Matrix Computation and its applications Dr. Vivek Aggarwal Prof. Mani Mehra Department of Mathematics Indian Institute of Technology, Delhi

Lecture - 50 Best approximation: least square method

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Hello viewers. So, welcome back to the course on Matrix Computation and its application. So, today we are going to discuss a very important application that is the Best approximation using least squares method. Now, suppose we have some data, this is my x- axis, this is my y -axis and suppose some data is given to me. Suppose I take one data point here, then I have this point, something like this one.

So, this is my, I can write this a  $(x_1, y_1)$  point, this is  $(x_2, y_2)$  and this is in the end, I have  $(x_n, y_n)$ . So, these points are the random points that are given and I do not know where they lie. They may lie on a straight line or they may be spread over the given xy plane. So, in this case now the question is that, we want to fit a line passing through these points.

So, I have written the passage through these points. So, I know that I can fit a line that is passing through all this point. So, this is possible, this is possible if all the points are

collinear, that is all the points lie in a line. So, in that case, what do we do? How will we find out what, we are going to do that let.

So, let us take a line that I am writing as y = ax + b. This is my line l. Now I will substitute the first point here. So, I will write

$$ax_1 + b = y_1$$
$$ax_2 + b = y_2$$
$$ax_n + b = y_n$$

So, I do not know whether these points are collinear or not, but I want to approximate these points with the line.

So, I want to fit a line that is passing through this point. So, it will pass through these points only when it is collinear, otherwise I want that line to pass from this one. So, this is what I want to fit. So, I can say that we want to fit a line from the given data. For given data points, maybe I can write this way now.

So, let us not claim anything, I will do with this one now first. So, I want to fit a line. So, I have taken a line and then I put the value here and suppose this is equal to this value.

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Now, from here if you see, I can write this in the matrix form. So, I will get the value here this is

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

So, this matrix A is of order of dimension n\*2.

Now, we are assuming here. So, assuming here, we are assuming that all x i's are distinct, it means  $x_i$  is not equal to  $x_j$  for any i j, it means they all are distinct. So, from here if you see then this is a system of equations.

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So, I can write this as A and maybe I can write this vector v is equal to Y this one I can write. Now, from here if you see, I am taking the second column is 1,1, 1 and the first column is  $x_1$ ,  $x_2$ ,  $x_3$  and I am saying that all these are distinct now from here I can say that the rank of A is 2.

Now, we have the rank of this matrix 2. So, this is basically like this system. I can say that the number of equations is greater than the number of variables. The number of variables is only 2, I want to find the value of a and b for this line ok. So, I assume that this is the line which is

going to fit the given data. So, I need to find the value of a and b. Now if this line is there I put the value of x all these x coordinates and suppose it is equal to  $y_1, y_2, ..., y_n$  ok.

So, this is the system we get where the number of equations is greater than equal to I can say the number of variables and this system is called an overdetermined system of equations. So, rank is 2. Now, from here if you see from here then this is equal to I am writing a and this is

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

Now two things happen. Now, in this case it is because the number of equations is greater than the number of variables. So, this system I can write this system as this is my equation number 1 and I can write this as 2, this I can write as a 3. Now, system 2 may have a solution.

Now the question is when it can have the solution? Now if the vector is so, if the vector is one,  $y_1, y_2, ...y_n$  this is the right hand side vector, I just take the transpose here. If the vector this belongs to column space of this vector, the column space of this

$$\begin{pmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_2 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \end{pmatrix}$$

because if you see this one it belongs to R<sup>n</sup>.

So, now if this vector belongs to the column space of this one, then the system has solution and in this case I know that this matrix is of dimension  $n^* 2$ . So, its rank cannot be more than 2, but here the column vectors are linearly independent.

So, the rank of this matrix is 2. Now from here we can say that if the vector this belongs to the column space then the system has solution, has in fact, unique solution and if this is there this is possible only when all the points, all the data points I can say, and this is possible only if all the data points are collinear. It means this system is going to have the solution when all the data points will lie in a line like this one.

