Matrix Solvers
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Lecture – 48
Conjugate Gradient Methods (Contd.) and Introduction to GMRES

Hi, we are looking into Conjugate Gradient Algorithm which is a class of Krylov subspace methods for symmetric a matrix. So, when you are solving x is equal to b using Krylov subspace based iterative methods if the matrix a is symmetric we have observed that few interesting properties come out. One is that the new residual vector is along that the present residual vector is along the next steps next basis of Krylov subspace at particular m level or residual vectors or orthogonal to each other. And also we have seen that the auxiliary vector p m has an a called p i has an a conjugacy that is p i dot a p j is equal to 0 if p i is not is equal to p j.

Utilizing this facts we have found out how alpha x and x r and p should be updated. And what should be the values of the updates.

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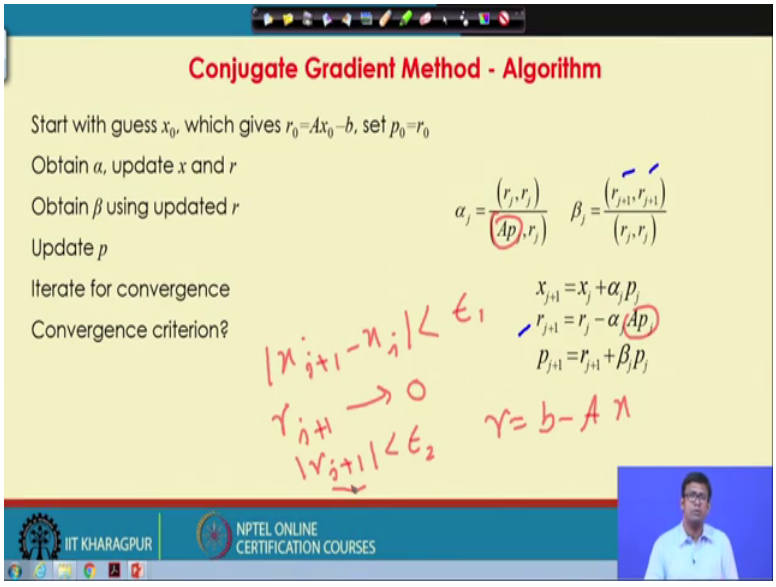

So, we summarize what we have found out the crux of that alpha and beta at any iteration stage or for any particular when you are going in Krylov subspace any particular basis of the Krylov subspace, we can write alpha and beta is r j dot alpha is r j dot r j divided by A p j dot r j and beta is r j plus 1 dot r j plus 1 divided by r j dot r j.

And r j is the residual and p is the auxiliary vector and x can be updated as the x j plus 1 is x j plus alpha j p j r j plus 1, r will be a residual will be updated as r j minus alpha j A p j p j plus 1 is equal to r j plus 1 beta j p j.

So, if we translate it is this into an algorithm all are basically vector operations vector vector products etcetera except we have to find out this A p matrix vector product which are used at couple of stages here. So, what you can do? You should start with a guess x 0 which will give us the initial guess r 0 which initial residual r 0 x 0 minus b and said the initial of auxiliary vector is same as the initial residual vector p 0 is equal to r 0 and then we will update everything update obtain alpha and update x and r which are updated based on alpha and then update beta. Once r is updated we get r j plus 1 we can calculate beta obtain b using the updated r and this is the updated r this is the updated r use the updated r to obtain b. And update p based on that.

So, start with 0 m is equal to 0, you obtain alpha 1 of t and if this is x 0 you have p 0 and r 0 everything there. So, with alpha 1 you find out x 1 is equal to x 0 plus alpha with alpha 0 rather plus alpha 0 p 0 and r 1 is equal to r 0 minus alpha 0 A p 0.

