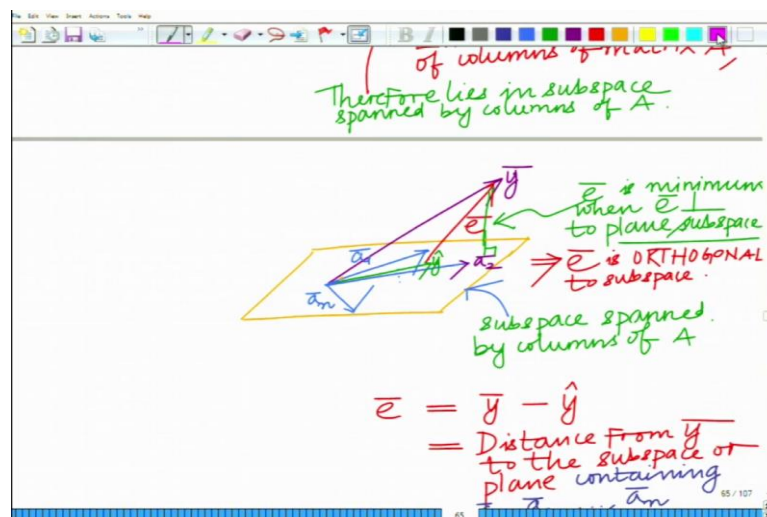
So these are the n columns of the matrix A and this is $\bar{y} - (x_1 a_1 + x_2 a_2 + \dots + x_n a_n) = \bar{e}$ and on expansion of this we get a linear combination of the columns of matrix A which implies that this always lies in the subspace spanned by the columns of A .

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So this can be represented pictorially if you take a plane which is nothing but a subspace. So let us say this is the subspace spanned by columns of A and you have your vector \bar{y} which does not necessarily lie in the subspace. So you are trying to form an approximation which lies in this subspace and let us say you denote this by \hat{y} . So $\bar{y} - \hat{y} = e$ is the corresponding error.

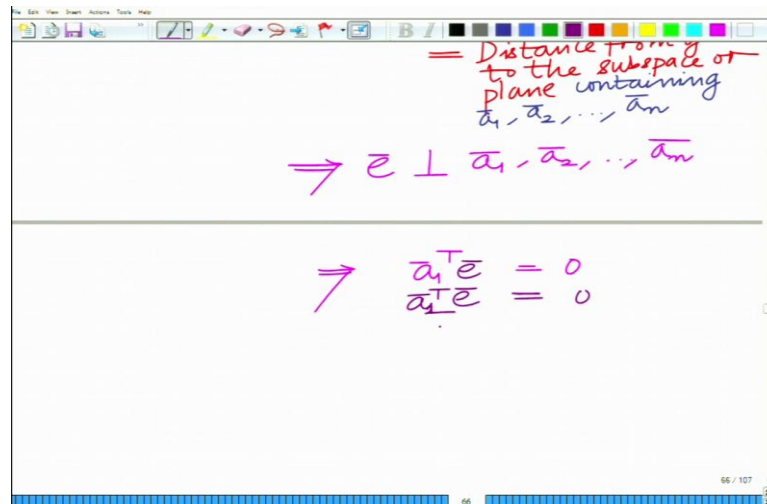
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So this is the distance from \bar{y} to the subspace or the plane that is spanned. Now we want to find the error and we want to minimize this error. And now you can see that this error

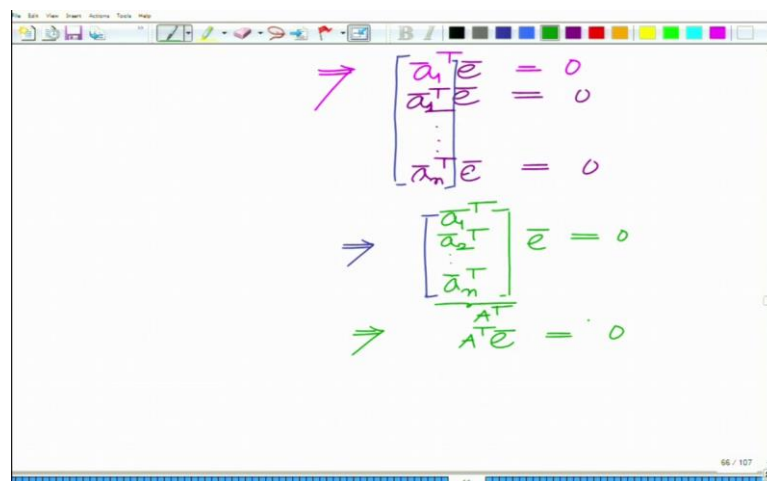
is minimum when the error is perpendicular to the plane or we can say that this error vector is orthogonal to the subspace.