If I see this one. So, these points I have taken are all lying in the line. So, if I fit a line from these points, then this system is going to have the solution. All the points lying completely on

the line. These points are completely on the line, not away from the line. This is my line and I can write that this is y = ax + b.

So, if this system is a solution then all the points are going to lie on the line. Now, but in general our data is spread over the whole domain xy, they are not lying on the xy on a line because these data points are coming from some experiment. So, in this case now, if the data points are not collinear, that is they are sparse, the points are spread all over the domain, the data points are spread in the xy plane. So, that is there which implies that the system Av=Y is inconsistent.

Inconsistent means this system is not going to have the solution. So, that is there. Now, in that case what we are going to do.

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Now, it means that in this case A v if I take y and taking its norm that is basically we are dealing with the ||Av-Y|| = 0, then the system is consistent and has a unique solution. But if we take  $||Av-Y|| \neq 0$ , then the system is inconsistent. So, this system I cannot solve with the method.

So, you can see from here that basically this is what is an error. Now from here what we are going to do is that if you see from here then I can write this as

$$||Y - Av||^{2} = |y_{1} - (ax_{1} + b)|^{2} + |y_{2} - (ax_{2} + b)|^{2} + \dots + |y_{n} - (ax_{n} + b)|^{2}$$

This if you see square, this is equal to  $y_1 - (a x_1 + b)$  because this is giving you the error basically. So, this is basically the error. This is basically the error. So, this is equal to square because I am taking the two norms here.

So, the error will be just this will be the error, this will be the error, this will be the error, this is the error corresponding to this x, actual value this one and by the line we are consuming this one.

$$|| Y - Av ||^2 = (e_1^2 + e_2^2 + \dots + e_n^2)$$

Now our so now, we come to know that I cannot fit a line which is passing through all this point. So, but that is not possible. So, now, we want a line which is passing through, which is passing close to all the points. This is what I can do. So, now, what I want that we want to minimize  $||Y-av||^2$ 

So, I want to minimize this one and I will minimize the value of a and b because that value I have to find the coefficients in the line a b, a x + b. So, I want to minimize this error basically. So, this is called minimizing the error. So, if I am able to minimize this one then I will get a line which is passing close to all the points and if you see now this one then this method is called we have least square method, the least square solution.

So, why is it called that? We are taking the square. So, this is the square of the error. If you see then this is a square of the error and I am finding the minimization. So, I am finding the least of all this one. So, that's why this name is called the least square method. So, our main purpose is here to minimize this error term, the square of the errors.

So, I want to do this one. So, that is called my least square method and this is the best approximation that we discuss now. So, let us just give one example of how it is happening here I just take one example.

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Suppose I take a line, suppose I have a point (1, 1), (2, 2), (3, 3), (4, 4), I have four points. And I know that these points are collinear points. The 4 points are there, but if you draw these points, then it is supposed one point is here another is here another is here. So, all the points lying on this line.

So, I know that this is a line y = x ok. Now I take that let, so, let us take a line y = ax + b. Now from here I can write. So

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a_{1} + b = 1
a_{2} + b = 2
a_{3} + b = a_{3} + b = 3
a_{4} + b = a_{4} + b = 4
\begin{bmatrix} 1 & 1 \\ 2 & 1 \\ 3 & 1 \\ 4 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix}
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Now, from here if you see I can solve this system, because here if you see from here then this vector can be written as a linear combination of these two. So, this vector lies in the column space of this matrix A. And now also if you see from here, I can solve it very easily by the standard method, I can write the augmented matrix.

