Advanced Numerical Analysis

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Lecture - 23
Discretization of ODE-BVP using Least Square Approximation and Gelarkin Method

So in my last lecture we looked at Least Square Approximation, method of least square approximations was used to discretize the boundary value problem. Now unlike orthogonal collocation or finite difference where we took some finite number of points and force the residual to 0. In this case we said that some of the square of something is similar to some of the errors that is, here integral square—integral of the square of residuals.

Now we wanted to minimize that instead of setting it = 0 into domain we wanted to minimize the square of the integral over the domain. So this was conceptually different from what we have done earlier. And we look at a specific problem. So, the problem that we looked at was a linear problem, so this was.

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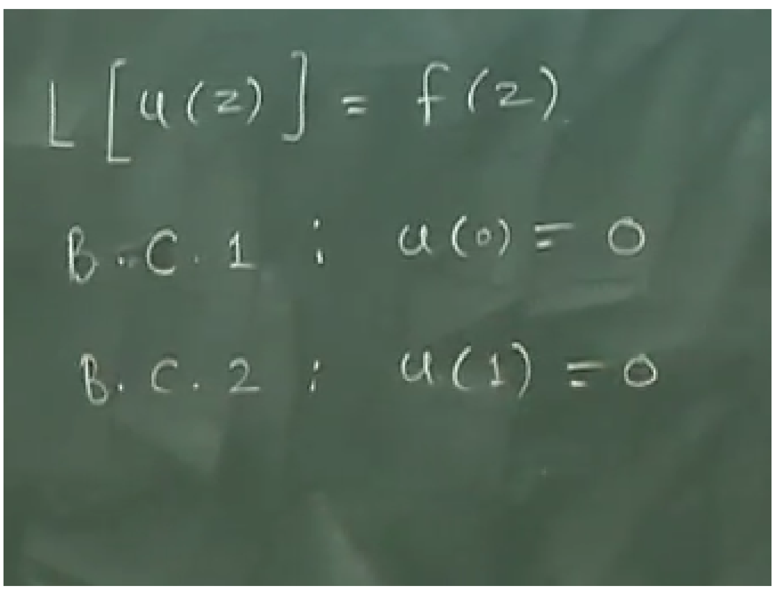

So we looked at solving this. So this was a boundary value problem, there are two homogenous boundary condition = 0. And then we wanted to get a solution for this problem. Now, we constructed an approximate solution not exact solution.

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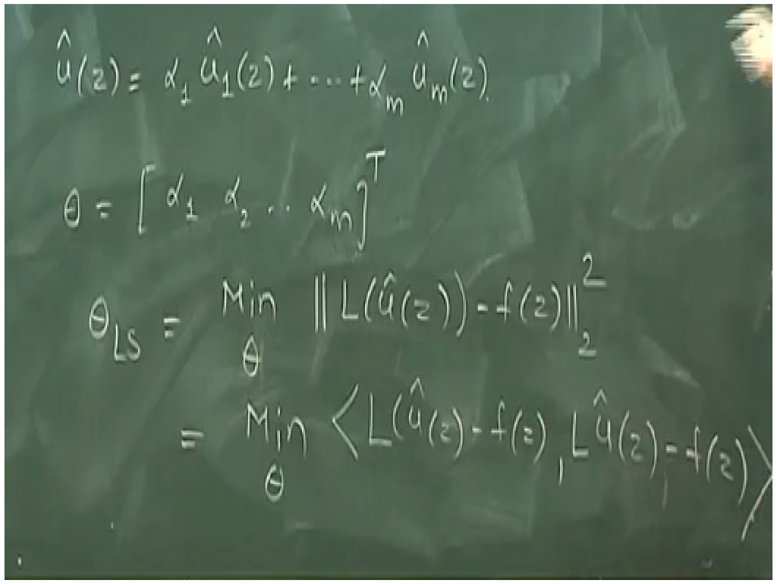

This approximate solution was u cap z was, there u1 cap to um cap or some known functions okay and idea was to find out unknown coefficients alpha 1 to alpha m such that. So we want to--if we say theta that is = alpha 1, alpha 2, alpha m, if we define this vector theta then we wanted to find out theta least square that was minimized with respect to theta norm of L u cap z – f z 2 square.

So this is nothing but a residual square or integral of the residual. This minimize with respect to theta inner product of L u cap z – f z. So in order to find out least square estimate such that—but we have chosen the basis function in this particular case, such that the boundary conditions are met. Okay. So, we at special case, and then with we derive the normal equation. We derive something that look like a normal equation. So basically idea was to minimize this with respect to theta.