Once you found r 1, r 1 dot r 1 divided by r 0 dot r 0 you find out beta; p 1 is equal to r 1 plus beta 0 p 0 update p and then go to j is equal to 2 3 4 up to m update p and iterate for convergence. Convergence means, what should be the convergence criteria? That is what we have the idea we got from the basic iterative methods. That mod of x j plus 1 minus x j is less than some small number epsilon; say epsilon 1 or the residual r j plus 1 must tend to 0, r is equal to b minus x. Once we have solved the equation r must go to 0 or we can also check whether r j plus 1 is less than a small number epsilon another small number epsilon.

We can fit a convergence criterion based on the difference of last 2 guess values or based on the absolute value of the or norm of the residual vector r. If the residual vector is very small it should go to we will say that it has been converged and converge in that way. So, we are basically what we doing? We are basically finding out different basis of the Krylov subspace A r 0 r 0 a square r 0 this and along each basis we are updating x. So, p is because we are updating along x along p, p becomes essentially the basis of Krylov subspace.

These are orthonormal to each other also. So, p becomes basically the normal basis of Krylov subspace we can orthonormalize it easily.

So, the instead of finding out the orthonormal basis v 1 v 2 v n, we will looking into the auxiliary vector p 1 p 2 p n and they become the basis now and we can say that p 0 is equal to r 0. So, r 0 is one of the vectors which will spend the Krylov subspace and how r 1 r 2 r n we see that we will finally, with this p we are spending the Krylov subspace.

So, increasing number of m we are approaching the right solution. So, that the residual r m goes to 0. So, now, if we look into the algorithm in a more formal form.

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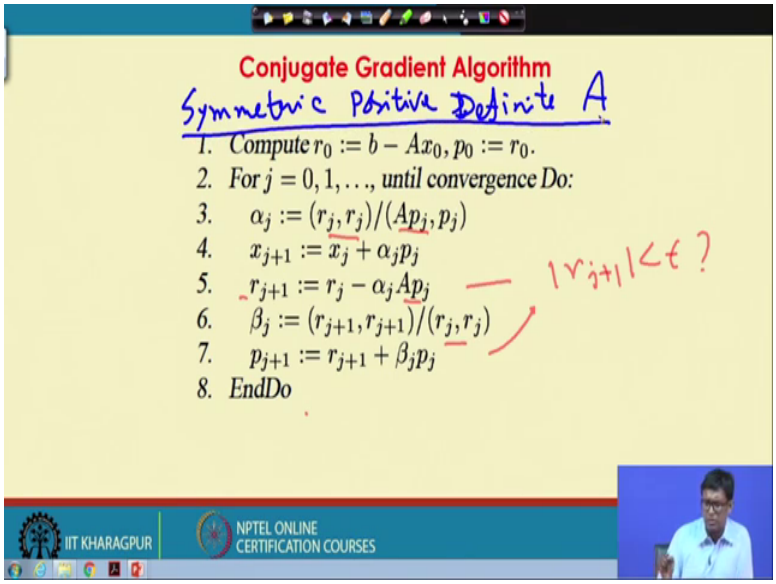

Compute r 0 is b minus A x 0 and p 0 is equal to r 0. For j is equal to 0, 1 until convergence that means, residual is. So, let us write down convergence we will can probably be checked here that mod r j plus 1 is less than epsilon you check it. Obtain alpha j is r j dot r j by A p j dot p j x j plus 1 is equal to x j plus alpha j p j; r j plus 1 is r j minus A alpha j A p j and once you obtain the r j plus 1 you already have stored r j dot r j.

This A p j, once you find this and utilize it here, so that you can avoid doing the matrix multiplication several times. You have stored r j dot r j and then r j plus 1 divided by this r j dot r j which you have stored you get beta j and p j plus 1 is r j plus beta j p j. And then you if a mod r j, so, here you check if mod r j is less than epsilon. If then EndDo,

you come out of the iteration loop say that the solution has converged else you keep on iterating it for the right solution.

