

Matrix Solvers
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Lecture – 27
Comparing GS and Modified GS

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Modified Gram-Schmidt

Algorithm

1. For $j = 1, \dots, n$ Do:
2. Compute $r_{jj} := \|\hat{x}_j\|_2$,
3. If $r_{jj} = 0$ then Stop, else $q_j := \hat{x}_j / r_{jj}$
4. For $i = j + 1, \dots, n$, Do:
5. $r_{ji} := (x_i, q_j)$
6. $x_i := x_i - r_{ji}q_j$
7. EndDo
8. EndDo

u_i Projection
 q_1, q_2, q_3
 $r_{ji} = \frac{u_i}{\|u_i\|}$
 $(u_i - \text{Proj}_{q_1} u_i) \perp q_1$
 $(u_i - \text{Proj}_{q_1} u_i - \text{Proj}_{q_2} (u_i - \text{Proj}_{q_1} u_i)) \perp q_2$
 $u_i - \text{Proj}_{q_1} u_i - \text{Proj}_{q_2} (u_i - \text{Proj}_{q_1} u_i) \perp q_1, q_2$
 due to orthogonal q_1, q_2
 $\perp q_3$

Welcome, in last class we were looking into modified Gram Schmidt algorithm. The idea of Gram Schmidt algorithm is to consider have a set of linearly independent vectors and then form a mutually orthonormal set of vectors out of that. This is done in a way you first the, first vector you consider the vector itself and then divide it by its length and get a normal vector or reunite vector on the direction. For the second vector onwards you take a vector project that vector along the already settled orthogonal vectors.

And subtract these components from that particular vector. And whatever will be remaining with you is perpendicular to the already settled set of orthonormal vectors. And this vector take this vector, divide it by its length you will get another unit vector now you get a set of orthonormal vectors up to this vector and move it for move forward.

So, what we have seen is that, as we take one particular vector v_1 for example, we take one particular vector v_i and we have a vector we have few orthogonal vectors q_1, q_2, q_3 so on. So, we project v_i on q_1 and this is say projection of v_i on q_1 . This is projection of v_i on q_2 . This is projection of v_i on q_3 . We subtract all these things from

v_i and get a new vector which is u_i and then q_i in the next orthogonal vector is u_i by mod of u_i .

However, when we subtract all these projections so, when we first take v_i and subtract its projection from q_1 whatever will get will be v_i minus projection of v_i on q_1 . This is perpendicular to or rather q_1 . This is perpendicular to q_1 then we subtract from this vector which is already perpendicular to q_1 , we subtract projection of q_1 on v_i . This is from this we again subtract projection of q_2 of u_i on q_2 . This will be perpendicular to q_2 this is also perpendicular to q_1 .

However, if we have number of vectors and why this is both perpendicular to q_1 and q_2 ; because whatever is perpendicular to q_1 has no component in q_1 . So, from this whatever you subtract will still remain perpendicular to q_1 ; however, in a numerical implementation what happens? When we do this for number of vectors it becomes perpendicular to q_2 , q_2 , but does not remain perpendicular to q_1 due to round of errors. So, the solution becomes that which is the modified Gram Schmidt algorithm that instead of projecting v_i every time and subtracting these projections from v_i , what you do you make this as $u_i = v_i - \text{projection of } v_i \text{ on } q_1$.

Then the next step in modified Gram Schmidt method will be u_i minus projection of u_i on q_2 . These 2 steps are similar; however, exactly same arithmetically we can see; however, as this is done as we are not subtracting anything from this projection which is v_i minus projection of v_i on q_1 , we are taking u_i and projecting u_i on q_2 and subtracting this from u_i the round of error we are making in this stage is again projected on q_2 and being subtracted. So, round of errors are in a sense being cancelled. And this always remains perpendicular to q_1 and q_2 . And this is the idea of modified Gram Schmidt method.

And we have a modified Gram Schmidt algorithm, where the dot product we take not with the initial set of vector. Rather the initial vector we subtract it is from the initial vector we subtract it is projection along one particular q . And then we take the modified vector for the dot product.