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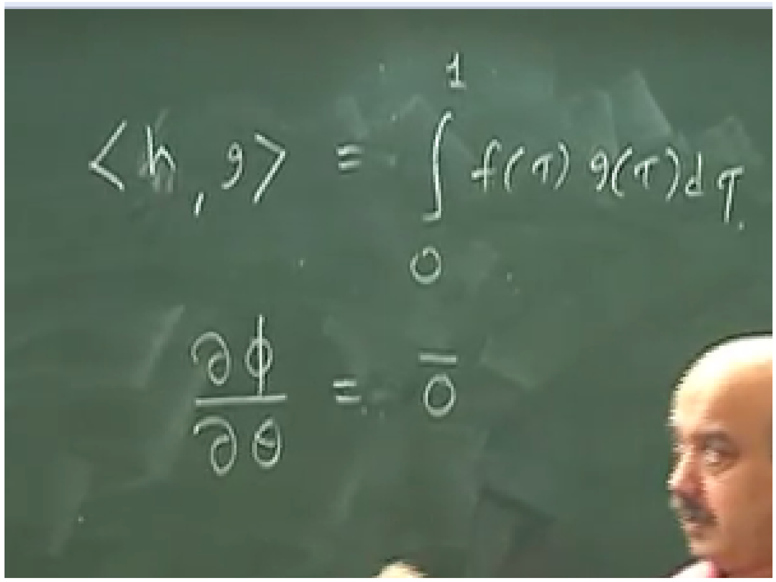

So here, between any f and g or say h and g inner product is defined as 0 to 1 f Tau; so this gave us the equation that was needed to solve this particular problem, okay. Now to minimize this or to get the solution if we take this as phi, if we take this objective function to be phi then we use the condition dou phi/dou theta = 0. This particular condition can be used and you can obtain alpha 1 to alpha m numerically.

But in the special case where L is the linear operator okay, we could get the so called normal equation, we can get the solution analytically. If it is not a linear operator, you will not be able to solve alpha 1 to alpha m analytically we will have to use some numerically optimization to get the solution. And then whether there will be a unique minimum and all that is not guarantee.

But in this case when L is a linear differential equation we could actually find solution to this problem, that is we could find theta least square analytically using equation that look almost like normal equation. So this was the way we went about during this. Well, there is a small verification, suppose what you do if you want to take a general case.

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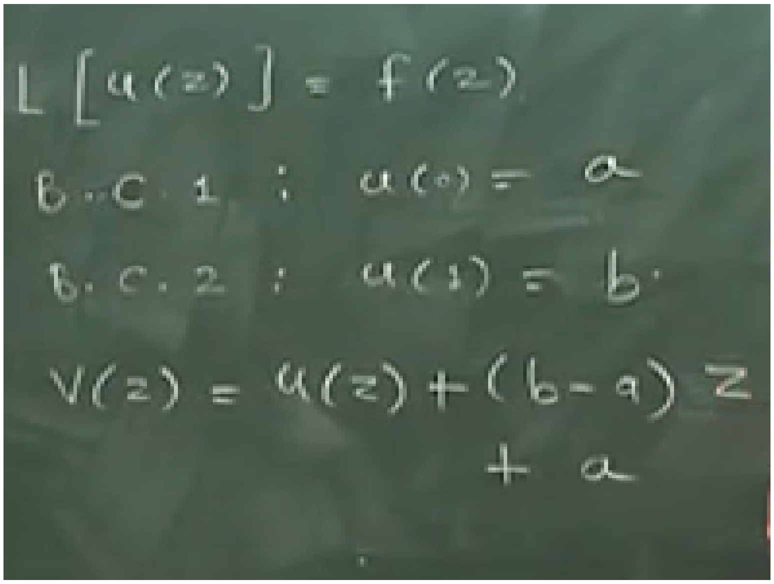

And see what if this is Alpha? What if this sum a, and this is sum b, they are = 0. Okay. Suppose this is = a, and this = b and so-- well in that case what we do is we do a simple linear transformation and then try to map it to 0 to 1. In such case, we define instead of u z, I will call a new function say v z which is. I will define a transformation; I will define a new variable v z which is u z + b-a times z + a. What will be v z? You know in terms of in this new variable.

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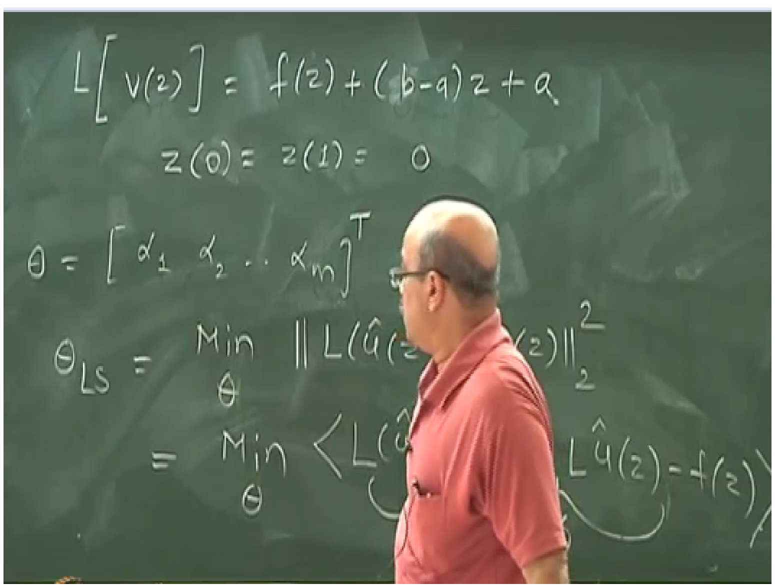

I will get – it is very easy to see that I will get L. Just check this. We will get z 1 and z 0. So you it can do a little bit of transformation. You can do a transformation here. At 0 u z z=0 okay. You will have—this is 0, okay. Sorry this is a, this is a, this will be okay. So now u z = v z+. Okay. So now it will follow. Now it will work out. So u z = v z + b-a time z and +a. So we take, let us take a specific operator that we looked at yesterday.

