Computational Fluid Dynamics

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Lecture No. # 29

Gradient Search Methods (Contd.)

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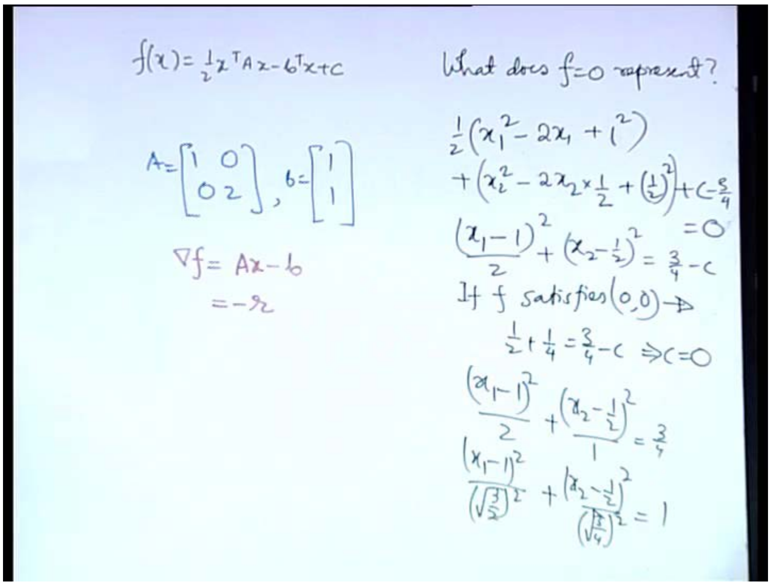

In our previous lecture, we introduced the concept of the gradient search based techniques, and we tried to illustrate one of those methods with the help of an example. So, we will continue with that example. So, in the example, our objective was to solve the system of equation A x equal to b, where A is given by this matrix, and b is given by this vector. So, what we first did is, we first obtain f (x), which is half of x transpose A x minus b transpose x plus C.

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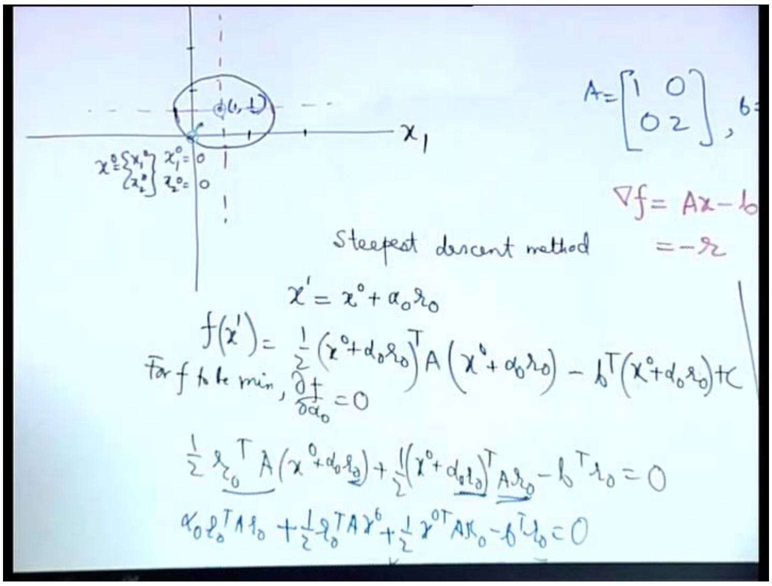

And we plotted f in the x 1, x 2 plane, by setting C equal to 0, we satisfied that f will pass the curve representing f will pass through (0,0). And so, it represented an ellipse with semi major axis length root 3 by 2, and semi minor axis length root 3 by 4. Now, the method that we are going to describe on the basis of this example is known as steepest descent method. In this particular method, what we will try to do? We will try to move along the gradient of the function f, which represents the steepest rate of change or maximum rate of change of the function f, the direction of the maximum rate of change of the function f.

We start with the initial guess, let us say this initial guess is x 1 0 equal to 0, and x 2 0 equal to 0 as an example. Now, in the next step, what we will do? We will update this x. So, we will come up with a new x, we will start from the x 0 point, which is (0,0) move in a direction of gradient of f and stop somewhere, where the function is a minimum, and that will be the new iterate, that will be the new value of x. So, x 1, these are x 0; so, x 0 means, the vector x 1 0 and x 2 0. Now, x 1, x 1 is a point in this plane, x 0 is another point, and the direction from x 0 to x 1 is along the gradient of f; gradient of f an r have the same direction, but of course, opposite sense, but it does not matter, because the direction is the same.

So, we can say x 1 is equal to x 0 plus alpha 0 into r 0. What is r 0? R 0 is gradient of f at x 0 that is minus r 0. So, we have to find out. So, what it says? X 1 minus x 0 is a vector, which is oriented along r 0, and which has the magnitude, which is governed by the coefficient alpha 0. So, you have to find out, what is alpha 0? So, what does alpha 0 tell? What does r 0 tell? R 0 tells, what is the direction in which you are moving that is gradient of f at x 0; how much you are going to move along that direction that will be given by alpha 0. So, f of x 1 is half x 0 plus alpha 0 r 0 transpose A… minus b transpose x 0 plus alpha 0 r 0 plus C.