So, this is the augmented matrix. I can write

[1	1	1		[1	1	1		1	1	1
2	1	2		0	-1	0		0	1	0
3	1	3	=	0	-2	0	=	0	0	0
4	1	4_		0	-3	0_		0	0	0

So, the rank of A is the same as the rank of the augmented matrix. I can write like this one. So, the system is consistent and if you see from here then if I want to find out the solution. So, the solutions will be a + b = 1 here and then I get b = 0. So, from here I will get a = 1. So, that gives me a solution, that a = 1, b = 0. So, I get the line a = x and I already know that this is the solution. So, this is a collinear point and we are able to solve these points.

Now, suppose we have points, maybe I just take points (0,1), (1,2) and (2,4). Suppose I take these points. I just take the three points and I just take the equation. So, now, I get

 $a \cdot 0 + b = 1$  $a \cdot 1 + b = 2$  $a \cdot 2 + b = 4$ 

So, I assume a line that is y = a x + b and from here I will get the matrix that is

[0]	1]	[0]	[1]
1	1	$\begin{vmatrix} a \\ b \end{vmatrix} =$	2
2	1	101	4

So, this is my system of equations and I know that this matrix is having the rank 2, no problem. Now from here I will write its augmented matrix.

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$$\begin{bmatrix} 0 & 1 & 1 \\ 1 & 1 & 2 \\ 2 & 1 & 4 \end{bmatrix}$$

So, that is I am writing  $\begin{bmatrix} 2 & 1 \end{bmatrix} \begin{bmatrix} 4 \end{bmatrix}$  That is my augment matrix. I will reduce the row echelon form. So, reduce this one it will be now in this case I just swap the first and the second row it is

$\begin{bmatrix} 0 \end{bmatrix}$	1	$\lceil 1 \rceil$		1	1	2		[1	1	2		[1	1	2]
1	1	2	$\rightarrow$	0	1	1	$\rightarrow$	0	1	1	$\Rightarrow$	0	1	1
2	1	4		2	1	4		0	-1	0		0	0	1

So, I can say from here that the rank of the augmented matrix is 3, but the rank of A is 2, if you see, this is the A matrix. So, rank is 2 and the whole augmented matrix the rank is 3.

So, in this case I can say that the system is inconsistent. So, this system is inconsistent, I cannot solve this one. So, it means that we cannot find a line which is passing through all this point ok. So, from here we find that the system is inconsistent. So, now our next step is we need to find a line. So, we need to find a line which passes closest to all the data points. So, this is what I need to do to find out the line fit.

So, this one we need to do. So, how can we do this one because I found that this system is inconsistent. So, if the system is inconsistent then how am I going to solve this system? So, that is one of the main questions for finding this system or the solution of this one.

So, now we are going to introduce an important thing: if you see from here, I have this matrix, this is my matrix. So, I have my matrix here. Now we have a, b is equal to y and my

$$\mathbf{A} = \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 2 & 1 \end{bmatrix} \text{ and my } \mathbf{y} = \begin{bmatrix} 1 \\ 2 \\ 4 \end{bmatrix}.$$

Now, I know these two vectors. So, this vector and these vectors are linearly independent ok and also so, this vector  $(0\ 1\ 2)^T$ , the first column. So, I can take transpose here and  $(1\ 1\ 1)^T$  this belongs to R<sup>3</sup> and is linearly independent. It means that they, so this span if I take these vectors and find their span is a subspace of R<sup>3</sup>.

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So, this is a subspace of  $R^3$  basically. Now if you see from here that this is a subspace (0 1 2) ok, this vector and (1 1 1). They are linearly independent as a subspace of  $R^3$ . So, let's get right here. So, I just take the three dimensional plane. So, the three dimensions we have are (x, y, z) and suppose this is some plane. I just made a plane here.

So, suppose this is a subspace made up of these factors because it will be a plane. Now I know that this vector, so, this system is inconsistent which implies that this vector  $(1 \ 2 \ 4)$  does not lie in the column space of the matrix A. It means this vector  $(1 \ 2 \ 4)$ . So, if I take any point. So, this  $(1 \ 2 \ 4)$  is not lying on this plane in this subspace.