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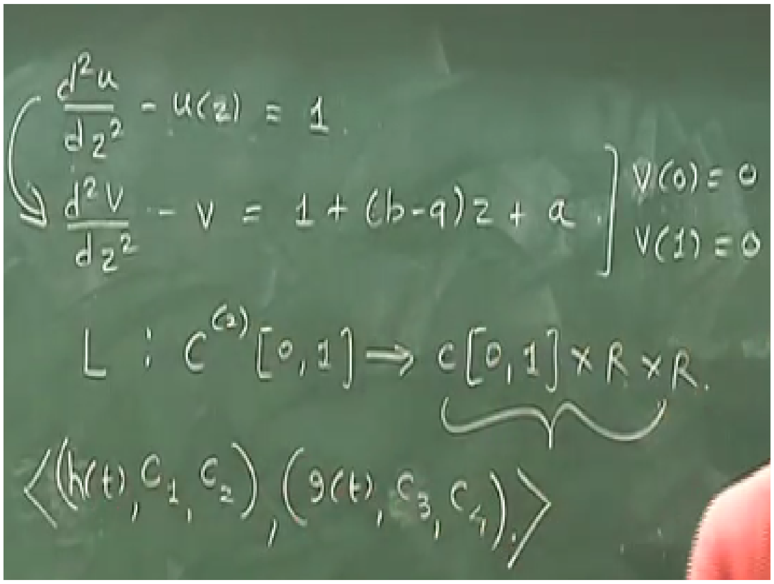

So instead of L, let us look at the specific problem that is d2 u/dz square – u z=1. This was the problem that we looked at. Okay, if you use this transformation then the transform will be d2 v/dz square – v = 1+b-a z + a, so this get transformed to this and you can check here boundary conditions gets. Boundary conditions in terms of u will become, in terms of V it become V 0 = 0, V 1 = 0. Just check here. So at 0 we have this nicely following and at 1 well will it be V z = -- at C = 1.

So if I put 0 here, if I put d here so b here so b=-- yeah 0, 0 will canceled and b, b will cancel and you will get 0, V 0. So the problem gets transform like this, so this is one way of dealing with the problem. The other way of dealing with the problem is modifying the definition of inner product. So now we have to work with – instead of working with the space of twice differentiable functions we have to work with product spaces and define a inner product slightly differently.

So this is one way of dealing with non-homogenous boundary conditions which you can do a transformation and then solve this problem. So when you take derivative of -- second derivative of this, this will disappear. I am taking second derivative of this. Second derivative of this will disappear this part will disappear. What remains is still d2/dz square and when you substitute this for u here, when you substitute this okay, it will be – of this which on this side will become +. So the problem gets transform to this problem, and the earlier solution will still work.

But there are more general ways of this, this looks like fix by which you know we have done transformation and we got this a better way is to change the definition of the inner product itself. So what we can do now is that this equation which we are looking at, this equation that we are looking at L is a map from. L is a map from twice differentiable continuous functions to set of continuous functions over 0 to 1 * R * R, this we have seen. So this is the products space.

And now, we have to define the inner product in slightly different way. So if I define the inner product, see this-- I have to define an inner product from this space and if I define a proper inner product on this space then I can solve the problem in slightly different way. So what I do now is I have to define an inner product of-- I want to define an inner product of a function say h t, then a scalar C1 and a scalar C2 with inner product of with g t, C3.

I have defined an inner product of this product space. I am defining inner product on this product space. Now, this in product will be modification of.

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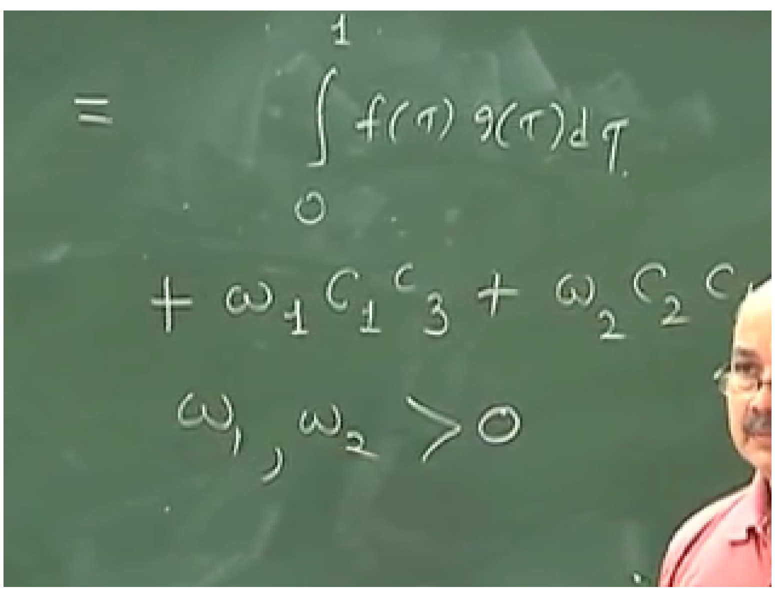

This inner product will be modification of this plus W sum positive weight which is W1 times C1, C3 + W2 times C2, C4. The inner product now is defined as integral of f t g t, inner product is defined as this is f t g t + W1 times C1 * C3, W2 times, W1 and W2 are positive weights, okay. So W1 and W2 are positive weights. So with this, what I can do is—earlier-- how did we derive-- how do we arrive at the optimality criteria?

