

Dynamic Data Assimilation
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Lecture - 17
Matrix Decomposition Algorithms Continued

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QR DECOMPOSITION: $m < n$

- $Z = Hx$, $H \in \mathbb{R}^{m \times n}$, $m < n$
- Then $H^T = QR$ as above, since $n > m$
 with $Q = [Q_1, Q_2]$, $R = \begin{bmatrix} R_1 \\ R_2 \end{bmatrix}$, $Q_1 \in \mathbb{R}^{n \times m}$, $Q_2 \in \mathbb{R}^{n \times (n-m)}$
 $R_1 \in \mathbb{R}^{m \times m}$ and $R_2 \in \mathbb{R}^{(n-m) \times m}$ is a zero matrix
- $Q_1^T Q_1 = I_m$ and $H = R^T Q^T$

$$\begin{array}{l} H \\ m \times n \quad m < n \\ \hline H \\ m \times n \quad m < n \\ \hline H^T \\ n \times m \end{array}$$

In the previous talk we talked about QR decomposition for the over determined case. QR decomposition can also be applied for the under determine case. I am going to quickly point out some of the key steps. Let again Z is equal to H of x , H is m by n , m is less than n , m is the number of observation, n is the number of unknowns. I have more unknowns than the number of observations. In this case, please remember I have done the QR decomposition of H m by n , when m is greater than n . We have already done with that. In this case I have H m by n , here m is less than n .

If I took the transpose of this H ; that is n by m n is greater than m . So, these two cases are the same if you interchange m and n . Therefore, QR decomposition of H for the over determined system, is the same as the QR decomposition of H transpose for the underdetermined system. That is a quick mathematical enterprise that you can utilize. If you utilize this you can see the QR decomposition for the lower triangular, for underdetermined case on the over determine case, are not too different from each other.

So, I can compute H transpose QR as above. Since in this case, n is greater than m by interchanging the role of m and n , I can apply everything that we saw thus far, Q again is Q_1 and $Q_2 R$ is again R_1 and $R_1 R_2$. R_1 is an upper triangular matrix. R_2 is a 0 matrix, $Q_1^T Q_1$ is I_m , and H is equal to $R^T Q^T$. So, essentially the whole thing flies without any much trouble at all.

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LEAST SQUARE SOLUTION – QR METHOD ($m < n$)

- $f(x) = \|r(x)\|_2^2 = (Z - R^T Q^T x)^T (Z - R^T Q^T x)$

$$= Z^T Z - 2Z^T R^T Q^T x + x^T (Q R R^T Q^T) x$$

$Z = Hx$
 $H: R^T Q^T$
 $\rightarrow (Z - R^T Q^T x)$
- $\nabla_x f(x) = -2QRZ + 2(QRR^T Q^T)x = 0$
- $\nabla_x^2 f(x) = 2QRR^T Q^T$
- x_{LS} is the solution of: $(R^T Q^T Q) = RZ$

So, in this case again, my f of x is equal to square of the normal residual. So, Z is equal to. So, let us go back to the previous case. The problem reduces to Z is equal to. I am sorry H is equal to R transpose Q transpose, in view of that $H Z$ minus H of x . I am sorry, in view of that Z minus H of x . I am sorry once again; let me correct myself Z minus H of x .

Z minus H of x , H is equal to R transpose Q transpose. Therefore, Z minus H of x now becomes R transpose Q transpose x , and this is what is used in here. So, f of x is the square of the sum of the errors represented this way. So, this is an alternate expression for the residual, which can be, when multiplied can be given by this. You can compute the gradient of this. This is independent. The first term is the independent of x . this is linear in x .

This is quadratic in x . From the module on multivariate calculus, we know how to compute the gradient of a linear function; we know how to compute the gradient of a quadratic function. By applying those rules, it can be verified that the gradient is given

by this expression, at the minimum gradient must be 0. I can also simultaneously compute the hessian. So, the solution for the least square problem is obtained by solving the gradient to be equal to 0, and that gives rise to this equation. So, $R R^T Q^T x$ that must be. I am sorry.

X must be equal to $R Z$ therefore, if I change if I can multiply both sides by R inverse.

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FORM OF THE LEAST SQUARE SOLUTION

- $y = Q^T x = \begin{bmatrix} Q_1^T \\ Q_2^T \end{bmatrix} x = \begin{bmatrix} Q_1^T x \\ Q_2^T x \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$ $y_1 \in \mathbb{R}^m, y_2 \in \mathbb{R}^{n-m}$
- $R R^T = \begin{bmatrix} R_1 \\ 0 \end{bmatrix} \begin{bmatrix} R_1^T & 0 \end{bmatrix} = \begin{bmatrix} R_1 R_1^T & 0 \\ 0 & 0 \end{bmatrix}$
- $\begin{bmatrix} R_1 R_1^T & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} R_1 Z \\ 0 \end{bmatrix} \Rightarrow \underline{R_1 R_1^T y_1 = R_1 Z}$, y_2 is arbitrary
- y_1 is obtained by solving a lower triangular system $\underline{R_1^T y_1 = Z}$ $\downarrow O(n^2)$

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If I multiply R inverse, I get the overall solution. So, to that extent, I am now going to express various operations, and here y is equal to Q transpose x , which is given by this partition form. R plus R transpose is essentially given by. So, there is no plus here. So, sorry there is no plus here. This is given by this matrix. There is $R_1 R_1^T$ 0 0. Therefore, if I assemble all these things I get this equation, which is the equation I need to solve. $R_1 R_1^T$ is a non singular matrix, if I multiply both sides by R_1 inverse, I simply obtain the least square solution by solving R_1 transpose, y_1 is equal to Z . So, this is again R_1 is upper triangular system R_1 transpose a lower triangular system. This can be solved in $O(n^2)$.

So, the whole theme of the exercises, whether it is over determined undetermined by invoking the QR decomposition of the rectangular matrix H in either case, one can reduce the solution least square problem, to one of solving a lower triangular system or an upper triangular system which is much easier to solve. This is the motivation for using the QR decomposition, because the pathway leads to a very simple problem in the end.

And we already know solution of upper triangular system lower triangular systems are very simple.