So, it may be somewhere here. Let us write that this is my vector  $(1 \ 2 \ 4)$  like this one and this is the subspace S. So, I just write it S. This is a subspace because if this point lies in this plane in this subspace then the system will be consistent, but now we know that this is inconsistent. So, it is not lying here.

So, what we are going to do is now, we are going to take the projection of this vector on this plane. So, we are going to take the projection of this vector over this plane. So, that this is the right angle. So, this is suppose my I have a system a v is equal to y then. So, this is my guess.

Now, this is the projection of this vector on this space. So, this is supposed to be my new y, I call it y hat. So, now, I can say that the y hat is a projection of y on the subspace S. So, now, we need to find how we can take the projections of this space subspace projection of this vector on the subspace S.

So, this is what we have done in theory. So, now, we do this one, I mean generalization. So, let us know how we can take the projection. Now we do generalization. So, how to take projection of y on the subspace S. This one we want to see ok. So, let us see how we can do this one.

Now, we just take the generalization. I have a ok, I have some maybe I just take x is equal to b, I will write this a general space. So, let us take this one. So, proof. So, here we are going to do it. Let us assume a system of equation Ax=b, where a is something like having two columns only because I know always having two columns.

So, it is going to have the  $a_1$  and  $a_2$ . So, these are the two columns is going to have because in this case we have always n \*2 and my x is 2\*1 and on the right hand side I have b that is  $b_1$ ,  $b_2$ , b. So, this is n\*1. So, always we are going to have now I know that this vector is now we know that that b does not lie in the column space of a.

So, that does not lie in the column space of an ok. So, now, I will just make a some three dimensional space and suppose this is my plane space s is equal to the span of a one a two and suppose this is my x I am just considering it in the three dimension and we have a vector which is lying here this is my vector b and I take its projection here and I get this vector this is my projection vector.

So, I call it maybe P and this is my basically b hat the new projection vector. So, this one I want to find and I know that this is equal to the error this part. Now we assume that a one and a two are 1 I, linearly independent because they are always linearly independent. So, we assume here that they are linearly independent.

So, the space subspace S is a 1, span by  $[a_1, a_2]$  and dimension of S will be 2 in this case now that is ok.

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So, now once we have the projection, the b dash, then we have our system, a new system, that is a new system that is having the same x, but on the right hand side we have a new b. So, in that case we need two solutions and that solution will be a new solution, that is x hat I am writing.

So, x hat is an, is an solution, is a solution of  $\hat{A}\hat{x} = \hat{b}$ 

So, this is the solution of this one. Now if you see from here this is the error e. So, what is e? e is basically if you see that is  $b - \hat{b} b - \hat{b}$ 

So, now from here, now we know that from the this place I know that  $\hat{b} \perp (b - \hat{b})$ 

I know that this is A x = b. So, from here I can write that  $\hat{b} \perp (b - A\hat{x})$ 

So, from here I can write now from this  $\hat{b} \hat{b}$  is lying in the subspace S. So, I can write that also

 $\hat{b} \in S \Rightarrow \hat{b} = c_1 a_1 + c_2 a_2$ 

So, from here I can write. So, this one I can write that  $c_1a_1 + c_2a_2 = \hat{b} \perp (b - A\hat{x})$ 

this one I can write.

And from here very easily I can write that, because this  $a_1$  and  $a_2$  already lying in this one,  $a_1$  and  $a_2$  are lying in this subspace and this vector error vector is perpendicular to the whole S because this is making the right angle triangle here.

So, this vector  $\hat{b} \hat{b}$  hat is lying in the S space and this vector is perpendicular to this one. So, now, from here I can say that the  $a_1 \perp (b - A\hat{x}) \Rightarrow a_1^T (b - A\hat{x}) = 0$  $a_2 \perp (b - A\hat{x}) \Rightarrow a_2^T (b - A\hat{x}) = 0$ 

so, in the matrix form

And from here I can write

$$\begin{pmatrix} a_1^T \\ a_2^T \end{pmatrix} \cdot \begin{bmatrix} b - A\hat{x} \\ b - A\hat{x} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

So, this is my vector taking the dot product with this vector and that is (0 0).