For f to be minimum, you must have del f del alpha 0 equal to 0. So, let us differentiate this with respect to alpha 0. So, we have half of r 0 transpose A x 0 plus alpha 0 r 0 plus half of x 0 plus alpha 0 r 0 transpose A r 0 minus b transpose r 0 equal to 0. So, if you take alpha 0 common, here there are two terms, which contain each contains half of r 0 transpose A r 0 combined with alpha 0. If you take alpha 0 common, it becomes r 0 transpose A r 0 plus half r 0 transpose A x 0 plus half x 0 transpose A r 0 minus b transpose r 0 equal to 0.

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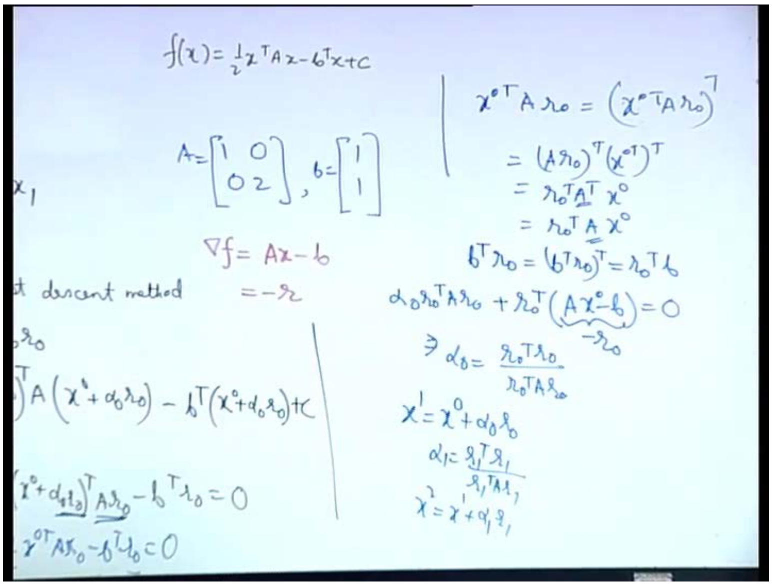

Now, using a similar manipulation, what we have done earlier also; you can show x 0 transpose A r 0 is equal to x 0 transpose A r 0 the transpose of that, because it is scalar, that is equal to A r 0 transpose into x 0 transpose transpose is equal to r 0 transpose A transpose x 0, and that is equal to r 0 transpose A x 0, because A transpose is equal to A, we are dealing with a symmetric matrix A transpose and A are the same. So, the second term and the third term combine together becomes r 0 transpose A x 0. And the final term b transpose r 0 is equal to b transpose r 0 transpose is equal to r 0 transpose b. So, if you combine all this, what you get is alpha 0 r 0 transpose A r 0 plus r 0 transpose A x 0 minus b is equal to 0; what is A x 0 minus b that is equal to minus r 0, because A x minus b is r minus r. So, this is minus r 0 therefore, alpha 0 is r 0 transpose r 0 by r 0 transpose A r 0.

So, with this, we can say that the new x - x 1 is equal to x 0 plus alpha 0 r 0. So, you move up to certain x, and that is the new x - x 1, and then you change your direction. Similarly, when you go on calculating x 2, the subsequent x, your alpha 1 will be r 1 transpose r 1 by r 1 transpose A r 1 and x 2 is equal to x 1 plus alpha 1 r 1. In this way, you go on having new choices of the point, till you come to the solution, so till you hit the bull's eye. So, in the first step, you move along the direction r 0; in the second step you move along the direction r 1; interestingly, there is a very important relationship between these two subsequent directions, direction of r 0 and direction of r 1.

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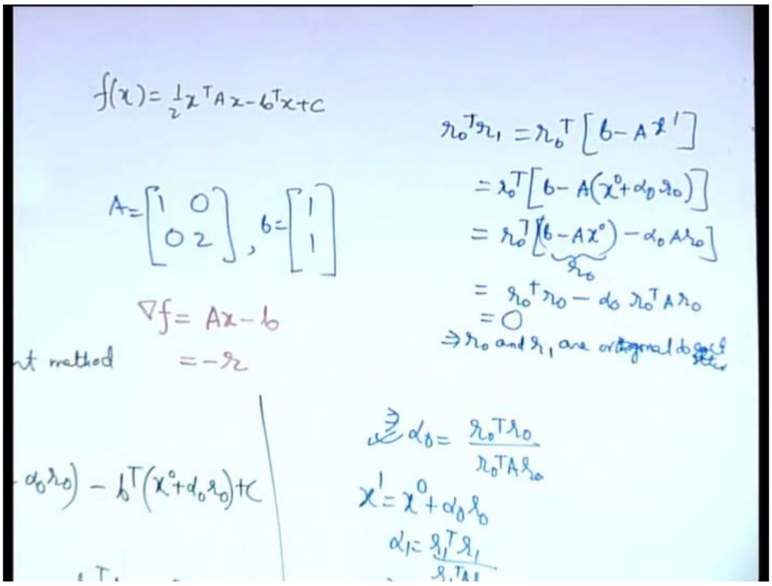

To understand that, let us calculate r 0 transpose r 1. So, r 0 transpose r 1 is b minus A x 1, because r is b minus A x. So, r 1 is b minus A x 1; in place of x 1, we can write x 0 plus alpha 0 r 0. So, r 0 transpose b minus A x 0 minus alpha 0 A r 0; what is b minus A x 0 that is equal to r 0. So, this is equal to r 0 transpose r 0 minus alpha 0 r 0 transpose A r 0; remember alpha 0 is the scalar. So, by using this relationship, alpha 0 equal to r 0 transpose r 0 by r 0 transpose A r 0, this becomes equal to 0. So, r 0 transpose r 0 equal to alpha 0 into r 0 transpose A r 0.