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Comparisons

A set of linearly independent vectors in R^4 may be chosen as:

$$a_1 = (1, \epsilon, 0, 0)^T, \quad a_2 = (1, 0, \epsilon, 0)^T, \quad a_3 = (1, 0, 0, \epsilon)^T$$

making the approximation $1 + \epsilon^2 \approx 1$ *→ mimics round off error*

Classical Gram-Schmidt gives the orthogonal vectors: *for $\epsilon = 10^{-6}$, $1 + \epsilon^2 = 1.0000000001$*

$$q_1 = (1, \epsilon, 0, 0)^T / \sqrt{1 + \epsilon^2}$$

$$q_2 = (0, -1, 1, 0)^T / \sqrt{2}$$

$$q_3 = (0, -1, 0, 1)^T / \sqrt{2}$$

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And now if we see the an example that we are considering a set of linearly independent vectors in R^4 . And we are taking 3 vectors one epsilon 0 0 1 0 epsilon 0 1 0 0 epsilon. Epsilon is a small number. And $1 + \epsilon^2$ is very small say for example; epsilon is 10 to the power minus 6. So, epsilon square is 10 to the power minus 12 is further small.

And we make the approximation $1 + \epsilon^2 \approx 1$. So, this approximation actually mimics round off error because for epsilon is equal to say 10 to the power minus 6, $1 + \epsilon^2$, which is 10 one point 10 to the power minus 12 right. So, 1.0000000001, this we are doing a round off error and we are considering this to be 1. So, though we though this is not any computed implementation; however, we are solving a problem in pen and paper, but we are doing a substitution of round off error here.

So, when in this case when we apply Gram Schmidt, classical Gram Schmidt technique we get the following orthonormal set of vectors q_1 is one epsilon 0 0 (Refer Time: 06:58). This was again a length one that is that is the approximation doing here. Its length is $\sqrt{1 + \epsilon^2}$ and we are considering it to be 1. $1/\sqrt{2}$ 0 0 1 by root 2 by root 2.

These are orthogonal set of vectors. And this are obtained after doing the mimicked round off error.

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Comparisons

A set of linearly independent vectors in R^4 may be chosen as:

$$a_1 = (1, \epsilon, 0, 0)^T, \quad a_2 = (1, 0, \epsilon, 0)^T, \quad a_3 = (1, 0, 0, \epsilon)^T$$

making the approximation $1 + \epsilon^2 \approx 1$

Classical Gram-Schmidt gives the orthogonal vectors:

$$q_1 = (1, \epsilon, 0, 0)^T$$
$$q_2 = (0, -1, 1, 0)^T / \sqrt{2}$$
$$q_3 = (0, -1, 0, 1)^T / \sqrt{2}$$

Modified Gram-Schmidt gives the orthogonal vectors:

$$q_1 = v_1/1 = (1, \epsilon, 0, 0)^T$$
$$q_2 = (0, -1, 1, 0)^T / \sqrt{2}$$
$$q_3 = (0, -1, -1, 2)^T / \sqrt{6}$$

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Now, if we look into the modified Gram Schmidt orthogonal vectors, they are not same as this. Because at certain step there is 1 epsilon square which appeared in Gram Schmidt method which did not appear in modified Gram Schmidt method. So, you did not have to neglect that epsilon square this thing this; however, if we write epsilon square in both the if we have not disregarded that epsilon square which is coming in classical Gram Schmidt method, we would have got the same set of vectors in both the cases. But as epsilon square is very small like a computer approximation we are doing 1 plus epsilon square is equal to 1.

This ideally should give right result and if we think of writing a computer program, we have to deal up with deal with systems where this type of situations will occur, where there will be numbers which are at which are not the exact number rather the numbers which are replaced by a truncated version of this numbers, where the round off error is already there, ok.

So, we see the modified Gram Schmidt solution. The first one is one epsilon 0 0, second one is same 0 minus 1 1 0 by root 2. The third one is change 0 minus 1 minus 1 2 by root 6. The third vector in Gram Schmidt and modified Gram Schmidt are different. And that is because of this approximation 1 plus epsilon square is equal to 1 is made somewhere here which has not been made in modified Gram Schmidt at that particular location and you cannot try it yourself we will see that this type is arising.

This is the solution is actually very straight forward. So, these are the different value of q_3 we are getting in Gram Schmidt and modified Gram Schmidt method.