This is the algorithm though the mathematical formulation deals with number of steps and manipulations using matrix algebra. The algorithm looks very simple. It is also extremely straightforward to write a computer program for this which will give us good result for and but this is always for this has to be remembered this is for symmetric positive definite, if A is not symmetric this algorithm will fail.

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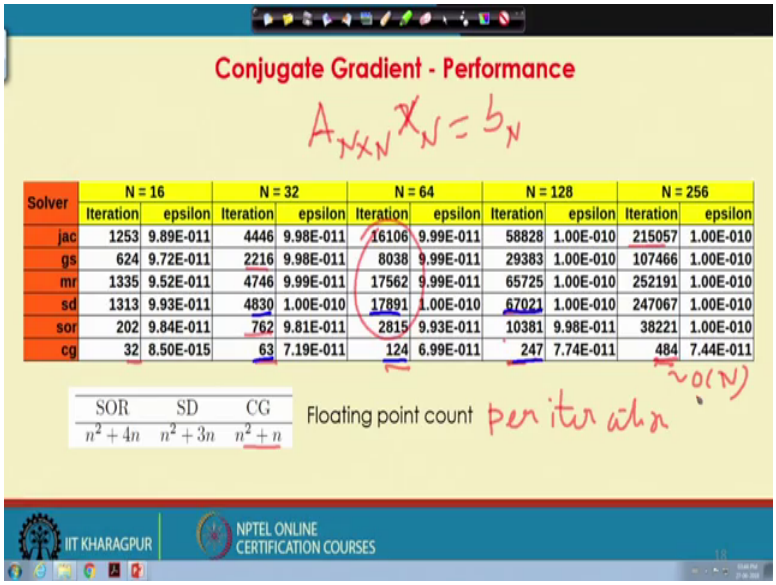

Now, let us look into the performance and which is interesting. So, there are few N into N matrix. So, we have a A N into N X N is equal to b N. We have a N into N matrix. And we started the changing the values of N from 16 to 256. So, finally, you are solving 256 into 256 equations. And the convergence criteria is kept very small 10 to the power minus 11 etcetera.

So, what we can see is that Jacobi takes 1253 iterations for this particular matrix. Gauss Seidel takes half of that, say SOR with optimum over relaxation further smaller value. However, minimum residual and steepest descent takes 1300 iterations. Conjugate gradient takes only 32 iterations and we can check this is twice N basically number of iterations.

For N is equal to 32 Jacobi, Gauss Seidel MR etcetera takes around Jacobi MR SD they are comparable takes around 400 4800 iterations, Gauss Seidel takes 2200, SOR with optimum over relaxation takes 760. And conjugate gradient takes 63 which is almost twice of N. And these things continue that the number of iterations in conjugate gradient is much smaller than the number of iteration in any i other of them.

So, it is for symmetric positive definite matrixes conjugate gradient, it is a very first solver. When Jacobi is doing 16000 iteration or 215057 iterations for a better convergence conjugate gradient is only doing 484 iterations. Another interesting thing we can see that if we compare between steepest descent or MR with conjugate gradient steepest descent with conjugate gradients steepest descent with conjugate gradient. The number of iterations are almost square root of that. So, the convergence rate is almost square for conjugate gradient compared to the steepest descent algorithm or even is very high compared to any other algorithm.

So, for symmetric a matrix this is one of the fastest solver till we know and the number of iterations are of the order of number of rows in the matrix. If we keep the convergence criteria smaller all these numbers will also fall down. However, this is very important aspect. Also there is a one matrix vector product and few vector products. So, if we compare the number of floating point count per iteration rather floating point count part we can see that it is of n square plus n which is actually less than successive over relaxation correlation or steepest descent.

So, conjugate gradient is a very first solver as well as the number of iterations number of floating point operations per iteration is small. So, number of iteration is small number of operations per iteration is small. So, in a as a whole it will give us a very first solver and extremely first solver and the number of iterations are usually of the order of n. Why is it first? For that we will quickly look into the convergence criteria of conjugate gradient method.