So, what does it show? R 0 transpose r 1 is 0 that means, if you multiply the elements of r 0 with the corresponding elements of r 1, both are vectors, you get the result 0; that means, just like physical vectors, it it is like a extension of the dot product, it is a sort of a inner product,, but if you consider it from simple conceptual considerations, it is just like a dot product, where you have that elements of r 0 multiplied with the corresponding elements of r 1, and the result is 0. So, that means, r 0 and r 1 are orthogonal to each other..

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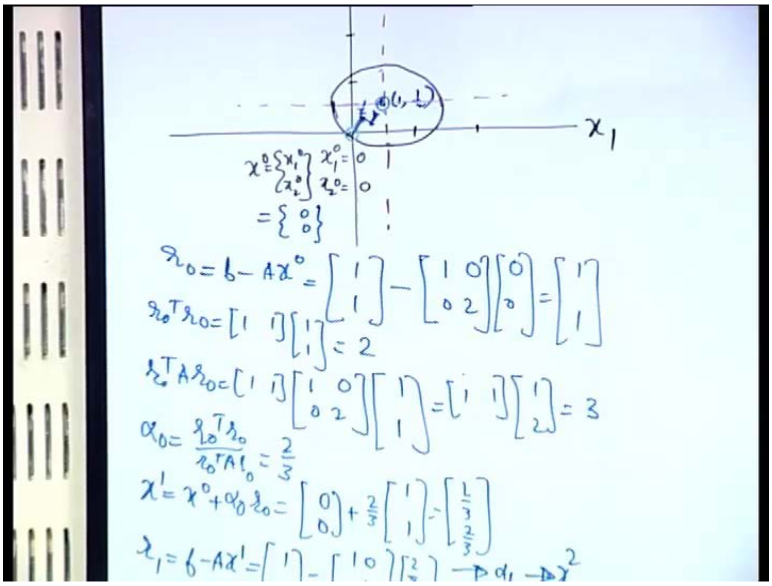

So, what we learn from this? First we moved along the direction of r 0, next we moved along the direction of r 1, which is x 2 minus x 1, and that direction will be perpendicular to this direction. In this way, we will be moving in mutually perpendicular directions in several steps may be depending on how many steps necessary, till you reach the solution. So, to understand how do we reach the solution using this steepest descent method, let us work out 1 or 2 steps may be, and the remaining steps you can complete. So, first step, what you have to calculate? You have to calculate alpha 0 that means, you have to calculate r 0 and r 0 transpose r 0 into and r 0 transpose into A into r 0. So, your x 0 is known, that is 0 0. So, what is r 0? B minus A x 0. So, that is equal to 1 1 minus… That is 1 1. So, r 0 transpose r 0 is equal to 1 1 into 1 1. So, that is 2. Then r 0 transpose A r 0;

A is 1 0 0 2 into r 0… So, 1 then it becomes 3. So, what is alpha 0? R 0 transpose r 0 by r 0 transpose A r 0. So, that is 2 by 3. What is x 1 - is equal to x 0 plus alpha 0 r 0, that is 0 0 plus 2 by 3 into r 0 is 1 1, so 2 by 3 2 by 3.

Then you can calculate, what would be the next calculation? What is r 1? So, r 1 is b minus A x 1; so, 1 1 minus 1 0 0 2 into two-third two-third. Let us not go into again these lengthy calculations, because we have by this time understood that what are the sequential steps? So, once you calculate r 1, you can calculate alpha 1, and then you can calculate x 2 by using this formula. In this way, you can calculate then alpha 2 and then x 3 and so on; till you find that you reach the solution; that means, when do you find that you reached the solution, your residual becomes 0, that is when you reach the solution.

So, as we can see through this example that it requires a substantial number of steps, even for such a simple equation, it requires a substantial number of steps to start with the initial guess point, and to come to the final solution. This may be further improved, and improvement of this aspect is considered in a method, which is also a a sub class of the gradient search based methods that is known as conjugant gradient method. So, let us look into the conjugate gradient method; and we will follow the method by using the same example that we have considered so far.

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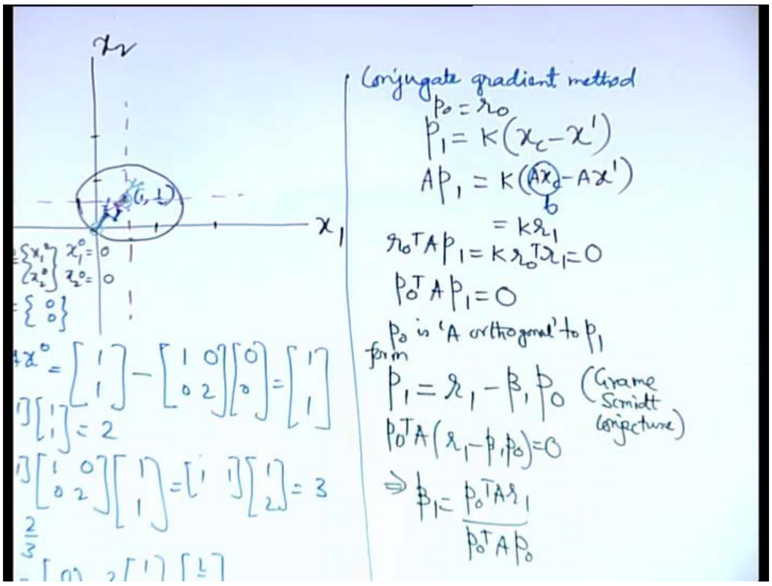