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Comparisons

Check Orthogonality:

- Classical: $q_2^T q_3 = (0, -1, 1, 0)(0, -1, 0, 1)^T / 2 = 1/2$
- Modified: $q_2^T q_3 = (0, -1, 1, 0)(0, -1, -1, 2)^T / \sqrt{12} = 0$

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And now if we check orthogonality the classical Gram Schmidt q_2 transpose q_3 is not giving me 0, rather giving me a half; however, the modified Gram Schmidt is giving me the right result. Because this epsilon square approximation is avoided in modified Gram Schmidt, which is not avoided in classical Gram Schmidt and once you do it practice this problem yourself, you will be able to identify that particular step where this is been done.

So, modified Gram Schmidt obviously, gives us much stable solution. This error will only come when we are when there is some epsilon square which is which neglecting which can hinder the problem, ideally it should not be because these are small value, but this is changing the solution.

So, we call this to be a numerically unstable method, because it might give good result classical Gram Schmidt might give good result in certain cases. But there are small changes in the vectors and it can give entirely different result. And the results will be wrong. In a sense that, vectors are not mutually perpendicular to each other; however, modified Gram Schmidt is a stable algorithm and it should give you right result in all the cases.

So now will know that if we have a set of independent vectors we can get a set of orthonormal vectors using those independent vectors how we can use it for the purpose of matrix solvers? So, what we will do? We will consider a matrix with independent columns.

And what is the importance of having a matrix with independent columns? It can be very easily shown you can take it like a small exercise yourself; that if the matrix has independent columns, and we solve $Ax = b$, x will have at most one solution, infinite solutions are not possible maximum there will be one solution if matrix A has independent columns. If the columns are equal to the number of rows, then there will be exactly one solution if the columns are less than the number of rows so that you have less variables, but more equations. Columns are less than the less than number of rows.

However, if the columns are independent you will still get one solution. And that is why in case of singular matrices when finding the particular solution, we remove the dependent columns from that. So, that we have a independent we only have independent columns in the equation. So, what will try to see is that we will form a matrix with independent columns and do a Gram Schmidt Gram Schmidt orthogonalization over that matrix.

So, the matrix will be transformed to a q matrix, or to a matrix with orthonormal columns. If it is a square matrix it will be square q matrix which is called an orthogonal matrix; however, So, you will get a matrix with orthonormal columns. Now solution is very easy because in a with a orthonormal basis, we have earlier seen that we can take the right hand side vector and project it on orthonormal basis. Projection with each of the bases will give me each component of the solution vectors. So, solution will be much simpler.

So, and there is a more formal way of proposing the solution here. So, what will do will start with the equation $Ax = b$. And now take A and do a Gram Schmidt orthogonalization on A . And see how the equation looks like and what are the ease in solving the equation.

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Q-R Factorization

Start with a matrix A with independent columns $v_1, v_2, v_3, \dots, v_k$. Let us run Gram-Schmidt orthogonalization steps on each of the vectors to get orthonormal vectors $q_1, q_2, q_3, \dots, q_k$.

$$v_1 = (q_1^T v_1) q_1$$

$$v_2 = (q_1^T v_2) q_1 + (q_2^T v_2) q_2$$

$$v_3 = (q_1^T v_3) q_1 + (q_2^T v_3) q_2 + (q_3^T v_3) q_3$$

$$\vdots$$

$$v_k = (q_1^T v_k) q_1 + (q_2^T v_k) q_2 + (q_3^T v_k) q_3 + \dots + (q_k^T v_k) q_k$$

Any vector b can be expressed in orthonormal basis as

$$b = (q_1^T b) q_1 + (q_2^T b) q_2 + \dots + (q_n^T b) q_n$$

Triangular Form

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So, this is called a QR factorization start with a matrix A with independent columns v_1, v_2, \dots, v_k , and let us run Gram Schmidt orthogonalization steps on each of the vectors to get a orthonormal set of vectors.

So, I have sorry, I will have the first vector v_1 it is very, very easily it can be orthonormalized, like will only take the length of that first vector and divide it by that and we will get the vector q_1 . And the relationship between v_1 and q_1 is q_1 is unit vector. So, $v_1 \cdot q_1$ is basically length of v_1 , a vector with unit vector dot product if there are on the same direction it is the length of v_1 along q_1 .