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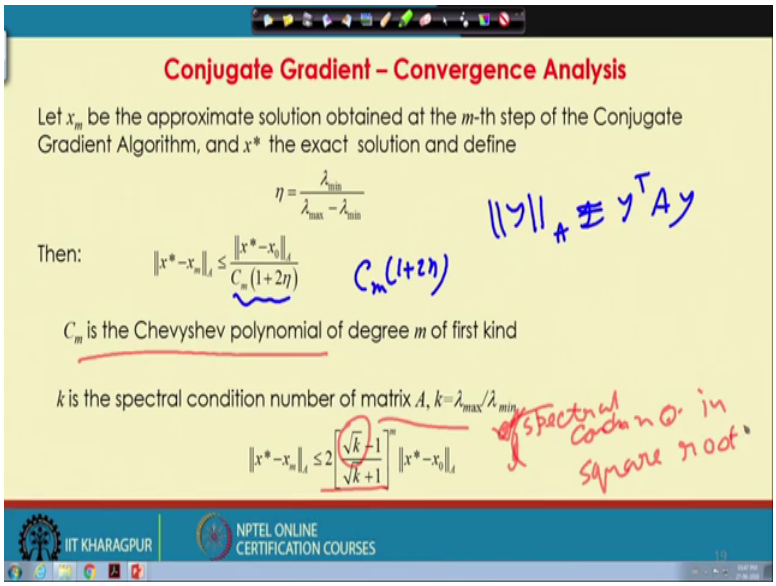

Let x m be the approximate solution and obtained at the mth step of conjugate gradient algorithm and x star be the approximate solution and we define eta is lambda mean by lambda max minus lambda mean. Then x star minus x m it is A norm. So, what is a norm; y's A norm is equal to y transpose A y.

So, x star minus x m's A norm is equal to x star minus x 0 x star is the exact solution x m is they mth iteration solution A norm by polynomial of 1 plus 2 eta and this polynomial C m. So, C m is a function of 1 plus 2 eta, it is not C m into 1 plus 2 eta C m is a function of 1 plus 2 eta.

This polynomial C m is known as the Chevyshev polynomial of degree m of first kind, not going into detail that is the polynomial of 1 plus 2 m. If you can simplify this that k being the spectral condition number lambda of matrix A, lambda max by lambda mean; x m by x star minus x m is of A norm is less than equal to twice root of spectral condition number minus 1 by root of spectral condition number plus 1 to the power m x star minus x 0 by A.

So, convergence is a function of I am sorry convergence remains a function of spect root of spectral condition number. And as small is this number it will converge first. Now, earlier for steepest descent we have seen that convergence is a function of spectral condition number. Spectral condition number is a number greater than 1 is the relation between lambda is lambda max my lambda means. So, it is always greater than 1.

Root of spectral condition number must be smaller than the spectral condition number. So, this particular coefficient which is being multiplied with x star minus x 0 to be see the mth order error must be smaller number than the coefficient which was multiplied with the same norm for steepest descent algorithm and how smaller? This is root of spectral condition number or a spectral condition number in square root.

So, in a way we can get the idea that the rate of convergence or the convergence factor will be rather rate of convergence or the convergence vector will be in a sense square root of that. Therefore, the number of iterations will be also square root of the number of iterations first steepest descent method. And that is why conjugated it is a very first solver because it is convergence depends on the root of the spectral condition number. And the number of iterations are almost square or of the order of square root of number iteration needed for spec steepest descent type of algorithm.

So, we get an algorithm which is robust which can handle any A which is symmetric positive definite and is a very first solver. What is the advantage in conjugate gradient method considering the fact that it is a Krylov subspace based method because Krylov subspace based methods need inversion of the Heisenberg matrix h m of a upper triangular matrix with one sub diagonal need inversion of that matrix. And the Lanczos algorithm needs a TDMA type of a method to solve this particular equation where h m is replaced by a tri diagonal matrix T m.