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THE LEAST SQUARE SOLUTION: $m < n$

- $X = QY = Q \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = [Q_1 \ Q_2] \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = Q_1 y_1 + Q_2 y_2$
- Since y_2 is arbitrary, there are infinitely many solutions
- Clearly, $x_{LS} = Q_1 y_1 = Q_1 (R_1^{-T} Z)$
- $\|x\|_2^2 = \|Q_1 y_1\|_2^2 + \|Q_2 y_2\|_2^2$
 $= \|y_1\|_2^2 + \|y_2\|_2^2$
 $\geq \|y_1\|_2^2 = \|x_{LS}\|_2^2$

$(Q_1^T Q_1 = I_m, Q_1^T Q_2 = 0, Q_2^T Q_2 = I_{n-m})$

This is another look at the least square solution. The least square solution is now given by x is equal to Q of y in the case of underdetermined system. y is $y_1 \ y_2$. Q is $Q_1 \ Q_2$. Therefore, x is equal to $Q_1 y_1$ plus $Q_2 y_2$.

Now, please remember y_2 is arbitrary. So, there are infinitely many solutions, and that is consistent with the undetermined system. In the case of there are infinitely many systems. Infinitely many solutions for the equations whether, because there are more unknowns than the known's from the previous analysis, we get the linear solution of the linear system, arising from the least square problem, is given by this; x therefore, the norm of X_{LS} .

So, this must be the norm of X_{LS} , the same X_{LS} in here that is equal to the norm of $Q_1 y_1$ square plus $Q_2 y_2$. $Q_1^T Q_1$ is I_m $Q_1^T Q_2$ is 0 $Q_2^T Q_2$ is I_{n-m} , I_m is the m th order unit matrix, I_{n-m} is the n minus m th order unit matrix. Q is an orthogonal transformation, ortho are the length is invariant orthogonal transformation. Therefore, this term reduces to this term, because of orthogonality. Again this term reduces to this by orthogonality.

So, y_2 is arbitrary; therefore, the least square solution is larger than, or equal to y_1 ones at the. The norm of the square of y_1 , we are going to any solution x is greater than the least square solution; therefore, the least square solution is given by the formula that we had already given which is here.

So, this corresponds to this therefore, any arbitrary there are infinitely many solution, any one of the infinite many solution has a norm, that norm is greater than least square solution. Therefore, the least square solution is the unique solution of minimum norm. So, that is the end gain the end result, and this is result of applying the QR decomposition to the underdetermined system as well.

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SUMMARY: QR ALGORITHM

- Over determined case $H \in \mathbb{R}^{m \times n}$, $m > n$
- Step 1: Compute $Q_1 \in \mathbb{R}^{m \times n}$ and $R_1 \in \mathbb{R}^{n \times n}$ such that $H = Q_1 R_1$ using Gramm-Schmidt orthogonalization method – See below
- Step 2: Compute $Q_1^T Z$ $(\tilde{R}_1^T)^T : (\tilde{R}_1^T)^T = \tilde{R}_1^T$
- Step 3: Solve upper triangular system $R_1 x = Q_1^T Z$ and $x_{LS} = R_1^{-T} (Q_1^T Z)$

So, summary of the QR algorithm over determine system H is, m is greater than n compute Q_1 compute R_1 ; such that H is equal to $Q_1 R_1$ using a method called Gramm Schmidt Orthogonalization. So, that is where we are now leading to, that is the reason for the summary. I only said that such a thing can happen, but we do not know how to make it happen. So, if I can express H as Q times R Q s orthogonal R is upper triangular, we saw all the beauties in the analysis, that essentially assumed I can do now it is time for us to be able to tell how to make the decomposition happen, that decomposition H is equal to $Q_1 R_1$; that is the reduced QR decomposition is often done by a very famous procedure called Gramm Schmidt Orthogonalization method. We will talk about it shortly.

So, once you have $Q^T R^{-1}$, I can compute $Q^T \text{transpose } Z$. Once you have $Q^T \text{transpose } Z$ that defines the right hand side. I need to solve the lower triangular system $R^{-1} x$ is equal to $Q^T \text{transpose } Z$, that gives us to the linear least square solutions $R^{-1} \text{minus } T$. Minus T means what. This is $R^{-1} \text{inverse transpose}$. It is denoted by, is also equal to $R^{-1} \text{transpose inverse}$.

So, these two operations commute; because they commute for simplicity, in mathematics we simply call it minus t. So, if I say minus T, is a combination of 2 operations the order in which you apply these operations is a material these two operators commute. So, the least square solution is given by your solution of a lower triangular system, which is given elegantly by this.

So, the whole method is beautiful and very nice. So, we need to concentrate on being able to express H as $Q^{-1} \text{ times } R^{-1}$, the reduced decomposition, and that is done by Gramm Schmidt Orthogonalization. So, that is our next term, given H How do we convert H into product of Q and R. So, we in our method, what is that we assume, let us pretend we can do the decomposition H is a QR Q and R, and how if I can do that, the solution algae, the solution, the structural solution becomes. After having achieved that it behooves us to ask a question, how do I make it happen, how do I make H x process the product of Q and R.

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SUMMARY: QR ALGORITHM

- Under determined case $H \in \mathbb{R}^{m \times n}$, $m < n$
- Step 1: Compute $H^T = Q_1 R_1$, $Q_1 \in \mathbb{R}^{n \times m}$ and $R_1 \in \mathbb{R}^{m \times m}$
- Step 2: Solve the lower triangular system $R_1^T y_1 = Z$
- Step 3: $x_{LS} = Q_1 y_1 = Q_1 (R_1^{-T} Z)$

So, this is the next part of the exercise. I also want to touch upon the under determine case, when H is, when m is less than n , it is an undetermined case. Again it is a complete summary of all the analysis we have done H transpose. So, whatever we did for H , now I am going to do for H transpose. Operation and H and operation of H transpose are not too different from each other, they are mathematically equivalent. Again H transpose can be expressed with the product of Q^T and R^T .

$Q^T R^T$ are given by these respective sizes. Solve the lower triangular system, and least square solution is given by $Q^T R^T$ inverse transpose time Z . So, with this we have completed a discussion of the QR transpose algorithm, QR decomposition algorithm modulo the method for decomposition; QR decomposition.