So, conjugate gradient method. So, in this method, what is done? First you calculate up to x 1 that is fine; then you try to make a modification, what modification? See, what we do? We first calculate x 1, and then we see that it requires a lengthy number of steps to reach the final solution. So, then somebody, who is very greedy wants to get a solution in one step that is, wants to get to the solution from the point x 1 directly. So, let us say this point is called as x C, which is the centre of this ellipse, which is a solution; reaching this point means, reaching the solution. So, in one step, if you want to move from x 1 to x C, so what you do is you do not go through all these steps in one step, you want to reach this solution; then what is the direction in which you move? You move in a direction, which is directed from x 1 to x C.

So, you move along a direction given by say t 1, which is a new variable, which is K into x C minus x 1, where K is just a scalar, because how much you have to move is something which has to be determined, but at least the direction is known from x 1 to x C. So, position vector of the second point minus position vector of the first point, because you introduce a new variable p 1, and you intend to move along that direction, you also have something which is p 0, and which you call same as r 0. So, p 0 is same as r 0, because for the initial direction, you do not have any difference in terms of the direction, in which you move for the steepest descent method, but from the subsequent steps, you try to change your direction. So, you have p 0 equal to r 0, p 1 equal to K into x C minus x 1.

Now, you can write a p 1 is equal to K Ax C minus A x 1; why you write it in this way is because you can then write it in terms of the residual. What is Ax C? Ax C equal to b, because x C is the correct solution. So, Ax C minus A x 1 is b minus A x 1, which is equal to r 1. So, this is K r 1. You know that r 0 transpose r 1 is equal to 0, which we have just proved. So, if you multiply both sides by r 0 transpose, then it will become 0. So, r 0 transpose Ap 1 is equal Kr 0 transpose r 1, which is equal to 0; and r 0 is nothing but equal to p 0. So, we can write p 0 transpose A p 1 that is equal to 0. So, p 0 transpose p 1 is not 0, but p 0 transpose A p 1 is 0. So, this is in linear algebra terminology is called as p 0 is A orthogonal to p 1; just a name.

Now, despite having a relationship between p 0 and p 1, this alone does not give you any clue of what is p 1, because that is essentially, your interest, that what is that next direction in which you are interested to move; once you reach x 1, from x 1 in what direction you are interested to move. So, you have to know, what is p 1? And at the most, what you have in your hand? You have r 1 as one direction, and p 0 as another direction, which is same as r 0. So, you form p 1 as a linear combination of r 0 and r 1, and try to satisfy this relationship. So, you form p 1 as r 1 minus beta 1 p 0. So, the whole purpose is that you are going to have a new direction; this new direction you can form by taking help of some known direction; known directions till now r 0 and r 1; r 0 is same as p 0. So, you make it as a linear combination of these two, and this is known as Grame Scmidt conjecture. So, then p 0 transpose A into r 1 minus beta 1 p 0 is equal to 0. So, you have beta 1 as p 0 transpose A r 1 by p 0 transpose A p 0.

So, if you know beta 1, then using beta 1, you can find out what is p 1, but the next thing is that you know that therefore, the direction in which you want to move, that is p 1, but how much that the next, you have to find out.

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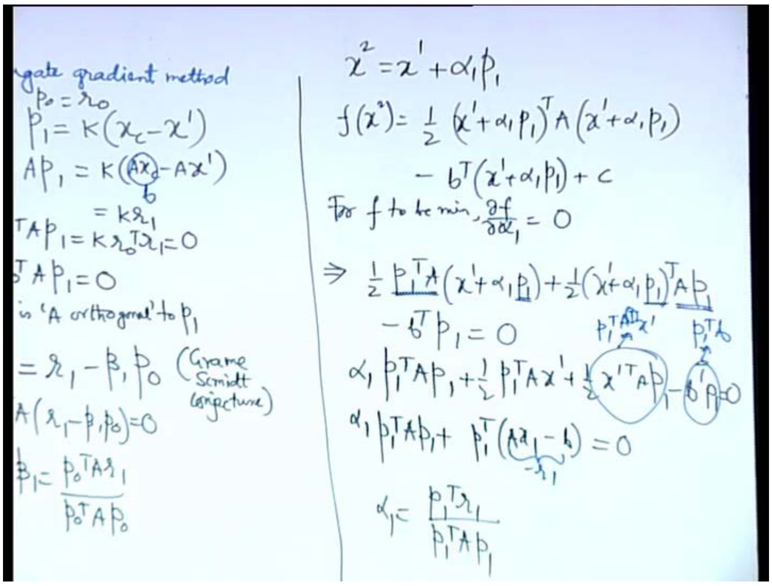

So, next you have to find out that what is the next point x 2? X 2 is equal to x 1 plus alpha 1 into p 1. See, here lies the difference between the steepest descent and the conjugate gradient method. In the steepest descent method, it was alpha 1 r 1. So, you moved along the direction of r 1. Now, you are not moving the direction r 1, but a different direction p 1 with a hope of reaching the point, the target, the solution directly in one step. So, the question will remain that what is this alpha 1? Again the basic principle is the same; alpha 1 should be such that f should be a minimum.