Inverting even or even applying like a T m inverse or h m inverse doing these things even if T m is a tri diagonal matrix. They are expensive then this particular method because it uses it does not use recursive method it does not use matrix inversion. It uses a method through which the auxiliary vectors are advanced utilizing the factor that they are a conjugate. And the residual vectors are obtained at next level assuming that one residual vector is orthogonal to all the previous residual vectors.

So, using this properties we can formulate linear relationships for advancing residual vector as well as the auxiliary vector and then we can very easily advance the x m plus 1 to the or the it or the solution x to the next iteration level and it converges very first due to the proper due to the as the function is convergence is a function of root of spectral condition number.

So, considering all this conjugate gradient becomes a very first solver and though it is a solver of that of Krylov subspace methods which belongs to Krylov subspace method. However, it does not explicitly find out h m inverse or solve T m y is equal to beta e 1 rather it uses some properties like A conjugacy of auxiliary vector and r'm's orthogonal to each other. And devices are faster way to solve the Krylov subspace problem.

Now, this is a very good method. However, this is restricted only for symmetric matrices. And now our question will be what will happen for a general sparse matrix which is not symmetric. So, what are the first methods based on Krylov space for that? And for that we will start looking into oblique projection methods. We will start a discussion very soon on oblique projection methods. And after that we will look into our different type of Krylov subspace method once we finish some discussion on oblique projection method different type of a Krylov subspace methods.

So, let us quickly look into one the new the generalize method for any matrix we will not restrict ourselves to positive to symmetric positive definite matrix for any matrix which is called a GMRES method or Generalized Minimum Residual method and it is an oblique projection method.

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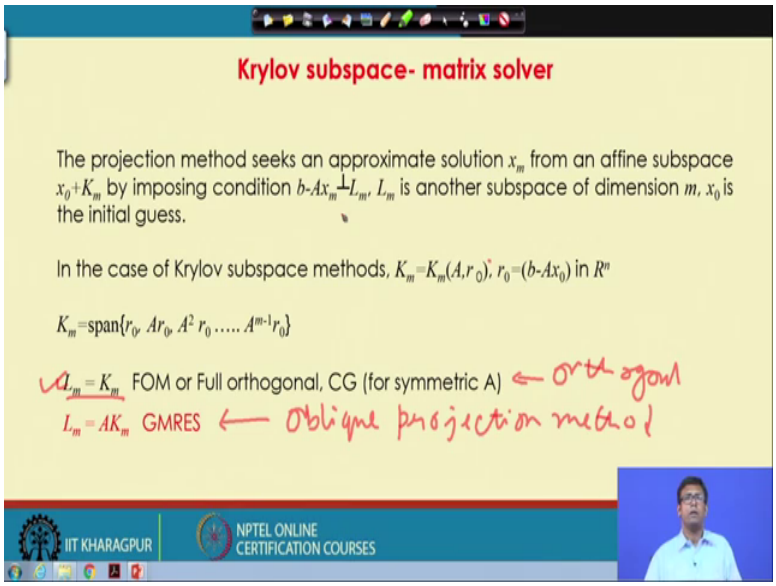

So, Krylov subspace matrix solvers this is a projection method that seeks an approximate solution x m from an affine subspace x 0 plus K m by imposing condition that b minus x m or the residual is orthogonal to L m, L m is another subspace of dimension m x, 0 is

initial guess. In case of Krylov subspace methods this space K m is K m of A and r 0, r 0 is the initial residual. Where k m is span by r 0 A r 0 A square r 0 A to the power m minus 1 r 0.

And till now we have looked into orthogonal methods, where L m is equal to K m which are called the orthogonal methods. And now we will look into GMRES which is an oblique method oblique projection method that is L m is not is equal to K m, b minus x m is not orthogonal to K m rather it is orthogonal to A K m.