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GRAMM- SCHMIDT ORTHOGONALIZATION

- Let $H = [h_1, h_2, \dots, h_n]$, $h_i \in \mathbb{R}^m$, $1 \leq i \leq n$, $m > n$
 $\text{RANK} = \min\{m, n\} = n$
- Let the columns of H are linearly independent
- Find $Q = [q_1, q_2, \dots, q_n]$, $q_i \in \mathbb{R}^m$, $1 \leq i \leq n$ and $\{q_i\}_{i=1}^n$ is an orthogonal system:

$$\begin{aligned} q_i^T q_j &= 0 \text{ if } i \neq j \\ &= 1 \text{ if } i = j \end{aligned} \quad \text{ORTHO NORMAL}$$
- Problem: Given $\{h_i\}_{i=1}^n$, find $\{q_i\}_{i=1}^n$ with the above properties

And that is given by the method called Gramm Schmidt Orthogonalization. So, now, I am going to conjure up case and illustrate how given a matrix H , and I can deliver the Q factor and the R factor. To that n , let H be a matrix, is the m by n matrix, each of the H is are a vector in \mathbb{R}^m . So, there are n vectors each of size n , each of size m . i runs from 1 to n , m is greater than n . So, there are n columns, each column have m rows.

Let the also. I am going to assume the columns are H are linearly independent. So, what does imply, H is a full rank. So, rank of H is equal to minimum of m n . In this case m is greater than n . So, minimum of m and n is n , if the rank of. I am sorry rank of H that is what I should have said. Rank of H is the equal to minimum of m and n is equal to m .

So, it is a full rank matrix, and that is guaranteed by the columns of H being linearly independent. Now you can see the basic concepts from vector space theory comes into play, right through. So, what is our aim? Our aim is to be able to find a Q matrix with n columns, which are q_1, q_2, \dots, q_n .

I would like the columns of Q q_1 and q_2 to be orthonormal system. In fact, it has been orthonormal system, that is given by the following if I take any 2 vectors with distinct entities i and j not equal $q_i^T q_j$ is 0. If i is equal to j $q_i^T q_i$ is 1. So, this is orthonormal. So, what is the problem? Given the columns of H , I need to find the columns of Q ; such that the columns of H are linearly independent, but the columns of QR orthonormal.

This is simply a procedure for converting a set of linearly independent columns, to a set of orthonormal columns, is a very simple procedure, and this procedure is very fundamental, is used repeatedly in several different applications in linear algebra. We have already talked about the applications, in solving linear least square problems. Now we are simply going to concentrate on how to do the decomposition itself.

So, let me go back and say this. So, given h_1, h_2, \dots, h_n find q_1, q_2, \dots, q_n , given that H are linearly independent. I need to find a set of vectors Q that are orthonormal.

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ALGORITHM – AN IDEA

- Set $q_1 = \frac{h_1}{r_{11}}$ with $r_{11} = \|h_1\|_2$ and $\|q_1\| = 1$
- Set $q_2 = \frac{1}{r_{22}}[h_2 - r_{12}q_1]$ – 2 unknowns: r_{12}, r_{22}
 Thus, $0 = q_1^T q_2 = \frac{1}{r_{22}}[q_1^T h_2 - r_{12}] \rightarrow q_1^T q_1 = 1$
 Therefore, $r_{12} = q_1^T h_2$ and $r_{22} = \|h_2 - r_{12}q_1\|$
- In general: j – unknowns ($1 \leq j \leq n$)
 $q_j = \frac{1}{r_{jj}}[h_j - \sum_{i=1}^{j-1} r_{ij}q_i]$ $q_i^T q_j = 0$ (2)
 $\Rightarrow r_{ij} = q_i^T h_j \quad 1 \leq i \leq j-1$
 $r_{jj} = \|h_j - \sum_{i=1}^{j-1} r_{ij}q_i\|$

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So, what is my first vector q_1 ? First vector q_1 is arbitrary I can start at any place. So, what I am going to do. I am going to start with q_1 is equal to my h_1 divided by the norm of h_1 , the divided by the norm of h_1 . Norm of h_1 refers to the length of the vector h_1 . So, r_{11} is the first element of R matrix, it refers to the norm of the vector h_1 , is the two norm of that. So, if I divide the vector by its norm I get a unit vector. So, q_1 is a unit vector. So, first vector q_1 is very simple, it is simply normalized version of h_1 . Now I need to compute q_2 . I am going to compute q_2 as a linear combination of h_1 and h_2 .

q_1 has already information about h_1 . So, I am going to now express q_2 as 1 over r_{22} times h_2 minus r_{12} times q_1 . Please remember q_1 is known, h_2 is known, r_{11} r_{12} is not known r_{22} is not known. So, there are 2 unknowns, r_{12} and r_{22} . How do I find these two unknowns? These two unknowns are found by imposing two condition. What is the first condition, q_1 q_2 must be orthogonal to q_1 that is give rise to value of one of the unknowns. Then the second one is obtained by forcing q_2 be of unit length. So, orthogonality condition, and the normality condition two conditions are enforced by fixing two parameters.

So, if I were to require q_1 to be orthogonal to give to, it requires 0 is equal to q_1 transpose q_2 the assumed to form of q_2 is above I substitute this in here. Therefore, why this is r_{12} , I would have q_1 transpose q_1 is 1 . Please remember that I have already utilized in here q_1 transpose q_1 is equal to 1 . Therefore, when I equate this to 0 r_{12} is simply q_1 transpose h_2 . So, I got 1 1 constant. What is r_{22} . Now I know r_{12} I know q_1 I know h_2 that is the vector, I can compute the norm of the vector, r_{22} essentially divides this vector by its length. So, r_{22} must be the length of that vector which is h_2 minus r_{12} to q_1 .

So, this gives raise to a formula for computing one of the core unknowns. This gives you a formula for computing the other unknown. So, from the known I am computing the unknown. So, here look at this now I have recovered q_1 , I have recovered q_2 I have recovered r_{11} , I have recovered r_{12} I have recovered r_{22} . So, I am recovering both the system simultaneously q and r . So, let us go back to a general, go to a general case when there are j unknowns. In other words I can now express q_j . So, let us pretend I have found out q_1 q_2 q_3 all the way up to q_{j-1} ; I am going to compute q_j . q_j is going to be expressed as a linear combination of all the previous vectors.

h_j has information about h_i ; therefore, I can express q_j by the linear combination that is given here divided by a constant r_{jj} from the previous calculations you can readily see r_{jj} is going to be the normalizing constant, r_{ij} are the constants used in which I am going to force the orthogonality. So, q_j has to be orthogonal to q_1, q_2, \dots, q_{j-1} . I am a $q_1^T q_2, q_2^T q_3, \dots, q_{j-1}^T q_j$ minus 1. So, there r_{ij} minus 1 constant that are required to force the orthogonality, one conscience is required to force the normality, and that is the that is a clear story. So, by multiplying q_j , by multiplying $q_i^T q_j$ for i less than j , and equating to 0, I compute all the values of r_{ij} to be $q_i^T h_j$.