So, f at x 2 is equal to half of x 1 plus alpha 1 p 1 transpose A x 1 plus alpha 1 p 1 minus b transpose x 1 plus alpha 1 p 1 plus C. Just substitute in place of x as x 2, which is x 1 plus alpha 1 p 1. So, for f to be minimum, del f del x 2 should be equal to sorry del f del alpha 1 could be equal to 0. So, what we get from here? Half of p 1 transpose A x 1 plus alpha 1 p 1 plus half of x 1 plus alpha 1 p 1 transpose A p 1 minus b transpose p 1 equal to 0.

So, we can now simplify, you can see that first you have with alpha 1 p 1 transpose A p 1, half of that; and then again another p 1 transpose A p 1, half of that. So, alpha 1 into p 1 transpose A p 1 plus half p 1 transpose A x 1 plus half x 1 transpose A p 1 minus b transpose p 1 equal to 0. So, alpha 1 p 1 transpose A p 1 plus… Now, you can reorganize these terms as we did earlier, you can take a transpose of this. So, if you take a transpose of this, it will become p 1 transpose A transpose x 1, and A transpose is same as A. So, plus this will become therefore, half p 1 transpose A x 1, this another p 1 transpose A x 1. So, total is p 1 transpose A x 1 from this term, and the last term b transpose p 1 is same as b transpose p 1 transpose. So, p 1 transpose b. So, p 1 transpose A x 1 minus b that is equal to 0, A x 1 minus b is minus r 1. So, the formula for alpha 1 that we get here is p 1 transpose r 1 by p 1 transpose A p 1. How to implement this? In practice, let us follow the previous example, using which we will try to illustrate.

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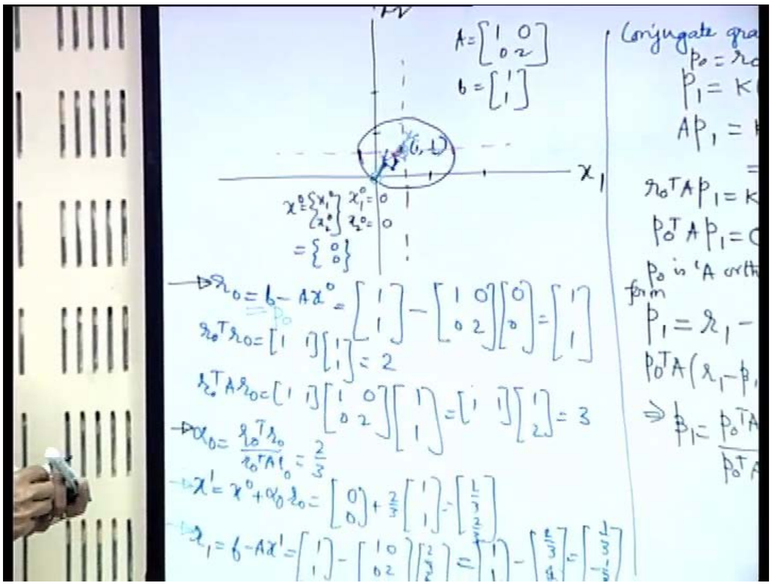

So, the same example, where we have A is equal to 1 0 0 2, and b is equal to 1 1 you have to find out the value of x. So, remember that the first few steps of the conjugate gradient method are same as the first few steps of the steepest descent method, up to which steps first calculation of r 0, which is already there; then alpha 0, and x 1 is equal to x 0 into alpha 0 r 0, and r 1 b minus A x 1. So, we will require r 1 and r 0, therefore, let us complete the calculation for r 1 before we proceed further. So, r 1 is b minus A x 1, so, 1 1 minus 2 3 and 4 3. So, what will be r 1 one-third and minus one-third.

So, up to these steps, we also had to calculate in the steepest descent method. Now, in the conjugant gradient method, the subsequent steps will require what? Next you will require the calculation of p 1; for that you need to calculate beta 1. So, let us calculate, what is beta 1 remember that r 0 and p 0 are the same. So, r 0 this is equal to p 0.

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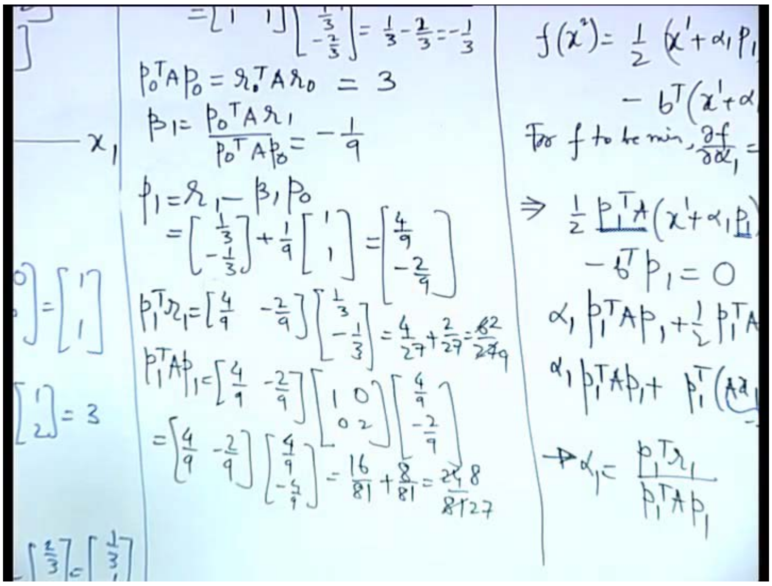