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So, this is my matrix, A transpose. So, from here I can write that, I very easily I can write that this is equal to

 $A^{\top}(b-A\hat{x})=0$ 

From here I can write this is A transpose, in the matrix form I can write. And that gives me that the  $A^{T}b - A^{T}A\hat{x} = 0$ 

$$A^{\mathsf{T}}A\hat{x} = A^{\mathsf{T}}b$$

and this one now since rank of a is 2, rank of A transpose A is also 2 and invertible.

So, this will be invertible. So, from here I can write that my  $x = (A^T A)^{-1} A^T b$  So, that will be my approximate solution for the given system, this one. So, using this one I am able to find  $\hat{x}$ . So, this is my  $\hat{x}$ . Now, so, from here you can see that and if you see from here this is  $\hat{A}\hat{x} = \hat{b}$ 

So, from here now what is  $A\hat{x} A\hat{x}$ ? So,  $A\hat{x} = A(A^T A)^{-1}A^T b = \hat{b}$ 

So, this equation I can give maybe I can give name 1. I have started from generalization. So, this is my basic generalization I have started. So, after that I thought maybe I should write it as one, this is my equation number 1, now this is 2 and I can write this as equation number 3.

Now, from here this is equal to this. So, from here I can write a projection matrix P which I apply on b, I get  $\hat{b}$ . So, where  $P = A(A^T A)^{-1} A^T$ . So, this is called a projection matrix. So, if I use this matrix on any vector. So, what is it to do? It will project that vector into the subspace made by the columns of A that we have already seen. So, that is why it is called the projection matrix.

Now, this is a projection matrix we have; now we have some properties of a projection matrix because if you see then I want to find out what are the properties of the projection matrix. So, let us see this one.

So, P is the projection matrix. So, if it is a projection matrix then some properties of the projection matrix that some important condition has to satisfy. First thing is that  $P^{T} = P$ .

So,this can be written as  

$$\left(A(A^{T}A)^{-1}A^{T}\right)^{T} = A^{T^{T}}\left((A^{T}A)^{-1}\right)^{T}A^{T} = A\left((A^{T}A)^{T}\right)^{-1}A^{T} = A(A^{T}A)^{-1}A^{T}$$

So, this is again the P. So, it is symmetric because we are taking the projection and taking the transpose. So, it does not matter if you take the projection 2 times.

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Now if you see from here if I have taken the projection of this vector and it reaches here. Now, I apply the same projection here, it is not going to change because this vector is already in the subspace S. It means that my  $P^2 = P$ . So, let us see this one. So,

$$P^{2} = \left(A(A^{T}A)^{-1}A^{T}\right)\left(A(A^{T}A)^{-1}A^{T}\right) = A(A^{T}A)^{-1}(A^{T}A)(A^{T}A)^{-1}A^{T} = A(A^{T}A)^{-1}A^{T} = P$$

So, P square is equal to P. So, from here we can see that this is my projection matrix. So, now, the thing is that that is how we are going to solve the system. So, this system we are going to solve. So, in the nutshell what we can say is that, now we have a system Ax = b and this system is inconsistent and this system is coming from least square.

Then we take

$$A^{T}AX = A^{T}b$$
$$\Rightarrow X = (A^{T}A)A^{T}b$$

that will be the corresponding approximate solution. So, this is my approximate solution of A x = b.

So, this is the solution after doing this one, we get that matrix now. This line will pass through the data closest to all the data. So, that is the meaning of least square. So, let us just quickly do one example.