So, I have computed j minus 1 such constant, then r_{jj} . So, this must be r_{jj} , is computed by the norm of the entire vector q_j , is therefore, r_{jj} is equal to h_j minus, thus the norm of the vector.

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QR – ALGORITHM – PSEUDO CODE

- Given $\{h_1, h_2, h_3, \dots, h_n\}$, $h_i \in \mathbb{R}^m$, $m > n$ linearly independent
- Find $\{q_1, q_2, q_3, \dots, q_n\}$, $h_i \in \mathbb{R}^m$, orthonormal

Step 1: Repeat the following steps 2 to 5 for $j = 1$ to n

Step 2: $v_j = h_j$

Step 3: For $i = 1$ to $j-1$

Compute: $r_{ij} = q_i^T h_j$

Update: $v_j = v_j - r_{ij} q_i$

Step 4: Compute norm of v_j : $r_{jj} = \|v_j\|$

Step 5: $q_j = \frac{v_j}{r_{jj}}$

R

H = QR

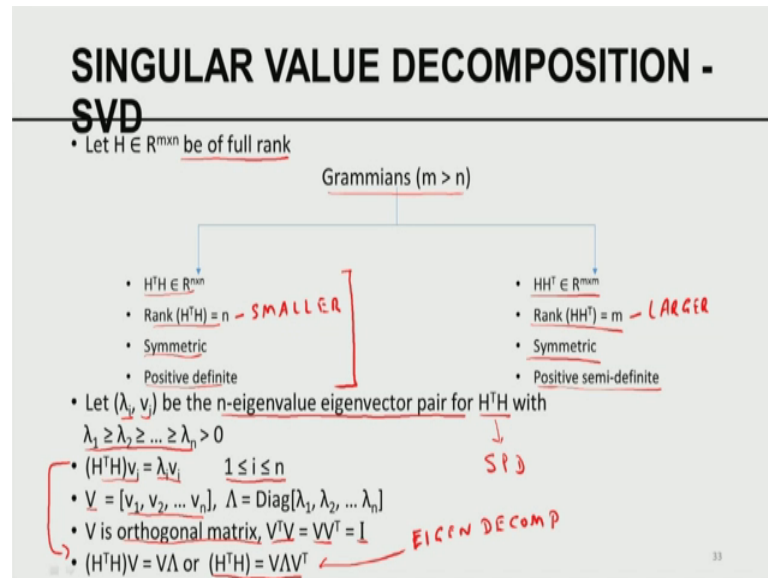
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So, I can now embed this in a pseudo code. Given h that are linearly independent, that are linearly independent. I want to find this are orthonormal, repeat the following steps 2 to 5 for j running from 1 to n . Step 2 v_j is h_j , for i is equal to 1. Now this must be v_1 must be equal to h_1 that is correct, sorry 1 second, what sorry once again, yeah that is correct.

v_j is right, because j is running from 1 to n . So, the overall do loop is on j that is right, that is correct the overall do loop is on j . So, step 2 v_j is equal to h_j ; that means, j is equal to 1. So, initially j is equal to 1 v_1 is equal to h_1 . Step 3 i for i is equal to 1 to j

minus 1, I am going to make v_j perpendicular to the previous vectors. So, that is how I compute this, and now compute the norm of v_j , and then q_j is given by this. So, this procedure is repeated, this procedure delivers q . It also delivers the matrix r as $r_{11} \dots r_{j-1,j-1}$, compute the norm this must be I am sorry $r_{j,j}$, or this is $r_{j,j}$. Therefore, in every case for every j I am trying to find all the i running from 1 to $j-1$ in here $r_{j,j}$ here.

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So, together I compute all the required quantities for every j , and that completes the procedure for computing the QR decomposition, with this algorithm, with this pseudo code, with this pseudo code sorry.

With this pseudo code, with this pseudo code we are able to express any H to be Q and R . R is upper triangular, Q is orthonormal, and this is the reduced QR decomposition. So, here we saw how to multiply, how to decompose H into a multiplicative decomposition QR . I have already utilized if H is equal to QR , how to utilize it in my solution process for the linear least square problems. These two together help you to solve the linear least square problem by the QR decomposition. So, that is method 2.

Now, I am going to go for the last of the three matrix decomposition methods, which is called the singular value decomposition. Singular value decomposition is economist SVD . This is the third alternative method for solving linear systems, I am going to assume my matrix H is again a full rank matrix. Given a rectangular matrix there are two

grammians $H^T H$ and $H H^T$. Both the grammians are of rank n are rank m there are full rank, both of them are symmetric, both of them are positive definite. In this case it is positive semi definite; if it is positive definite means all the Eigen values are positive. If it is positive semi definite means the Eigen values are 0 or positive that is the only difference between the two. And when m is greater than n when m is greater than n this is the smaller grammian.

Because n is smaller. This is the larger grammian. When the rank of $H^T H$ is n , it has n non 0 Eigen values, when the rank of $H^T H$, the rank of H itself is n . Therefore, the rank $H H^T$ is deficient, if this rank deficient some of the Eigen values in this case are allowed to be 0; that is why it is symmetric and positive semi definite. That essentially comes from the rank conditions for product of matrices and the given rank of and the given rank of H , at the given rank of h .

Because we are considering the case m is greater than n ; that is fixed, but these two are two different grammians, one is smaller another is larger, because it is cheaper to work with smaller matrices. Now I am going to consider first the analysis, Eigen analysis of $H^T H$. So, consider $H^T H$, which is there an n by n matrix. $H^T H$ by this definition is $S P D$; therefore, it has the n Eigen values which are the largest of them is λ_1 the smallest of them is λ_n , even the smallest of them is strictly positive.