So, next let us calculate, what is beta 1? To do that, what we need to calculate? Numerator p 0 transpose A r 1 p 0 transpose A r 1, this is equal to 1 1, this is p 0 A r 1 one-third minus one-third, this is one-third minus two-third. So, this becomes one-third minus two-third minus one-third. Then denominator in the formula for beta 1 is p 0 transpose A p 0. So, p 0 transpose A p 0, we have already calculated it in the steepest descent method, because p 0 transpose p 0, A p 0 is same as r 0 transpose A r 0, because p 0 and r 0 are the same. So, let us not just waste any time for calculating it, we have already calculated it. So, this is same as r 0 transpose A r 0; so, for that we have the result already as 3. So, beta 1 is equal to p 0 transpose A r 1 by p 0 transpose A p 0 is equal to minus 1 by 9.

So, that will lead to the calculation of p 1; p 1 is equal to r 1 minus beta 1 p 0. So, r 1 is one-third minus one-third minus beta 1 plus 1 by 9, p 0 is same as r 0, that is 1 1. So, this becomes one-third plus 1 by 9, so 3 plus 1 - 4 by 9, and minus one-third plus 1 by 9 minus 3 plus 1 minus 2 by 9. So, once you have calculated p 1, what what you next should calculate alpha 1. So, for calculation of alpha 1, you require in the numerator, so this is the formula for alpha 1, this is the formula for alpha 1; in this particular formula, you require p 1 transpose r 1, and p 1 transpose A p 1, so p 1 transpose r 1 is equal to…

P 1 transpose r 1; r 1 is one-third minus one-third. So, 4 by 9 into 1 by 3, that is 4 by 2 into 7 minus then sorry plus 2 by 9 into 1 by 3 plus 2 by 27, that is 6 by 27, that is 2 by 9; p 1 transpose A p 1, so 4 by 9 minus 2 by 9 A - 1 0 0 2 and p - 1 4 by 9 minus 2 by 9.

This will become 4 by 9 and minus 4 by 9, 4 into 4 - 16 by 81 plus 4 into 2 - 8 by 81 24 by 81 8 by 27. So, next we can calculate, what is alpha 1?

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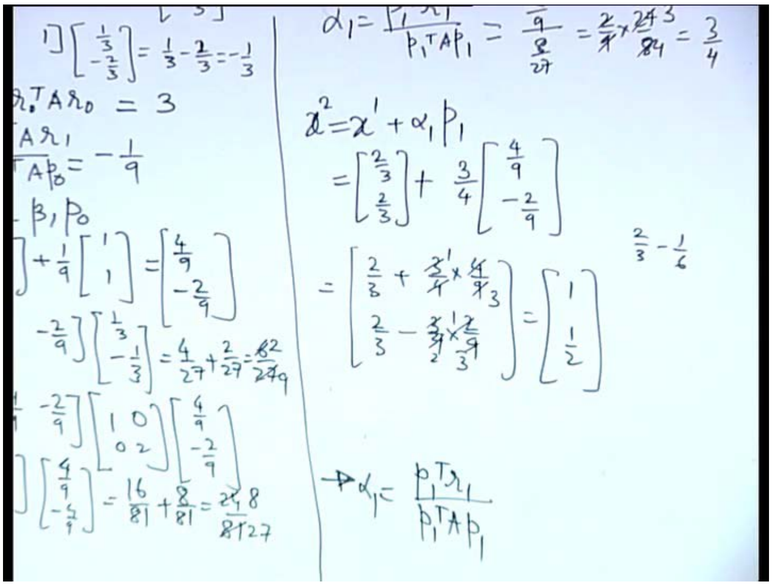

Alpha 1 is p 1 transpose r 1 by p 1 transpose A p 1; so 2 by 9 by 8 by 27, so 2 by 9 into 27 by 8, that is equal to 3 by 4. So, x 2 is x 1 plus alpha 1 p 1; what was x 1? X 1 was two-third and third plus alpha 1, that is three-fourth into p 1 4 by 9 minus 2 by 9. So, that is two-third plus 3 by 4 into 4 by 9 that is the first point. So, two-third plus one-third that is one and the other point is two-third plus 3 by 4 into minus 2 by 9.

There is some 2 by 3 minus 1 by 6 that is equal to half right. So, you can see that in one step, it has reached the solution. So, the conjugate gradient method is supposed to work with a greater speed for reaching the solution speed means, less number of steps that is what we call as speed, it is not the computational of speed. Now, we have seen the gradient search based method that is the steepest descent methods and the conjugate gradient method. Now, let us try to assess the applicabilities of these methods. So, let us work out one or two examples to see how they work, how efficiently they work and so on.