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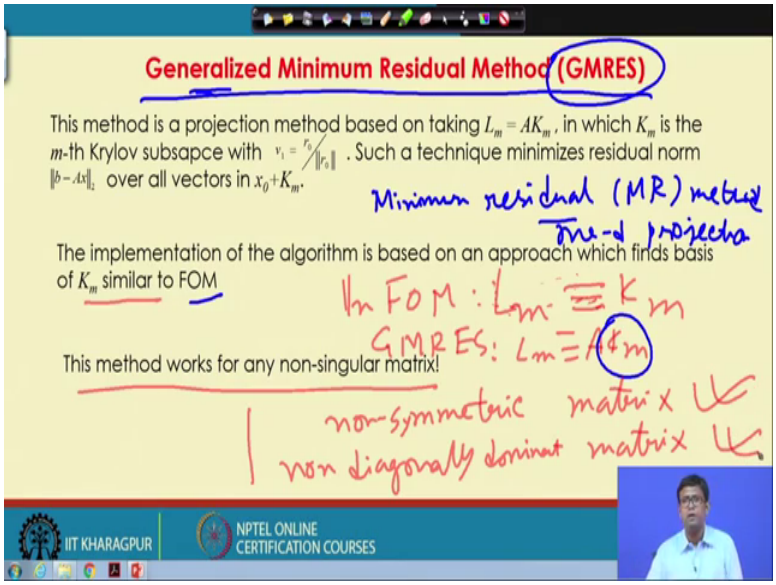

So, let us see what do you we mean by that. The idea of generalized projection method generalized minimum residual method is this method is a projection method based on taking L m is equal to A K m in which K m is the mth Krylov subspace starting with the first basis of Krylov that Krylov subspace b 1 is r 0 by mod of r 0 first orthogonal unit based orthonormal basis of that. And through this technique, so, starting with v 1 is equal to r 0 by mod r 0 we will find out one basis for K m and rather we will later we will find out other orthonormal basis for K m and find out the K m and then we will get L m is equal to A K m. And propose a general projection method and this method is called Generalized Minimum Residual method or GMRES.

This technique minimizes residual norm of b minus A x over all vectors x 0 plus K m. So, instead of minimizing x transpose A x minus x transpose b, what we are doing for conjugate gradient method? Now we are minimizing b minus x. And if we try to relate

this with the general projection methods we will see that this minimization happened in Minimum Residual or MR method. Now, M R was a one d projection method. When we try to generalize MR, we get the generalized minimum residual the generalized minimum residual method, GMRES. From one d to multi dimensional general projection method if we go we get GMRES.

The implementation of this algorithm is based on an approach which finds the basis of K m first which is similar to FOM, Full Orthogonal Method. In full orthogonal method K m was is equal to L m. In FOM, full orthogonal method K m was same as L m. Here, we will find out K m exactly the way same way or rather I will write it opposite. In full orthogonal method L m is same as K m. Here, we will find out K m which is similar to FOM. However, in GMRES we will find out L m which is not K m rather is equal to A K m, but the but how will we find out K m? That will be same as FOM.

So, all the Heisenberg matrix all the basis of the Krylov subspace everything will be exactly same how we have found out our Krylov subspace and the Heiseberg matrix basis V m and H m in full orthogonal method all will be exactly same. Now, once we have found out K m we will do something else. And the best thing about this method is that this method works for any nonsingular matrix.

So, we are now not limited to symmetric matrix for non symmetric matrix, for non-diagonally dominant matrix, for all these matrices. This method works for all these matrices. If you remember MR, minimum residual method was also effective for all this matrices. However, that was dependent on that is typically slow method because convergence rate is dependent on the spectral condition number of A transpose A, where the spectral condition number usually becomes much higher than the spectral condition number of A.

So, it is a minimum residual method was a slower method considering other methods of that particular class. However, this GMRES is will be faster than minimum residual method, but as minimum residual method it can work for any type of nonsingular matrix.