We define the residual square, we define the residual square and then we took derivative with respect to theta, you remember that? We took derivative with respect to theta, theta was nothing but alpha 1 and alpha 2, they are multiplying coefficients with the basic functions, okay. So now with this, with this modified definition of the inner product what happens is--

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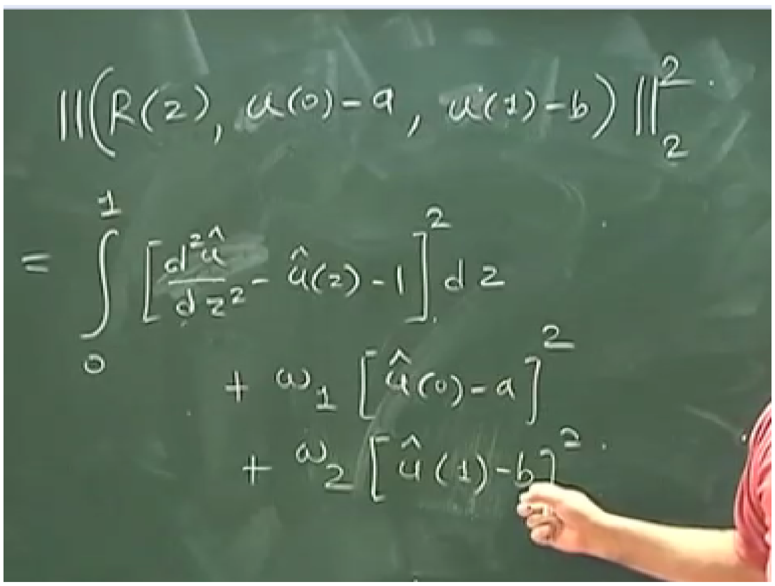

The residual square that is 2 norm of residual this is = residual. Okay. Actually residual will be-- will have to be defined-- so I should say residual and okay. Now I am taking three residuals. One residual is over the domain. Okay. Now, that is that will be taken care by integral over 0 to 1. And the two residuals at the two ends two boundary points. Okay. I am defining two residuals and now I am going to take square of this.

So my objective function which I minimize is going to be this plus this plus this. So the way will change is this integral will be it will be, so this will be = 0 to 1. Okay. See now, just look at this. This was already there earlier. We are minimizing this earlier, right? In addition, now I have two terms. I am minimizing difference between u 0 and a, and u 1 and b, okay. Now when I actually minimize this so, how do I get theta? What is my approximate solution?

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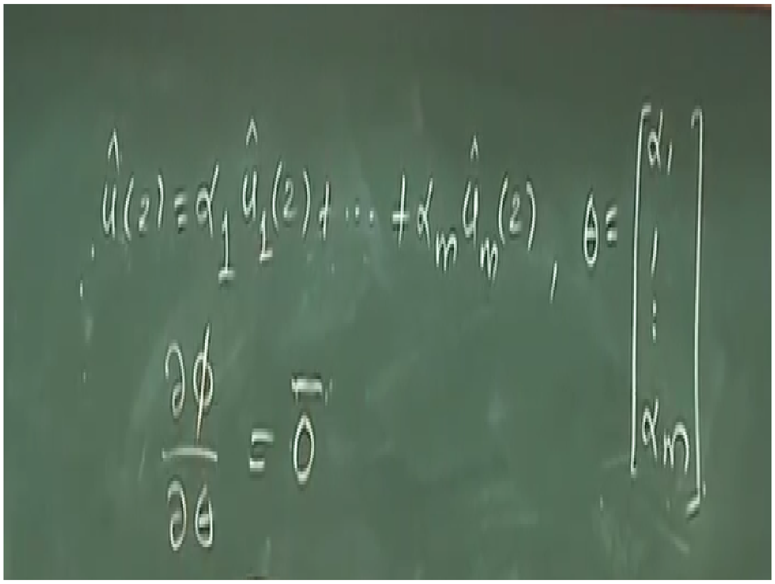

My approximate solution is u cap z is alpha 1, okay. And my theta is this vector alpha 1 to alpha m. Okay. And here this residual square, okay this residual square I am going call as phi and then how do I get the conditions to, how do I get conditions to solve the problem, that is dou phi/dou theta = 0. But now phi is going to be this. So they are two additional terms. Okay. Now the trouble with this approach is that the boundary conditions will not be exactly met.

The boundary conditions will be met in the square sense. This equality may not be there. Well, you can make it, you can make it, go closure and closure by increasing this weights, if you put more weight to this the optimizer will try to squeezing them make sure that u cap 0 and u cap 1 are closure to each other, okay. Now by this approach I do not have to choose the functions which are given this = this and this = this.

Let us say I am choosing shifted general polynomials. The two boundary points are not A and B. But by this approach I can choose the coefficients that some of the square of you know, difference between the solution and the exact boundary condition is minimized and together with the differential equation is obeyed the least square sense not exactly equal to. When I minimize this, this term will not be = 0 because I am minimizing. I am finding a lease square solution. Okay.

True solutions for this problem will be some – in an infinite dimensional space I am taking a finite dimension approximation, okay. So that is how I get a solution here, so that is one way to solve this problem. Now there is one more variant of this method, okay. This is the method of least square and you will get of course that equation by which you can get analytical solution theta if L is a linear operator then you will get a close form solution for theta.