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So this \bar{e} is orthogonal to the subspace, this implies that \bar{e} has to be orthogonal to each of the vectors in the subspace as shown in slide. We know that two vectors are orthogonal when their inner product is 0.

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So this implies $A^T \bar{e} = 0$ as shown in slide.

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Handwritten derivation on a whiteboard:

$$\Rightarrow A^T(\bar{y} - A\bar{x}) = 0$$

$$\Rightarrow A^T\bar{y} = (A^TA)\bar{x}$$

$$\Rightarrow \boxed{\hat{x} = (A^TA)^{-1}A^T\bar{y}}$$

Least Squares (LS) solution

But, $\bar{y} - A\bar{x} = \bar{e}$ so this implies $A^T(\bar{y} - A\bar{x}) = A^T\bar{e} = 0$. Now you observe that the best vector \bar{x} that minimizes the error is $\bar{x} = (A^TA)^{-1}A^T\bar{y}$. So this is nothing but again the least square solution, so intuitively what the least square solution is doing is basically finding the best approximation to \bar{y} in the subspace that is spanned by the columns of the matrix A. And therefore the distance of \bar{y} to the plane is minimum when the error vector is perpendicular to the plane. Now $\hat{y} = A\hat{x} = A(A^TA)^{-1}A^T\bar{y}$.

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Handwritten diagram and equations on a whiteboard:

Diagram: A 3D coordinate system showing a plane (subspace) and a vector \bar{y} outside it. The projection of \bar{y} onto the plane is labeled \hat{y} . The error vector \bar{e} is shown perpendicular to the plane.

$$\hat{y} = A\hat{x}$$

$$\hat{y} = A(A^TA)^{-1}A^T\bar{y}$$

\hat{y} = Projection of \bar{y} in subspace of a_1, a_2, \dots, a_n

$$\Rightarrow A(A^TA)^{-1}A^T = \text{projection matrix}$$

For subspace spanned by a_1, a_2, \dots, a_n

Now, if you look at this plane again you can also say that \hat{y} is the projection of \bar{y} in the subspace spanned by the columns of A, so when you multiply this matrix by \bar{y} you get

the projection. So this matrix is the projection matrix, that is $P_A = A(A^T A)^{-1} A^T$ is the projection matrix for the subspace that is spanned by the columns of A.

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The image shows a handwritten derivation on a whiteboard. At the top, the formula $P_A = A(A^T A)^{-1} A^T$ is boxed in purple. Below it, the product $P_A \cdot P_A$ is calculated. The first P_A is written as $A(A^T A)^{-1} A^T$. The second P_A is written as $A(A^T A)^{-1} A^T$. The A^T of the first term and the A of the second term are crossed out, leaving $A(A^T A)^{-1} A^T A(A^T A)^{-1} A^T$. The $A^T A$ terms in the middle are simplified to the identity matrix, resulting in $A(A^T A)^{-1} A^T = P_A$. Finally, the result $P_A^2 = P_A$ is boxed in purple.

$$P_A = A(A^T A)^{-1} A^T$$

$$P_A \cdot P_A = A(A^T A)^{-1} \cancel{A^T} A \cancel{A^T} A(A^T A)^{-1} A^T$$

$$= A(A^T A)^{-1} A^T A(A^T A)^{-1} A^T$$

$$= A(A^T A)^{-1} A^T = P_A$$

$$P_A^2 = P_A$$

So one of the most interesting properties of the projection matrix is that $P_A^2 = P_A$, in fact, $P_A^n = P_A$ for any integer $n \geq 1$. So this is the intuition behind the least square solution. So we will stop here and continue in the subsequent modules. Thank you very much.