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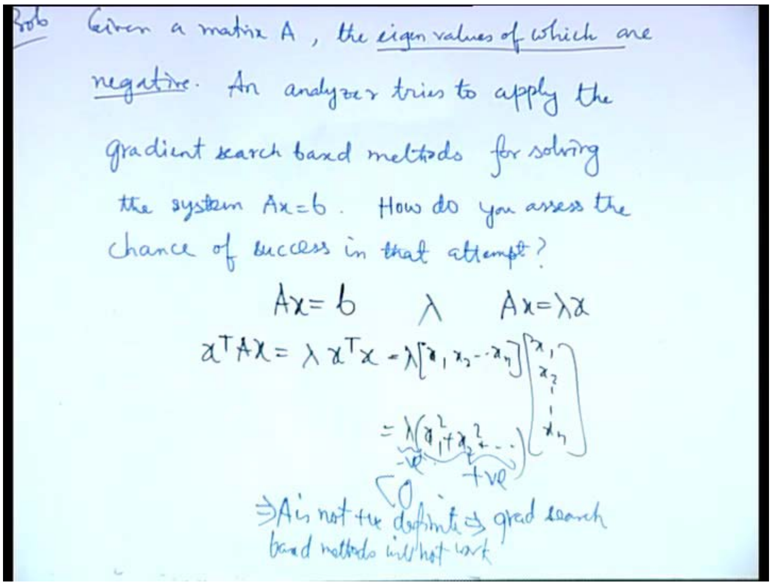

So, let us consider a problem; given a matrix A, the Eigen values of which are negative. An analyzer tries to apply the gradient search based methods for solving the system A x equal to b. How do you assess the success of that attempt the chance of success in that attempt?

So, in many cases, people try to use a method; in many cases, people are unsuccessful, because they have implemented the method wrongly; in some other cases, they are unsuccessful, because the method is wrong for that particular situation. So, when you say the question, how do you assess the chance of success in that attempt, you have to assume that, otherwise if he or she implements the method, there is nothing wrong with the implementation; of course, otherwise you can say that, I assess that there is no chance of success in the attempt, because the person is very dull or inefficient. So, it is not like that. So, you have to assume that the person is efficient in terms of implementing the method as it is, but even then whether you expect success or not, that is what you have to predict.

So, the clue should come from this particular statement, the Eigen values of which are negative. So, what is the consequence of a coefficient matrix, which is having negative Eigen values? So, you have A x equal to b, and the corresponding Eigen value if you have lambda for the matrix A, then you have A x equal to lambda x. Now, for the gradient search based methods, you have to recall that what are the basic conditions that need to be satisfied for the method to be applicable; one is a has to be symmetric, another a has to be positive definite, because we have shown that the symmetric condition is good enough to have the gradient of the function f equal to 0 corresponding to A x equal to b,, but that does not ensure a minimization; a minimization on the top of that is ensured by a positive definiteness of A over and above the symmetry requirement. So, we have to ensure that A is positive definite; how do we ensure? If you have an arbitrary vector x, then x transpose A x should be greater than 0.

Now, if you have x transpose A x here, that is nothing but lambda into x transpose x, what is x transpose x? It is positive or negative? It is always positive, because an element of x is multiplied by the corresponding element of x only. So, x transpose x is what? You have x 1, x 2 in this way x n, that is multiplied by x 1, x 2 in this way x n. So, it is lambda into x 1 square plus x 2 square, it is just like making a dot product. Now, this will be negative here, because this is positive, but lambda is negative; it is negative. Even if one Eigen value is negative that can make this x corresponding x transpose A x as negative. So, that means, it is not, A is not positive definite, which implies that the gradient search based method will not work.

Fortunately in computational mechanics problems, most of the coefficient matrices that you derived from the discretization of a physical problem, many of those will be symmetric and positive definite; and therefore, you can use this method, but you have to keep in mind that that is not an assurance you have to first assess whether the coefficient matrix is symmetric and positive definite. Symmetry assurance is obvious; you can just directly observe and find out whether it is symmetric or not, but for assessing the positive definiteness, you have to be a bit more careful.

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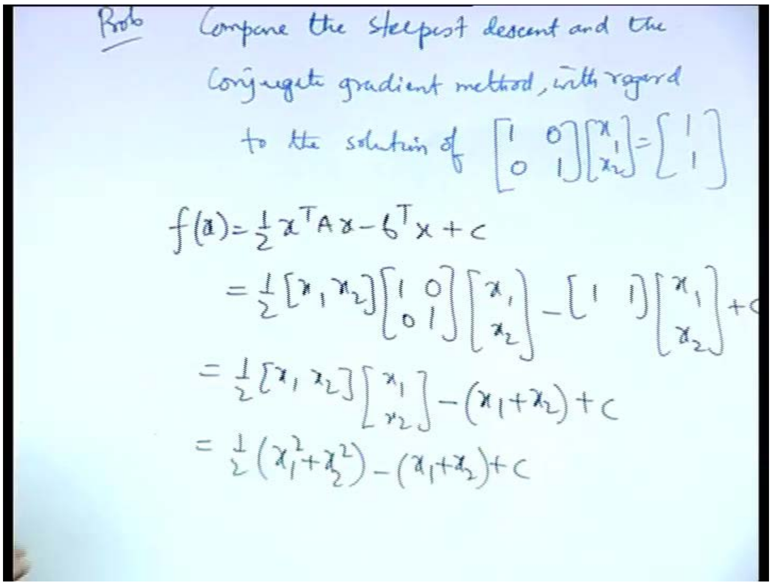

Let us consider another problem… Compare the steepest descent and the conjugate gradient method with regard to the solution of… This. So, let us find out what is f (x)? Half of x transpose A x minus b transpose x plus C. So, half of x 1 x 2 into 1 0 0 1 x 1 x 2 minus b transpose x plus C; this minus x 1 plus x 2 plus C, so half of x 1 square plus x 2 square minus x 1 plus x 2 plus C. To have a visualization of the method, we will try to plot f equal to 0 in the x 1, x 2 plane as we have done in the previous, in one of the previous examples.