If λ_i is an Eigen value, let V_i be the corresponding Eigenvector corresponding Eigenvalue λ_i for each i Eigenvalue pair. So, if these are the n different Eigenvalue Eigenvector pair for $H^T H$, it; that means, $H^T H V_i$ is equal to $\lambda_i V_i$; that is the fundamental relation that comes from the definition of Eigenvalue. There are n such relations; I am going to by invoking to matrix relation, succinctly denote the den relation is our own single relation. To that end I am going to concoct a matrix V . The matrix V is simply n by n matrix, whose n columns are the n Eigenvectors of $H^T H$ λ is a diagonal matrix whose diagonal elements are λ_1 to λ_n .

So, V is a n by n matrix diagonal matrix λ is also n by n matrix. We have already alluded to the fact, that the Eigenvectors of a real symmetric positive threat matrix are orthogonal to each other. Therefore, V is again an orthogonal matrix. Now you can see

orthogonal matrices are occurring again and again, 1 is you are decomposition. Now in Eigen decomposition of symmetric positive definite matrices, there are very many different uses of orthogonal matrices in different applications. If V is orthogonal v transpose v and $v v$ transpose is for the identity. Therefore, this relation can be expressed succinctly as H transpose $H V$ is equal to v lambda. If a post multiply both sides by v transpose, both this relation comes to be; that means, H transpose H is equal to v lambda v transpose, this is called the Eigen decomposition of H transpose H . This is called the Eigen decomposition.

So, so far so good, what does it tell you? Given any matrix H of size m by n , H is a full rank. I can consider I can compute two grammian smaller larger, compute the Eigen structure of the smaller grammian. I can express the grammian as the product of v lambda v transpose; V is the matrix of Eigen vectors of the grammian lambda is the diagonal matrix of Eigenvalues of the grammian. So, this is the very basic fundamental results, that comes from the symmetric possible, theory of symmetric positive definite matrices.

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EIGENVALUES AND VECTORS OF HH^T

- Define $u_i = \frac{1}{\sqrt{\lambda_i}} H v_i$, $u_i \in \mathbb{R}^m$, $1 \leq i \leq n$
- $(HH^T)u_i = (HH^T) \frac{1}{\sqrt{\lambda_i}} H v_i$
 $= \frac{1}{\sqrt{\lambda_i}} H (H^T H) v_i$
 $= \frac{1}{\sqrt{\lambda_i}} H \lambda_i v_i = \sqrt{\lambda_i} H v_i = \lambda_i u_i$
- Thus, (λ_i, u_i) , $1 \leq i \leq n$ are the eigenvectors of HH^T
- The rest of $(m-n)$ eigenvalues of (HH^T) are zeros

Handwritten notes and diagram:

Diagram showing \mathbb{R}^n space with vector v_i and \mathbb{R}^m space with vector u_i . A mapping H is shown from v_i to u_i . Handwritten equations: $(H^T H) v_i = \lambda_i v_i$ and $(H H^T) u_i = \lambda_i u_i$. A note says: m eigenvalues, $(m-n)$ ARE ZERO EIGENVALUES.

Now, I know V , I know lambda, I know H . So, I am going to now consider a linear transformation define a vector u_i is equal to 1 over square root of lambda I lambda is are positive I can take the square root H is I m by n matrix, V_i is a m n by 1 vector. So, $H V_i$ is a m vector, this is the constant. So, u_i are m vectors I would like to remind you. So,

this converts your vector from this transformation converts the vector from \mathbb{R}^n to \mathbb{R}^m . So, this is \mathbb{R}^n , this is \mathbb{R}^m . If there is V_i , this is u_i this transformation H , helps to convert an n vector into a m vector; that is a linear transformation u_i . Now I am going to multiply $H H^T$. Please remember $H^T H$ is a smaller the Grammian, this is the larger of the Grammian. I am going to take the larger the Grammian that is m by m matrix; I am going to multiply that by m vector.

I already know the value of u , I substitute this value which is here. I now simplify, if I simplified it and I am, I get $H H^T u_i$ is equal to $\lambda_i u_i$, I am going to let you follow through the simplification procedure, its a very simple sequence of arguments in matrix algebra. So, what does this tell you? This essentially tells you the following, if V_i is such that $H^T H V_i$ is equal to $\lambda_i V_i$, that immediately tells you $H H^T u_i$ is equal to $\lambda_i u_i$; that is a fundamental result. So, that goes to tell you if V_i is are the Eigenvectors of $H^T H$, u_i are the Eigen vectors of $H H^T$, but they share the same Eigenvalue. So, they share the same non 0 Eigenvalues. This matrix must have m Eigenvalues.

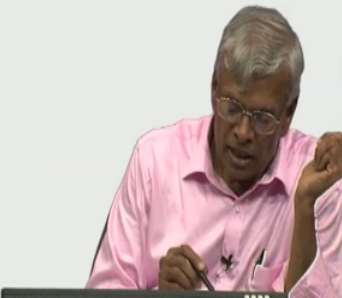
This matrix must have n Eigen values, m is larger than n . So, in this case they share the same set of non zero Eigenvalues the m minus n Eigenvalues are 0, are 0 Eigenvalues in here, 0 Eigenvalues; that is where the semi definiteness comes into play. therefore, $\lambda_i u_i$ are the Eigenvectors of Eigenvalue Eigen vectors of $H H^T$, the rest of the $m - n$ Eigenvalues of $H^T H$ are 0. So, we talked about the semi definiteness of this, positive to semi definiteness of this matrix $H H^T$.

Now, these are the general results. I would like to concentrate on the definition of this, and that is what is going to help us to be able to look at the linear transformation leading to SVD.

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EIGENDECOMPOSITION OF HH^T

- Set $U = [u_1, u_2, \dots, u_n] \in \mathbb{R}^{m \times n}$
- $u_i = \frac{1}{\sqrt{\lambda_i}} H v_i \Rightarrow U \Lambda^{1/2} = H V$
- $U^T U = (H V \Lambda^{-1/2})^T (H V \Lambda^{-1/2})$
 $= \Lambda^{-1/2} V^T (H^T H) V \Lambda^{-1/2}$
 $= \Lambda^{-1/2} V^T V \Lambda^{-1/2}$
 $= I \text{ (because } V^T V = I)$
- Columns of U are orthonormal



So, let u_1 to u_n be a matrix U , u_i is equal to please remember, this is equal to this is equal to $H v_i$ a 1 over square root of λ_i $H v_i$ $H v_i$. So, $U U^T$ you can readily see is I therefore, $U U^T$ has also the orthogonal property that 1 would require, I would like you to follow through this simple relation. So, that essentially tells you the columns of u are also orthonormal. So, we have proved the properties of v , we have proved the properties of u , u and v are related to the metric H transpose H , and $H H^T$ transpose. So, we have seen all the Eigen structure, Eigenvectors of the two grammians H transpose H and $H H^T$ transpose.