For v_2 , v_2 is constituted sorry q_2 is rather q_2 is constituted as take v_2 project it along q_1 subtract that part for it. You will get the part which is perpendicular to q_1 perpendicular to take v_2 project it on q_1 subtract that projection from v_2 . So, we will get a component which is perpendicular to v_2 and get q_2 out of it. So, v_2 can be decomposed in this 2 orthogonal vectors q_1 and q_2 . Similarly, for q_3 how do we get q_3 we took v_3 project it on q_1 and q_2 subtracted this projections from v_3 , what is remaining with us v_3 minus the projections normalized it got q_3 .

So, v_3 is again composite of 3 vectors. Or you can be decomposed into 3 orthogonal directions q_1, q_2, q_3 . Similarly, we move ahead v_4 , there will be 4 vectors in which v_4 can be decomposed q_1, q_2, q_3, q_4 . And v_k k th vector will be decomposed in all k

independent orthonormal vectors. So, if a vector is like v_1 there is only one basis vector which express v_1 .

For v_2 there is only 1 2 there are 2 basis vectors q_1 and q_2 which gives you v_2 . For any vector b on a orthonormal basis, q_1 to q_n it can be expressed as $q_1^T b$ q_1 which is projection of b along q_1 and on that direction. Projection of b along q_2 on that direction, and similarly projection of b along q_n and on that direction.

So, we can write v_1 is $q_1^T v_1$, $q_1^T v_2$ is q_1 , because it is only it has q_1 and q_2 components into q_2 and so on. So, we get a triangular form of equations here. The equation set gives us a nice triangular form. Remember, v_1 v_2 to v_k are columns of a matrix A and we are thinking of solving $Ax = b$. So, if we put this the right hand side as the column of matrix A , if in case substitute it what happens then?

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Q-R Factorization

$v_1, v_2, v_3, \dots, v_k$ and $q_1, q_2, q_3, \dots, q_k$ are column vectors. The matrices A and Q are related as:

$$\begin{bmatrix} | & | & | & \dots & | \\ v_1 & v_2 & v_3 & \dots & v_k \\ | & | & | & \dots & | \end{bmatrix} = \begin{bmatrix} | & | & | & \dots & | \\ q_1 & q_2 & q_3 & \dots & q_k \\ | & | & | & \dots & | \end{bmatrix} \begin{bmatrix} q_1^T v_1 \\ q_1^T v_2 \quad q_2^T v_2 \\ q_1^T v_3 \quad q_2^T v_3 \quad q_3^T v_3 \\ \dots \\ q_1^T v_k \quad q_2^T v_k \quad q_3^T v_k \quad \dots \quad q_k^T v_k \end{bmatrix}$$

$A = QR$ where Q is orthonormal matrix and R is triangular Lower triangular

$A_{m \times n} = Q_{m \times n} R_{n \times n}$ for n columns in R^m $m > n$

So, v_1 v_2 up to v_k and q_1 q_2 q_3 up to q_k are column vector. The matrix A and Q this is column of this vectors are sorry, this is columns of A and this is columns of Q , Q is the vector with orthonormal columns. So, the matrices A and Q are related as this columns v_1 v_2 up to v_n is equal to the columns q_1 q_2 q_3 . Because if I go back sorry, v_1 is $q_1^T v_1$ q_1 , v_2 is $q_1^T v_2$ q_1 plus $q_2^T v_2$ q_2 .

So, the column v_2 is something into column q_1 plus something into column q_2 . So, in that sense if we go we can write that the matrix A , this is the matrix A , this is the matrix Q multiplied by a triangular matrix. So, v_1 is $q_1^T v_1$ q_1 , v_2 is $q_1^T v_2$ q_1 plus $q_2^T v_2$ q_2 . These

are the column vectors. This is not a single entry this is rather a column a vector. The vector $q_2^T v_2$ is equal to $q_1^T v_2$ plus $q_2^T v_2$ into q_2 is combination of these 2 columns so on.

So, we get a equation where we write a is equal to Q into R , where Q is an orthonormal matrix and R is the triangular matrix. So, our R is rather direct to write a lower triangular matrix lower triangular matrix. And we get if A is m into n ; that means, A has m rows and n columns. So, there are n independent columns and each are in all the column vectors are members of vector space R^m .