And once you get that close form solution alpha 1 to alpha m will if you put those values back, you will get this least square solution of. Okay. So by this approach now, I could choose a polynomial expansion, nothing steps me I can choose a polynomial expansion here. So this function could be, you know 1 t 1 z z square z cube up to z the power m. And then I can minimize this objective function with respect to alpha 1 to alpha m and get my solution. Okay.

So earlier, particularly for Taylor series approximation and for approximations using orthogonal collocation, we where only considering you know, interpolation solution mainly considering the polynomial approximations, here too if you want to work with polynomials in principal you can work with polynomials not an issue. Okay, so that will not be a limiting factor.

So but we might, we can as well choose some convenient base like sin cos or shifted general polynomials and work with that. Okay. So this almost now brings us close to end of this discretization. There is one more point to be discussed now. This is—there is a method called Gelarkin method and I am going to just briefly touch up on this method.

In Gelarkin method, we do not attempt to minimize, we do not attempt to minimize this. Okay. In least square method we try to minimize the some of the errors, okay. Gelarkin's method is just an extension of, just an extension of the idea of projection, okay just an extension of idea of projections. Now, I am not going to derive it in any way I am just going to propose this method. And what is the basis for this method? Should be now clear to you when I write the equations.

The basis is idea of projections. Okay. So what I am going to do in Gelarkin's method, what is different here is that we do not put this objective function or we do not put any of the minimization problems and so on. But we use one factor. See, what we know in projections?

That, the error should be orthogonal to the subspace prime by the basis, okay whatever is the subspace you have given.

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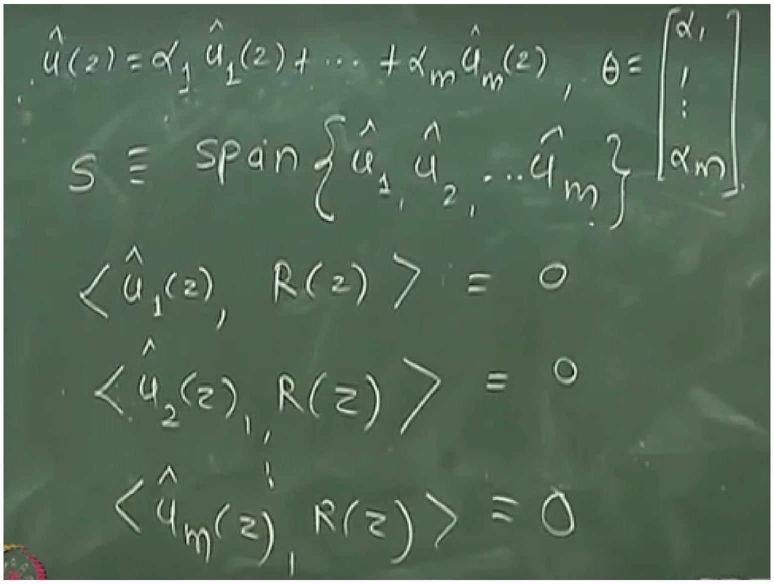

So here, if I take a set -- If I take a subspace S which is defined by span of u1 cap u2 cap, um cap, okay. Then I could derive an approach. Let us say I have defined my inner product like this. Okay. I have defined my inner product like this. I am not interested in minimizing the square of the residuals. But what I am interested in doing is just using the fact that when you do projections the error is orthogonal to this subspace. Okay.

So what I am going to do there is I am going to say that u1 z = R z, this is = 0. I want the error to be orthogonal to the subspace prime by okay this u1 to um. So I am just taking this basis vectors and I am forcing the condition that this to be = 0. Okay. This I have to use together with my two boundary conditions to solve the problem. Now you may not be able to force it = 0 for all the points, in some cases.

Because in some situation where you boundary conditions, you may want force this = 0 only at m-1 vectors and then two points come from the boundary conditions, because two conditions will arrive at the boundary conditions. I will look at specific problem to just given you an insight. Let us go back to the TRAM. Now this particular condition, this particular approach of solving will reduce to least square problem when the operator is linear. Okay.

When the operator is linear, least method and Gelarkin method will be become identical. But when the operator is not linear, okay so you will get the solution which is different. So this is, this can be applied, Gelarkin method can be applied to any other operator which is not necessarily a linear operator. It could be a non-linear differential equation and you are trying to solve it.

And basically what we will do is, we do not get into minimizing the residual we just say that the error between the solution and the subspace okay, the error is orthogonal to the subspace prime by the basis function of the solution, that is the simple solution which is used. So this is—let us go back to the TRAM problem and now that you have solved it using orthogonal collocation and finite difference will be able to appreciate this third method.

How do you choose this basis function, you know, how do you choose them in the orthogonal, there are different ways of choosing the basis function here, we are actually get into Gelarkin method is belongs to the class of finite element method and you will—because it involves this particular method would involve integral over the entire domain, these methods tend to give very accurate solutions, and I am not going to get into the details of how do you choose this basis functions.

There are some continuous basis functions which are like cap function and so on. So if you want to know more about this, it is there in the notes, you can check this. Also book by Gilbert Strang, okay his latest book on Applied Linear Algebra and his first book on the Linear Algebra with Applications. Both of them give you very, very good introduction. I think the latest book on Computational Science and Engineering.