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SVD OF H

- $u_i = \frac{1}{\sqrt{\lambda_i}} H v_i \Rightarrow H v_i = u_i \sqrt{\lambda_i}$
- $H V = U \Lambda^{1/2}$ or $H = U \Lambda^{1/2} V^T$ is called the SVD of H

$$H = [u_1, u_2, \dots, u_n] \begin{bmatrix} \lambda_1^{1/2} & 0 & \dots & 0 \\ 0 & \lambda_2^{1/2} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \lambda_n^{1/2} \end{bmatrix} \begin{bmatrix} v_1^T \\ v_2^T \\ \vdots \\ v_n^T \end{bmatrix}$$

$\Lambda^{1/2} = \begin{bmatrix} \lambda_1^{1/2} & & \\ & \ddots & \\ & & \lambda_n^{1/2} \end{bmatrix}$
 $\lambda \rightarrow H^T H$
 $\sqrt{\lambda_i}$ - Singular Values H

- $H = \sum_{i=1}^n \sqrt{\lambda_i} u_i u_i^T$
- λ_i are eigenvalues of $H^T H$ and $\lambda_i^{1/2}$ are the singular values of H by definition

Now, we are going to concentrate on what is the singular value decomposition of H , that comes from basically the definition of u_i under the relation to V_i , please remember this that is the way we define u_i . So, this by cross multiplying both sides by square root of $\lambda_i I$ this can be rewritten as $H V_i$ is equal to $u_i \lambda_i I$ this is for each i . So, this relation if I concoct for all i , can be written in a matrix form as $H V$ is equal to $U \Lambda$ to the power half, what is λ to the power half, λ to the power half is simply the diagonal matrix, which is λ_1 to the power half, λ_2 to the power half, and λ_n to the power half, the square root of the diagonal matrix Λ .

V is orthogonal. So, I can multiply both sides by V^T , if I multiply both sides by V^T because $V V^T = I$, I get this relation look at this. Now H I have now expresses the product of $U \Lambda$ to the power half and V^T , and this decomposition is a new decomposition, it is not LU , it is not Cholesky, it is not QR , it is a new animal, is a new form of decomposition, it is a multiplicative decomposition.

This decomposition is called singular value decomposition of H , why this is called singular value; λ s are the Eigenvalues of $H^T H$. So, square root of λ are called the singular values H . We have already alluded to these things in our module on matrices, because square root of λ_i or the singular values of H this is called singular value decomposition. therefore, H can be expressed as a product of the matrix U , the product of λ to the power half, and the product of V^T like this, if I do the multiplication you can readily see H can be expressed as a product of square root of λ_i . So, that is a scaling factor u_i , is a column vector, V_i transposes a row vector. So, this is an outer product matrix.

Each matrix is multiplied by square root of λ_i . So, this is the weighted sum of outer product matrices, where λ is are the Eigenvalues of $H^T H$, are the Eigenvalues of $H^T H$. I am sorry I have Eigenvalues of A , let me correct that once second Eigenvalues of. This must be $H^T H$, λ_i are Eigenvalues of $H^T H$ and λ_i to the power half or the singular values of H by definition. therefore, this expression, this expression, this expression. They are all called singular value decomposition of H , is a very powerful device. In fact, it is 1 of the most fundamental algorithms in numerical linear algebra, 1 of the important application of this in numerical linear algebra is the following.

Suppose somebody gives you a rectangular matrix H , and asks you to find what is the rank of H . A computational process for determining the rank of H is to compute the grammian $H^T H$, and do an Eigenvalue decomposition, and organize the Eigenvalue in the decreasing order. The number of nonzero are the number of positive Eigenvalues is equal to the rank of the matrix. Therefore, this algorithm for computing the rank of the matrix, using SVD is a very stable procedure for computing the rank. Not only it is used in computing the rank, but also it can be used in solving the least square problems.

So, the Gramm Schmidt procedure, the SVD the things that we have developed, even though we have developed within the context for specific aspect of inverse problems, these algorithms are so fundamental to numerical linear algebra in computation, each 1 of these find multitudes of application. That is why these are considered to be some of the nuts and bolts of computational linear algebra.

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SVD BASED SOLUTION OF LEAST SQUARES

- $Z = Hx$, $H \in \mathbb{R}^{m \times n}$ – full rank
- $H = U\Lambda^{1/2}V^T$, $VV^T = V^TV = I_n$, $U^TU = I_m$
- $f(x) = (Z - Hx)^T(Z - Hx)$

$$= (Z - U\Lambda^{1/2}V^T x)^T(Z - U\Lambda^{1/2}V^T x)$$

$$= Z^T Z - 2Z^T U\Lambda^{1/2}V^T x + x^T (V\Lambda V^T)x$$
- $0 = \nabla_x f(x) = -2V\Lambda^{1/2}U^T Z + 2(V\Lambda V^T)x$
- x_{LS} is the solution of: $(V\Lambda V^T)x = V\Lambda^{1/2}U^T Z$
- $x_{LS} = V\Lambda^{-1/2}U^T Z$

$H = U\Lambda^{1/2}V^T$
 $V^T x = \Lambda^{-1/2} U^T Z$
 $V V^T x = V \Lambda^{-1/2} U^T Z$
 $x = V \Lambda^{-1/2} U^T Z$
 (Annotations: $\Lambda^{-1/2}$ is SCALING, V and U are ROTATION)

$(V^T V \Lambda V^T) x = V^T V \Lambda^{1/2} U^T Z$
 $\Lambda V^T x = \Lambda^{1/2} U^T Z$
 $\Lambda^{-1/2} \Lambda V^T x = \Lambda^{-1/2} \Lambda^{1/2} U^T Z = \Delta U^T Z$

Now, what I have to come back and close the loop. I have expressed H in the form of SVD . If I am able to express H in the form of SVD , how does it help me to solve the linear least square problem that is what I would like to come back to, because the whole aim in these lectures is to solve inverse problem.