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Now, suppose I have the data points (0, 1), (1, 1), (2, 1), (3, 1). Suppose I take four points and these are data points. So, the question is fit a line. So, one wants to fit a line. So, let I take a line y = ax + b. So, from here I will get my system

a.0 + b = 1a.1 + b = 3a.2 + b = 4a.3 + b = 4 (Refer Slide Time: 53:20)





system now. I want to solve this system.

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So, I will use the octave for this one because we have to do a lot of calculations here. So, in this I will just because any student who has a difficulty with Octave or MATLAB, then he or she can take the help of my another course that is scientific computing using MATLAB.

So, you can go through a few videos that teach how we can work in MATLAB or Octave. So, now, we are going to define the matrix A here. So, this is the matrix I am going to have. So, matrix A is basically I am writing 0 1 and then 1 1 and then 2 1 and 3 1.

So, this is the matrix we got now on the right hand side I have a vector b. So, that is the column vector. So, I will just take the vector 1 3 4 4. So, 1 3 4 4 m this vector now I know that I want to take the I want to just check whether this is going to have a solution or not. So, I found the augmented matrix.

So, I just write A that is an augmented matrix and that matrix I can write as A here and then b. So, this is my augmented matrix and there is an inbuilt form that is the row reduced echelon form of the matrix A ok. So, this is what I just wrote. So, I found this value.

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So, this is basically from here I found that the system is inconsistent because the rank of A A, if you see the rank of AA is 3 and the rank of if I found A, then you can check from here that it is 2. So, the system is inconsistent. I can write that the system is inconsistent.

Now, what do we need to do? We have to apply the least square method. So, what I want to do is that now I will take the matrix. I get the matrix I found first. I found the transpose. So, I will take A this into A. So, that is my matrix A transpose A. So, maybe I can write here I can just write B is equal to transpose because some commands may be not here. So, it is a transpose of the matrix B.

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So, I can write B into A, actually I have not written the star here. So, no problem. So, this is my matrix and I know that this matrix will be invertible. So, I need to find the solution. So, I have to solve this one now to find the solution I have to find A transpose A, x is equal to A transpose b, I have changed the system basically and now from here I can find x bar is this is my A transpose A inverse A transpose into b.

So, that will be my solution in this case. So, I need to find out this value. So, this is my inverse, I have taken A transpose A. I just found a transpose this one now I want to find the inverse of this. So, I can find, I can write the inverse of B as the inverse of the matrix B, B star sorry B star a not B B star a or I can write this answer and this one.

So, that is my inverse. Now from here I can now write the inverse B because I need now we have A inverse B into A transpose because I need to find. So, I have taken this value, now I have to multiply by A transpose into b.

So, this one I need to do. So, I have to do multiplication. Now first I will just take it. So, this matrix and multiply by a transpose. So, that is B. So, this is my matrix and now I just take the answer and multiply by B. So, that is my solution. So, from here if you see that a is 1 and b is 1.5.

Now, if you see from here my x bar is coming 1 and 1.5. You can see from here 1 and 1.5. So, which implies that my line is 1. So, x plus 1.5 that is y is equal to this 1.

So, that is my line because a value, the value of a is 1 here and b is 1.5. So, this is the line which goes closest to all these points. It will never satisfy these points because if you put x equal to 0, here y is 1.5, but our data point was 1. If you put x equal to 1, it will be 2.5 and our data is 3, but this is the line which goes closest to all these points and that is the least square solution.

So, this is the best line fit line fit for the given data and this is the way we can find out the solution of this type of least square solutions now from this. So, this way we can find all this one and this is the way we have been able to find the solution. So, this is the least square solution and now I think we should stop now.

So, in the today's lecture we have discussed a very important application about that if we have a data points then how we can fit a line which is either passing through all the points, but if it is not passing through all the points then it should pass closest to all the point and that is done by the method of least squares. And then we have discussed how if the system is inconsistent then how we can solve those systems with the help of the projection.

So, I hope you have enjoyed this lecture, thanks for watching.

Thanks very much.