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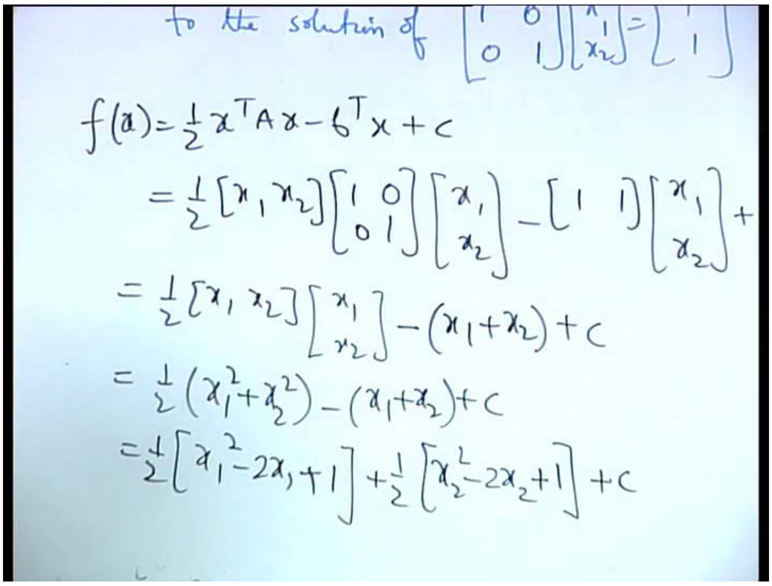

So, to do that, we will write half of x 1 square minus 2 into x 1 plus 1 plus half of x 2 square minus 2 into x 2 plus 1 plus C.

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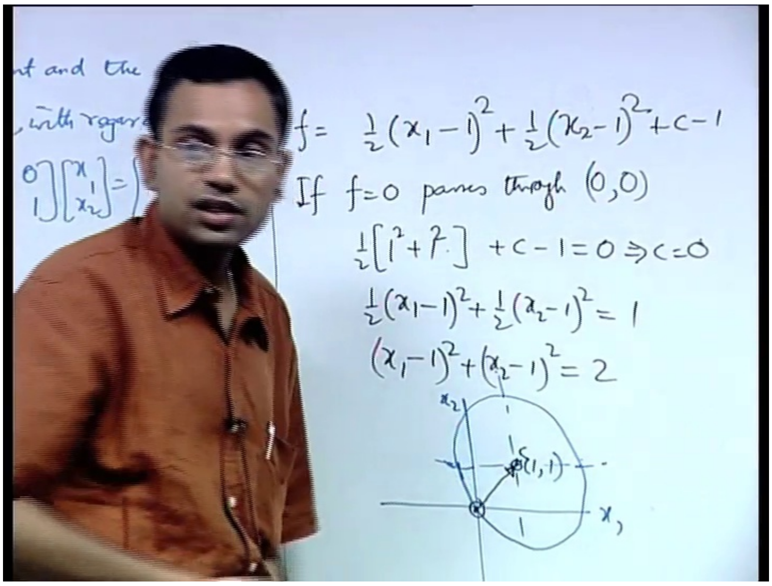

So, f is equal to half into… There is one adjustment of minus 2 plus C minus 2, so half of x 1. So, half plus half 1 sorry yes minus 1, so half of x 1 minus 1 whole square plus half of x 2 minus 1 whole square plus C minus 1. So, if you want to have if f equal to 0 passes through (0,0) which is your initial starting point then you have 1 square plus 1 square sorry half into 1 square plus 1 square plus c minus 1 is equal to 0 that means, C equal to 0. So, then you have half of x 1 minus 1 whole square plus half of x 2 minus 1 whole square is equal to 1. So, x 1 minus 1 whole square plus x 2 minus 1 whole square is equal to 2 right. So, it represents what? Represents a circle in the x 1, x 2 plane; circle has centre of (1,1). So, this is (1,1) and radius of root 2; it is very difficult to draw a circle, every time you try to draw a circle, it becomes an ellipse may be if you try to draw an ellipse, it becomes a circle.

But let us try to understand the basic essence out of it. So, you have the starting point (0,0), this is the bull's eye that you have to hit; you know, this is the solution. So, in the steepest descent method, you are moving along the direction of the gradient of n, which is what, which is normal to the curve. So, you move along the direction. So you will definitely hit the centre, because in one step, you are able to reach your goal; the steepest descent and the conjugate gradient method for this case will be the identical. So, when you say, the compare the steepest descent and the conjugate gradient method with regard to the solution of this; they are absolutely identical, because in this special case you are lucky enough to have it as a circle, where the normal direction and the radial direction are the same. So, that you reach the center in (( )). So, this is a very special example, a very simple example, where you can say that in identical steps, you can reach the solution for both the methods, without working out the further details.

So, we stop our discussion on the solution of the system of the algebraic equations here. So, so far we have studied the diffusion type of problems, their discretization, and solution of the discretized algebraic equation. So, our next agenda will be to go one step forward, and try to see how we discretize the convection diffusion problems, that we will do in the next class. Thank you.