He has latest book on Computational Science and Engineering and the other one is on Linear Algebra, the second one gives very detailed introduction to this topic. But this becomes little bit more involved. I just want to mention this before for the sake of completeness.

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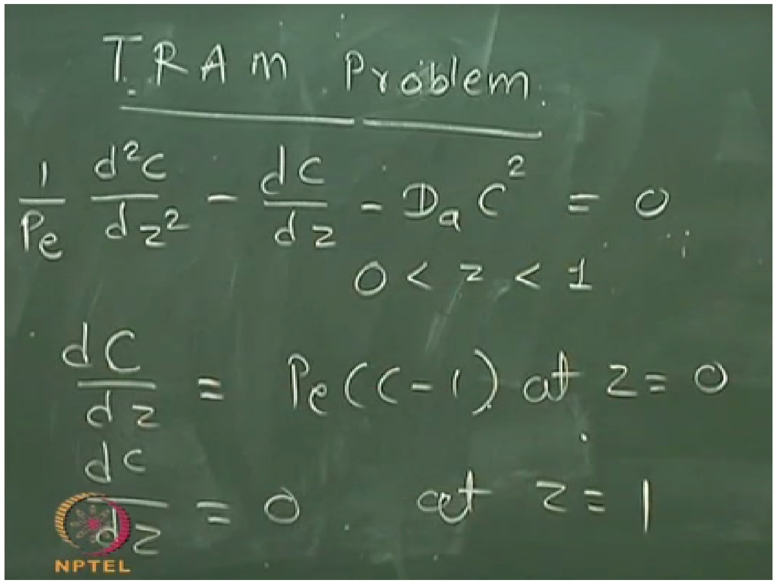

So if we go back a TRAM problem, so this is 1/ peculate number * d2c/dc square. So these are the problem with two boundary condition dc/dz = peculate number * C-1 0 and dc/dz = 0 at z=1, you already know about this problem. And I am going to do here now is.

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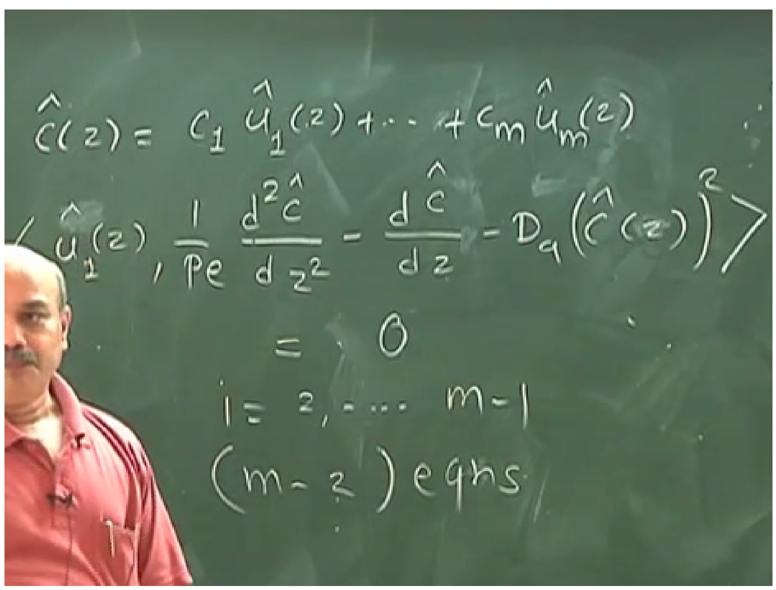

My solution here is going to be-- this is going to be my approximate solution, okay. And to get the equations what I do here is to get the equation, so this integral or this inner product, this inner product is equated to, right hand side is 0 for i=2 m-1. So we equate this to 0 for i=2-1. Now this is, you know even if you take some nice functions just remember, that I have to take second derivative of that first derivative of that and then square of this function.

And then calculate all the integrals, okay. It is a fairly involved job in terms of computing the coefficients. Finally, what you are going to get is a m-1 non-linear equations in m-1 unknown. Sorry, m-1 unknown equations in m unknowns. One minute, we will get m-2 equations because we are starting with 2 and going to m-1, okay. So putting this will give you m-2 equations in m unknowns, okay. m unknowns are alpha 1 to alpha m, okay. The rest of the equations will come from boundary conditions.

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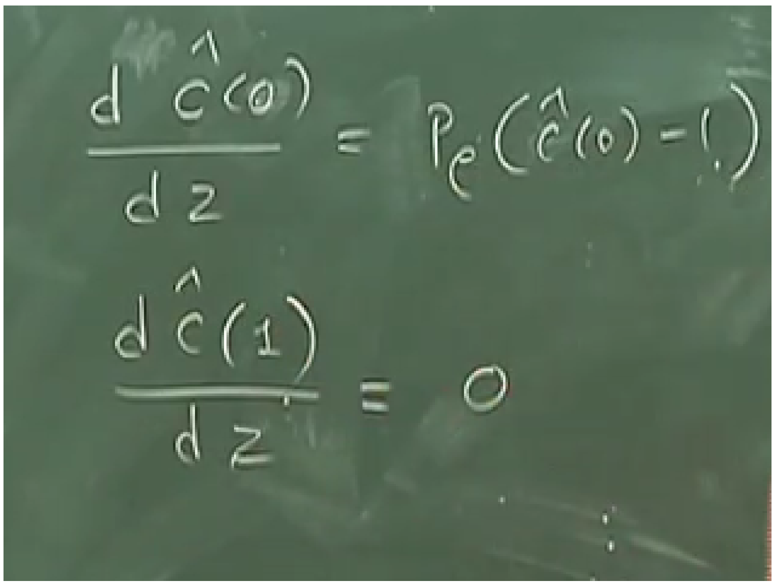