So, $H^T H$ is equal to $H^T H$ of x I want to solve, H is a full rank. I can express H as SVD $U \Lambda^{1/2} V^T$. Here $V V^T = V^T V = I_n$, $U^T U = I_m$.

u is I_n , the orthogonality of u and v are already established. So, f of x is equal to Z minus H of x transpose Z minus H of x , but I can express H as u lambda to the power half v transpose, u lambda to the power v transpose. I multiply both sides, I utilize all these properties, it can be shown f of x is essentially this term.

This is the constant term; this is the linear term that is a quadratic term. So, if I compute the gradient and equated to 0, the gradient of this expression is given by. The linear term is given by the first term, the quadratic term is given by this this must be a plus instead of a minus. Therefore, if I solve this system I simply have v lambda v transpose, x is equal to v lambda to the power half u transpose Z . I can multiply both sides on the left by v transpose, I can multiply. So, if I multiply both sides by v transpose, v transpose v lambda v transpose x must be equal to v transpose v , lambda to the power half u transpose z , but this is I , this is I though that reduces to v u transpose. I am sorry 1 second.

That leads to, this is I , that is way also equal to I . We are left with lambda v transpose x is equal to lambda to the power half u transpose Z . now I can multiply both sides by lambda to the power inverse, lambda inverse. So, if I multiply lambda inverse lambda v transpose x is equal to lambda minus 1 lambda to the power half u transpose Z . This is equal to I , this is equal to lambda to the power minus half. You can readily see that is equal to lambda to the power minus half, I hope you can see, that may be, maybe I will write that clearly.

This. So, this is equal to, this is equal to lambda to the power minus half u transpose u transpose Z . therefore, v transpose x is equal to lambda to the power minus half u transpose Z . I again multiply both sides by v , v v transpose; x is equal to v lambda to the power minus half, lambda to the power minus half u transpose z . So, this gives it x is equal to v lambda to the power minus half u transpose Z , say that is the least square solution. Therefore, if I am able to express my H , to be equal to u lambda to the power half v transpose, v transpose. I have found u , I know lambda to the power half, I know v transpose I use v , I use lambda to the power half here and u . So, all the factors are used here. So, I can readily use the factors that I find in the SVD , and express my least square solution to be this.

Now, this are the very beautiful interpretation. So, Z is the observation vector V is given to me, u transpose is an orthogonal transformation, orthogonal transformation essentially rotates they do not elongate or shrink. So, u transpose Z is simply a rotated vector Z , then I multiplied by λ to the power minus half diagonal elements. So, that essentially scaling. So, this is rotation.

So, I am going to give a geometric feeling. This is rotation, multiplying this is scaling, and then V is again orthogonal that is again rotation. Therefore, the least square solution, is obtained by first rotating the given observation, and scaling the given observation by the diagonal matrix, which is the inverse square root of λ , and then again rotation by v . So, you get the least square solution; that is a beautiful way to be able to express the least square solution, using the method of singular value decomposition.

So, it has a beautiful geometric view as well, in addition to be able to analytically express the solution in some perform. Now look at this now, in here I do not have to solve any system. In the previous case I have to solve, either a cholesky decomposition, I had to solve an upper triangular system lower triangular system.

In the case of QR decomposition I had to solve an upper triangular system. Here I do not have to solve any system. Why, the inverse occurs only for λ to the power minus half. What is λ to the power of minus half? λ to the power minus half is equal to λ to the power half inverse. Inverse of a diagonal matrix is they are essentially inverse of the diagonal elements, inverse of the diagonal elements, there are n elements I can compute the reciprocals of each, stick them along rely of this. So, that is the only inverse I need to compute.

So, there is no cost associated with computing inverse except for n reciprocal computation. So, once u λ to the power half, and v are available, it is simply. You do not have to do any operation except rotation simple scaling, and another rotation, but I want to quickly add, to compute u λ and v , we have to solve an Eigenvalue problem. Eigenvalue problems are intrinsically more expensive. Therefore, this method could overall be very expensive, but this is a very good stable method and very often recommended as one of the alternate methods.

So, among the three methods we have seen; the cholesky, the QR and the S V D. QR and S V D relate to orthogonal transformations. Any algorithm in matrix theory that involves

orthogonal transformations, are generally more stable numerically. therefore, these methods, these two lateral methods are much preferred. The method of normal equation based on cholesky method is very good method, but its subjected to lot more numerical round of errors. So, the three methods have different strengths and weaknesses.

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ALGORITHM - SVD

- Given $H \in \mathbb{R}^{m \times n}$

STEP 1: Compute $H = U\Lambda^{1/2}V^T$

STEP 2: Compute $U^T Z$ – (rotation)

STEP 3: Compute $y = \Lambda^{-1/2}U^T Z$ – (Scaling)

STEP 4: Compute $x^* = Vy$ – (rotation)

• Cholesky –

• QR } with

• SVD }

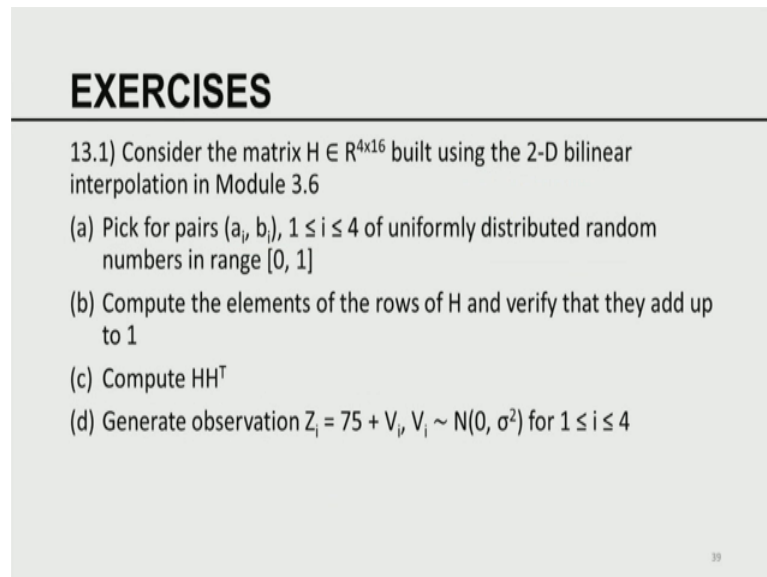
But before I go to compare I would like to summarize the S V D quickly here, H is U lambda to the power half v transpose.