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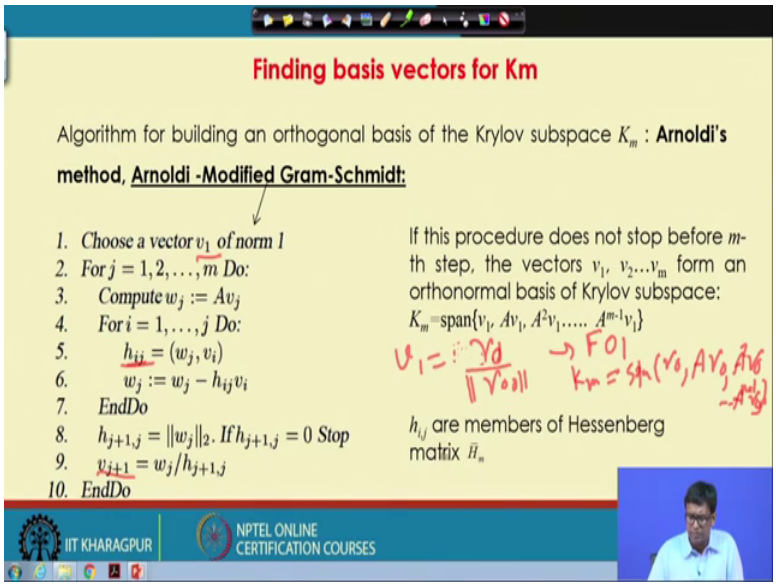

So, finding basis for K m is same as what we have done in Arnoldi's method. Arnoldi modified GYram-Schimdt method which is the say which will be continued to full orthogonal method later that you start with a create a vector of norm 1 and then you find out w is equal to find out h i j which are the parts of the Heisenberg matrix, h i j. And you find out v j which are the basis vectors for the orthonormal basis of Krylov subspace.

And you start with v 1 is equal to mod r 0 sorry v 1 is equal to r 0 by mod r 0, we will follow full orthogonal method where, the Krylov subspace is span of r 0 A r 0 A square r 0 so on A to the power m minus 1 r 0.

So, you start with the initial guess to be initial first vector the v 1 to be the initial residual normal in normalized form and you get the basis vectors of the Krylov space you need for solving x is equal to b. And h i j are the members of the Heisenberg matrix h bar m.

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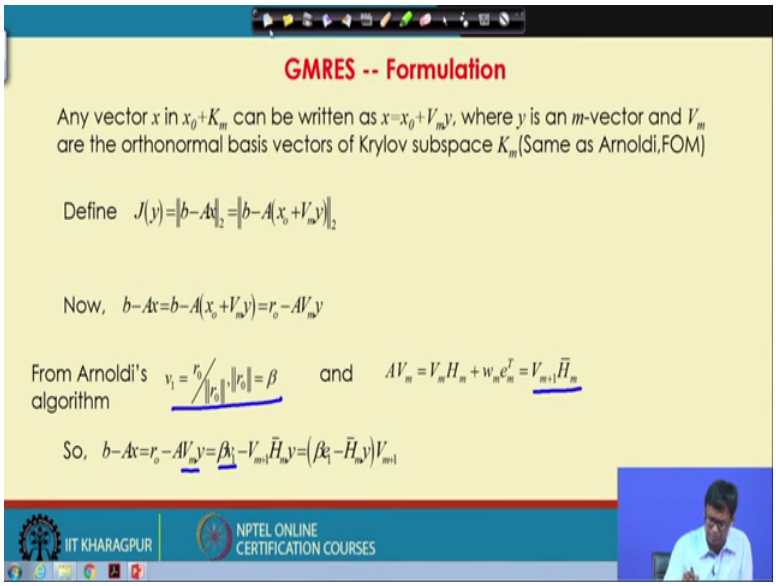

So, we will use H bar m and H m H bar m we will use the H bar m and H m in some cases. From H bar m if we remove the last row it becomes the another Heisenberg matrix, so which is H m. Any vector x in x 0 plus K m can be written as x is equal to x 0 plus V m y, where y is a m vector and V m are the orthonormal basis functions of Krylov space. And this is same as Arnoldi or FOM method.