So these two equations together with m-2 equations will give m equations in m unknowns, what are the m unknowns? Alpha 1 to Alpha m, so these are non-linear equations and the terms that appear in the coefficients of this non-linear equations will be all integrals which you have to integrate which you have to find out. Okay, so numerically this particular scheme is very, very involved but the dividends are very high. Okay.

You get good solution that is why you know the finite element methods FEM methods are, so where is this finite business come? When you construct this basis functions you divide the domain into a finite number of elements and on each one of them you define some nice functions which are orthonormal and those functions are use to. See for example one could use one of the, one of these function one of the popular functions are.

I mean you might wonder why, where is the discretization, where is the finite element business coming here. Okay.

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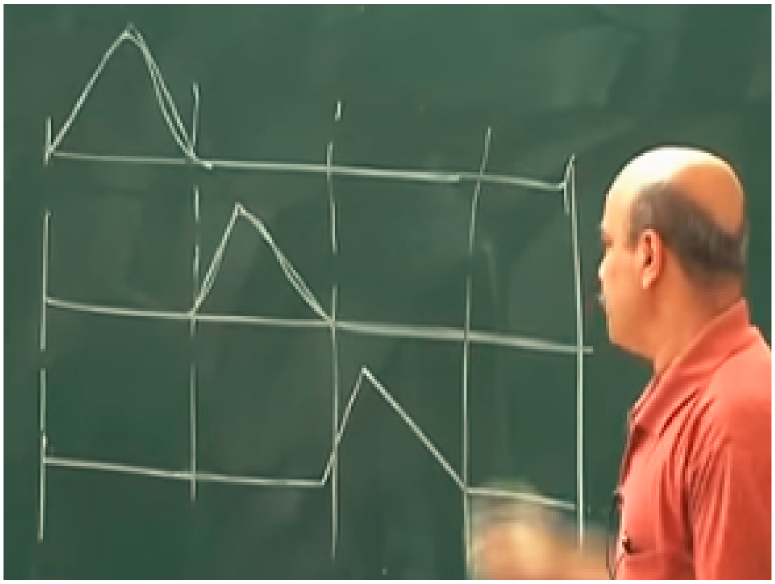

So you define functions over this domain which look like this and so on. You divide it into finite domains so this is divided into say 3 or 4 domains so this is, this is one this is second, this is third so you have this cap functions which are continuous at these points where linear in this region. So you have to divide the integral from integral over, over the domain 0 to 1, you have to divide between this point to this point this point to this point and this point to this point.

You can divide the integral in three parts and divide in each integral okay. And then likewise we will do it for everyone of them. Okay. **"Professor – student conversation starts"** (()) (31:06) These are not differentiable, so there are ways to construct different functions. I am just giving you a just idea. So you can construct differentiable function you can construct smooth functions which are okay. And then those smooth basis functions can be then, so you can construct smooth functions, not an issue. **"Professor – student conversation ends"**

So just to give you an idea you can construct a basis which looks like this or finite domain. So this function basis over only some domain it will be non—derivative will haven non-zero it will have 0 value else were. Okay. That is why it makes it into finite. So because the function value is

0 from here to here, you do not have to evaluate the integral. Okay, just have to evaluate between this point and this point.

And because of this, this special clause of function that you consider what happens is that finally the equations which you get have some kind of a Spark's structure, okay. And you can exploit that to solve some big problems. So I am going to stop this Gelarkin's method only here. I just wanted to connect everything into place, you know. I am not getting more into Gelarkin method because it, if I have to now expand on the finite element method it will be fairly complex, it will not be as easy as orthogonal collocation and finite difference.

Finite difference and orthogonal collocation are very finite difference is the easiest to understand where I would in terms of understanding complexity I will put orthogonal collocation next, it is not that difficult to understand, it is basically interpolation and you know you are just transforming the problem into set of non-linear algebraic equation. Here too you will find the non-linear algebraic equations.

The coefficient will be integrals and those integrals will be fairly complex to evaluate. They are quite cumbersome. So it is not that if you write a program for this, so that is why you get now commercial programs which can actually do all the integrals and solve them, okay. So all those together will give you set of equations which have to be solved simultaneously to arrive at the solution.

You can do that yeah. That m is notional. See, you can have—the problem is that here these equations can be forced only at the internal segments not at the boundary points, so the boundary points you will need to enforce the boundary conditions. Okay. So unless you use some trick what we did earlier. We had modified the inner product definition right. That trick could be used. You could modify the inner product definition to include the two endpoints then you know, the then boundary conditions are satisfied in the least square cells, not exactly. Okay.

So you could play all those tricks of modifying the inner product definition and then including the two endpoints and then, all that is possible. Okay, so now—because this why that is possible because each of this functions, see if you look at this function here, this function is defined over the entire domain. Okay. So this function is defined over the entire domain. So you-- inner product can be modified to include this point this point and integral over this point. Okay. So then this, this inner product here will get modified with two additional terms for the endpoints, okay.