That is the S V D decomposition, compute u transpose Z that is rotation I am sorry U transpose, see that is simply a rotation, I have already talked about that in the previous slide. This essentially a scaling and this is essentially another rotation. Therefore, we can very easily see the extra, is the least square solution. So, with this we have covered three methods cholesky sorry. With this we have covered three method; cholesky, QR, and S V D, these two involve orthogonal methods, orthogonal matrices. This method essentially is a variant of L u decomposition. Cholesky method is computationally not stable in the sense of numerical round off, as QR and S V D.

So, then you are trying to learn these methods, it is better to take 1 particular problem and solve it by three methods. When you when I say solve it the three methods I have given you algorithm for each of these. So, you can develop your own subroutine to do cholesky, your own subroutine for QR, your own subroutine for S V D. So, this way you can develop your own mathematical packages ground from ground up. So, that you do

not have to depend on, any built in library; such as MATLAB library or C library or Fortran library, this way you can develop mathematical software to solve data assimilation problems from ground up rather independently from, by using most of the basic algorithms.

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EXERCISES

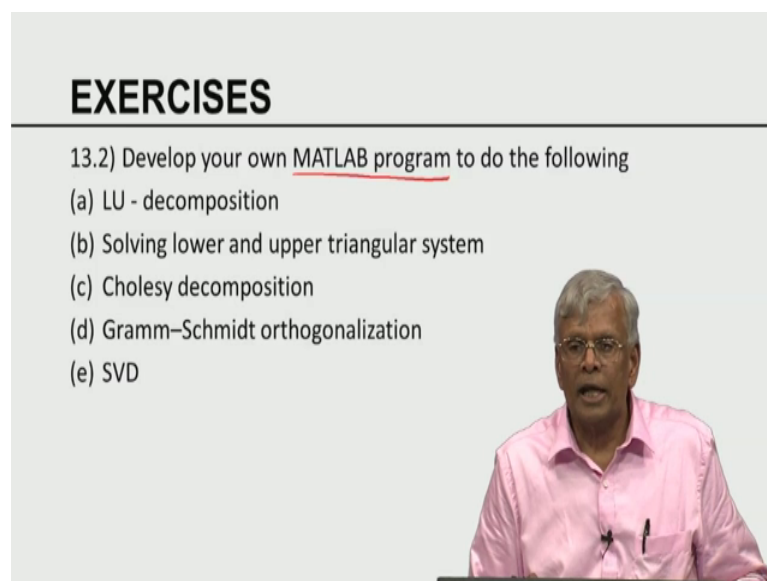
13.1) Consider the matrix $H \in \mathbb{R}^{4 \times 16}$ built using the 2-D bilinear interpolation in Module 3.6

- (a) Pick for pairs (a_i, b_i) , $1 \leq i \leq 4$ of uniformly distributed random numbers in range $[0, 1]$
- (b) Compute the elements of the rows of H and verify that they add up to 1
- (c) Compute HH^T
- (d) Generate observation $Z_i = 75 + V_i$, $V_i \sim N(0, \sigma^2)$ for $1 \leq i \leq 4$

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There are lots of exercises we have we have given. I would like to encourage the reader to work or through all these examples.

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EXERCISES

13.2) Develop your own MATLAB program to do the following

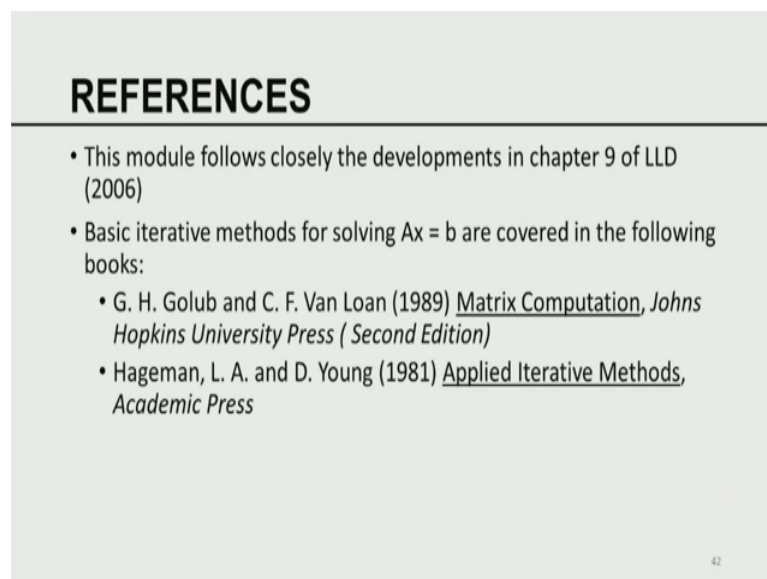
- (a) LU - decomposition
- (b) Solving lower and upper triangular system
- (c) Cholesy decomposition
- (d) Gramm-Schmidt orthogonalization
- (e) SVD

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In fact, working through these examples is a fundamental aspect of thorough understanding. I also would like you to develop your own MATLAB program that is the important thing; you can develop your own MATLAB program. You may say hey MATLAB as already has this program why do I do this, but that is an exercise. Suppose you want to go to work forever national agencies such as the meteorological forecasting agency. They may try to develop all these systems ground up independent of any existing libraries, because they would like to have a better control over everything.

So, in order to be employed, in order to be able to develop such systems, you must do an exercise in developing these programs, L u decomposition, solving lower upper triangular systems, cholesky decomposition, Gramm Schmidt method, S V D. I would like you to be able to program these methods, and compare them, and that is a very good part of the exercise.

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REFERENCES

- This module follows closely the developments in chapter 9 of LLD (2006)
- Basic iterative methods for solving $Ax = b$ are covered in the following books:
 - G. H. Golub and C. F. Van Loan (1989) Matrix Computation, Johns Hopkins University Press (Second Edition)
 - Hageman, L. A. and D. Young (1981) Applied Iterative Methods, Academic Press

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These are other examples these modules follow closely developments in chapter 9 of our book. We are not considering iterative methods. Iterative methods for solving linear systems are covered in several excellent textbook, Golub and Van Loan, as well as Hageman and Young. So, in view of time, we will not be able to cover the iterative methods. Dark methods we covered iterative methods are pursued in here. With this I believe, I have provided you a very good summary of matrix method, especially a direct methods to solve linear least square problems.

Thank you.