Now, if we define J y as b minus A x l 2 norm or if I substitute x is equal to b minus x 0 plus V y's l 2 norm. Now, b minus A x is equal to b minus A x 0 plus V y m which is r 0 minus A V y m. From Arnoldi's algorithm, we have seen that v 1 is r 0 by mod of r 0 and mod of r 0 is given as beta.

So, we can write and we have also seen from Arnoldi's algorithm V m is V m H m w m e m transpose which is V m plus 1 into H m, but the full Heisenberg matrix.

So, if we substitute this here we can write b minus A x is r 0 minus A V m y and A V m right this A V m can be substituted as V m plus 1 H m bar. And r 0 can be written as beta v 1 which comes from here r 0 is equal to beta v 1 which is e 1 becomes the first unit vector 1 0 0 this is b e beta e 1 minus H m bar y V m plus 1; V m plus 1 is the basis of the orthonormal basis of Krylov subspace. So, we got an expression for b minus A x.

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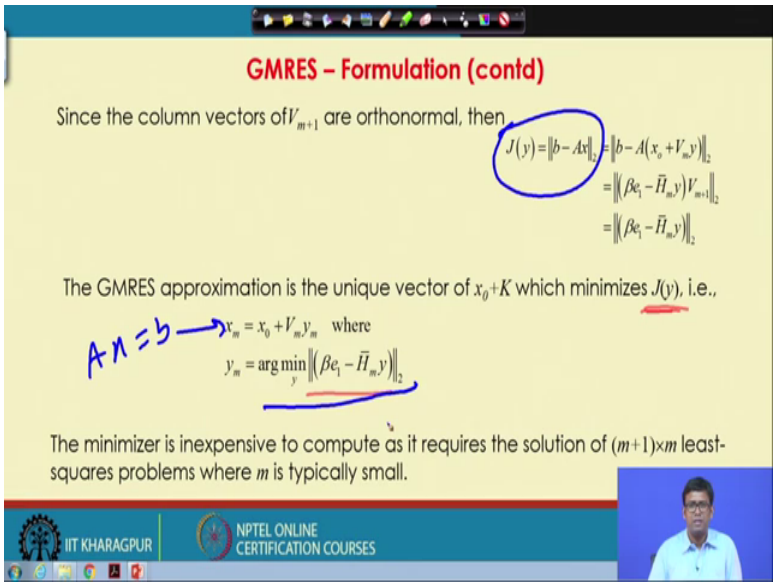

Since, the column vectors of V m plus 1 are orthonormal, we can write J y is b minus A x second norm is b minus A x 0 plus V m y second norm and beta e 1 minus H m bar y V m plus 1 second norm. There a relation we exactly got beforehand that beta b minus A x is beta e 1 V m minus 1.

So, since V m plus 1 has orthonormal columns this is beta e 1 minus H m bar y. Now, the GMRES approximation is finding out the unique vector x 0 plus K which will minimize J y that is x m will be x 0 plus V m y m, where y m is the value of y for which beta e 1 minus H m bar y is minimized minimal. And this is the idea of the GMRES method that you find out minimum of minima of J y which is beta e 1 minus H m bar y and you start that J y is equal to beta minus A x 2.

Find out the minima of that which is finding minima of beta e 1 minus H m bar y. And with this y m, V m you have already found out using Arnoldi or FOM type of method. With this y m you find out x m is equal to x 0 plus V m y m which is the solution, this x m is the solution of A x is equal to b approximate solution of A x is equal to b.

Now, this is instead of solving x is equal to b what you have to do is you have to find out minima of beta e 1 minus H bar m y. However, the minimizer is inexpensive to compute as it requires solution of m plus 1 into m least square problem where the value of m is typically small. And with this idea we will move further and we will see how we can for propose an algorithm for GMRES and what are the convergence criteria for that.

Thank you.