So, A is m into n Q is m into n and R is n into n . So, if we have n independent columns in R^m ; that means, either columns are equal to rows or columns are less than number of rows. So, A will have a shift like this A is m into n . m is greater than equal to n because there are n independent columns. So, m can be at most m , this equal to Q sorry, Q is also m in to n a rectangular matrix into r which is n into n which is a square matrix a small square matrix.

So, this is a triangular lower triangular matrix and a triangular matrix must also be a square matrix. So, A is a rectangular matrix that is obtained as another rectangular matrix Q into square matrix square lower triangular matrix R . Now if I substitute this into the equation Ax is equal to b . Because one idea is that if we have orthonormal columns, it is easy to solve the equations. We have we have to like we have $q \cdot x$ is equal to c you only have to take c and project it along each columns $q_1 \ q_2 \ q_3$. So, $c \cdot q_1$ will give you x_1 $c \cdot q_2$ will give you x_2 so on. So, solution becomes only a projection operation.

And now we saw that how from A is any general rectangular matrix, we have to convert it into a transform A to AQ matrix. Then that is doable as a is equal to Q into R , where R is the lower triangular square, square matrix R is a rectangular matrix. So, if we write Ax is equal to b as QRx is equal to b . And see how to solve this equation. And we will also see whether we can take advantage of that that q is orthonormal and so, finding solutions are easy.

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Q-R Factorization for matrix equation

For the equation $Ax=b$, QR factorization writes it:

$$(QR)x=b$$

using a modified Gram-Schmidt process on A

This equation can be represented as:

$$Qc=b \rightarrow Q \text{ is orthonormal}$$

$$Rx=c \rightarrow R \text{ is lower triangular}$$

The first equation can be solved as projecting b on Q as $c=Q^T b$

$$c_1 = q_1^T b, c_2 = q_2^T b, \dots$$

The second equation, $Rx=c$, can be directly solved as R is lower triangular matrix.

So, Ax is equal to b on QR

factorization on that will give us QRx is equal to b . Which can be represented as a system of 2 equations first is Qc is equal to b with Rx is equal to c . Now Q has so, there are 2 things this Q is orthonormal and R is lower triangular. So, the first equation Qc is equal to b can be solved as projecting b on Q . What is known to us? b is already known to us from the matrix A we you learn a Gram Schmidt process and get the orthonormal matrix Q . So, this can be obtained using a say modified Gram Schmidt algorithm Gram Schmidt process on A .

So, take a take a matrix A and modified Gram Schmidt algorithm Gram Schmidt on A , A you will get the Q matrix. And in this steps you can find out what is the R matrix. Now Q is an orthonormal matrix. So, Qc is equal to b can be solved as just projecting c on q . So, we can write c_1 is equal to $q_1^T b$ c_2 is equal to $q_2^T b$ and so on. And then we have the equation Rx is equal to c , which is the lower triangular system. So, you can find out c from them, the last equation or if we look into R , sorry.

So, this is a lower triangular say matrix; that means the first equation so, r has a shift like this. $R_{11} \ r_{12} \ r_{21} \ r_{22} \ r_{31} \ r_{32} \ r_{33}$ and here we have $x_1 \ x_2$ this is equal to $c_1 \ c_2$. So, I can directly find out x_1 is equal to c_1 by r_{11} , then x_2 is equal to $(c_2 - x_1 r_{21}) / r_{22}$ and so on. So, the second equation Rx is equal to c can be directly solved as R is a lower triangular matrix.

So, $Ax = b$ equation for any rectangular or for a square matrix also becomes easily solvable or other than Gauss elimination Gauss Jordan or the third one we discussed about LU LU decomposition or TDM TDM is restricted only for tridiagonal matrix, but general purpose we have seen Gauss Jordan Gauss elimination and LU decomposition. Other than this methods, we can also use the QR decomposition method in which we can solve a equation system and the efforts are not that involved like Gauss elimination efforts are probably simple, simpler than Gauss elimination you are not actually counting the number of steps, but this can be an exercise that count the number of steps involved in a QR factorization.

However, if we have or in some way you already have the QR factorization of a matrix, we can solve the equation very quickly. In a sense, $Rx = c$ is directly solvable. If there are n questions in n steps. So, we can solve that in order of n steps. And then $Qx = c$ is equal to $Qc = b$ is also solvable. We only have to project b along each of the q 1 and the solutions will be there.

But a n like LU decomposition the solution is simple when you have LU decomposition already, but LU decomposition itself is a costly process. Similarly QR decomposition the solution is simple, if we have already have the QR decomposed form. But solve getting QR decomposition needs a Gram Schmidt process, which is relatively costly process, ok.

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Q-R Factorization for normal equations

For the equation $A^T A \hat{x} = A^T b$, QR factorization writes it:

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

$$\Rightarrow (QR)^T QR \hat{x} = (QR)^T b$$

$$\Rightarrow R^T Q^T QR \hat{x} = R^T Q^T b \quad \text{Now, } Q^T Q = I$$

$$\Rightarrow R^T R \hat{x} = R^T Q^T b$$

or, $R \hat{x} = Q^T b$

This equation is directly solvable as R is lower triangular

Handwritten note: \hat{x} is best estimate of $Ax = b$ with least square error

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So, the further important thing happens if we sorry, if we think of QR factorization of normal equation. And normal equation is instead of $Ax = b$ is not solvable. The columns are independent, but the columns do not span the entire \mathbb{R}^m rather columns do not span entire \mathbb{R}^m therefore, $Ax = b$ does not have any solution.

So, x is equal to b is not soluble. So, what do you do then we try to find out the best estimate of x we get the normal equation $A^T Ax = A^T b$. x is the best estimate is equal to b , QR estimate this not actually we use $Ax \approx b$. x is best estimate of Ax is equal to b with least square error. So, also from a least square method we can get this system of equation. And we have $A^T Ax \approx A^T b$. So, for the equation, this is not $A^{-1} b$ I am sorry this will be $A^T b$.

So, we have the equation $A^T Ax \approx A^T b$. And now you put the QR decomposition here. So, which is $Q^T Q R x \approx Q^T b$. And transpose of a product is product of the transposes, in in the different order. So, this is $R^T Q^T Q R x \approx R^T Q^T b$. And now what we know is $Q^T Q$ is an identity matrix. So, we get $R^T R x \approx R^T Q^T b$. Cancel R^T from both the sides. So, we have $R x \approx Q^T b$.

And we again end up with a lower triangular matrix, but now the solution now we do not have to do any projection of 2 or we do not need to solve $Qc = b$. We only have one equation which is of lower triangular form $R x \approx Q^T b$. And this equation is directly solvable as R is lower triangular form. So, QR factorization actually is much useful if we have the normal equation. We will later see that many very sophisticated solution techniques are not if that efficient for normal equation because this $A^T A$ matrix is a complicated matrix to deal with one self.

However, if we have and QR decomposition, the $A^T A$ matrix we need not have to deal with that rather we deal with $R x \approx Q^T b$. And very easily we can solve this equation this is again $n \times n$ steps. We can solve this equation because R is a rectangular matrix system. So, this is one of the largest utility of QR decomposition when you are trying to solve normal equation $A^T Ax \approx A^T b$.

So, with this lecture we finish most of the direct solvers we planned to discuss here. And we go through the set of direct solvers which we have done through the set of direct solvers here; which are Gauss elimination then LU decomposition Gauss Jordan TDMA, or tridiagonal matrix algorithm we have seen it for one specific purpose. When the matrix is tridiagonalized. And we have discussed about variant of tridiagonal matrix algorithm which is not a direct solver which is actually an iterative solver; however, that TDMA can be used when the matrix is not tridiagonal rather penta diagonal or septa diagonal form.

And we have and now looked into another matrix solution technique which is QR decomposition. So, next part of this course we will discuss with iterative solvers. But before going into iterative solver we will have a brief review of Eigenvalues and eigenvectors of matrices which we will do in next few classes. Because they are important in iterative solvers, also they will help us to understand the behaviour of iterative solvers from the understanding we have already developed on Ax is equal to b systems using direct solvers. So, next class we will start discussing on eigenvectors and Eigenvalues.

Thank you.