And then you can have, you do not have to have force this, you can just force 1 to m and be done with it, that is also possible. Okay. But in that case—see if you do this, these two will be exactly satisfied. If you do it the other way, you know where you include those two as some of the squares in the inner product definition then they will be satisfied in the least square cells not exactly satisfy. Okay.

So they looked at – now let me sum it up what we have looked at is – the method of discretizing problems from – so what happens here even in this case, you start with the problem which is in infinite dimensions, you concept an approximation which is finite dimensional and then finally what you are going to get here after you do all these integral and everything, what are you going to get here? You are going to get m equation m unknowns.

In this case there will be non-linear equations. Okay. If L was the linear operator if this square was not there, you will get linear equations and you can solve them very easily okay. But we have this square here, so because of that you will get all kinds of square terms you known alpha 1, alpha 2 and you will have to do complex integrals of you know, u1 square u2, u2 square u1 all kinds of terms will appear in the integrals.

Now because you get, because of that you will get non-linear equations. But is happening if you realize is that a problem which was originally in the infinite dimension space is transformed into a finite dimensional algebraic equation solving problem. Okay. So I am transforming the problem which was originally solving boundary value problem, differential equation is getting transformed into problem of solving m equations in mms. Okay.

So the transform problem looks completely different from the original problem, solving non-linear algebraic equations is completely different problem from the original problem, okay. So there are some issues like errors in discretization. So when you actually solve the problem, okay. See there are variety of errors that creping.

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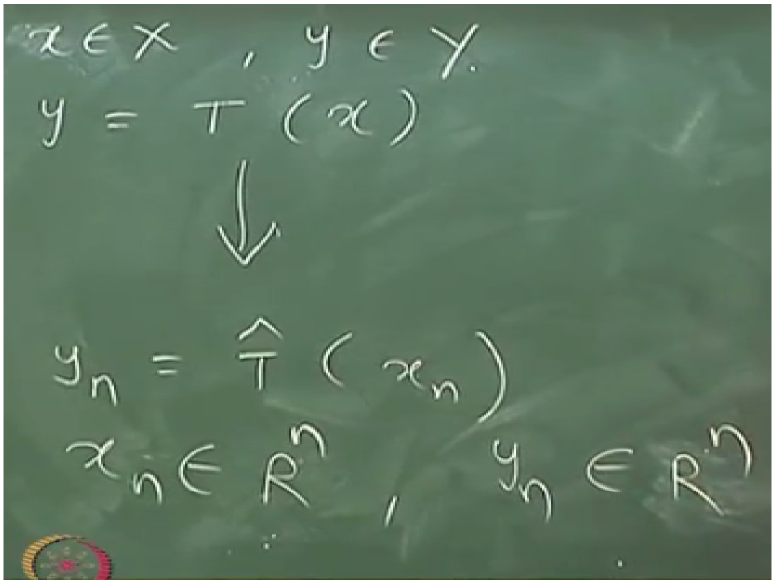

See we said that we wanted to solve Y inverse problem y = T if x where x belongs to some space x and y belongs to some space capital Y, we wanted to solve this problem. Okay. But we are not able to solve the original problem in most of the cases. In, you know you might wonder well IU am doing a course on solving partial differential equations and linear partial differential equations, okay. I can solve the analytically I can do all these series expansions, then why do I need all these. Just go back and check when you can solve those problems analytically?

You can solve those problem analytically when the boundary conditions are very nice, geometry have simple, okay when the geometry is simple. If I ask you to solve Laplace equation to be formulated for this room and if you do not approximate walls to be smooth walls, suppose I want to say there is a small notch here and then it comes out and then okay. My boundary is no longer straight wall.

Then suppose I have a problem, see if I take a reality that well, then you know the conductive the conductive heat transfer from this wall is different at different places, okay. In some region there is wall okay, so the, they will not be heat transfer they will not be convective heat transfer; there will be something like you know insulation okay. But in between there are windows, so if I take all these realities into account my boundary conditions even for the simple Laplace problem linear operator will be very complex and I will not be able to get those close form solutions.

This close form solution work, they are very nice they give us insight okay and when you can approximate geometry to be spherical, cylindrical okay or perfect you know, square or some parallelogram you can actually solve those problems very—but those you should look at them at some kind of limiting conditions. Approximate in this room okay with smooth walls and you know only one kind of boundary condition across this wall and all these walls are exactly constant temperature, this is a simplification.

And probably it was relevant you know 40-50 years back when computing was difficult. Now you can compute, you can say that, well there is a small notch here and I want to compute for this, what happens here? Okay, so when even for a linear problem when the analytical solution can be found for nice boundary conditions they may not be compatible when the boundary conditions become weird.

So even for linear partial differential equations you would need to solve them numerically. The class of problems which can be solved analytically is very small. Most of the problems you know in real life have to be solved using numerical methods. So you better understand the numerical methods. So what we are doing here is we are actually transforming this as I said into yn = T tilde xn, where xn typically belongs to some finite dimensional space.

And Yn belongs to some finite dimensional space, well do not confuse this x—this y and this x and this y, probably maybe I should use other notation X and some different kind of Y. okay. So this is some finite dimensional space, this is some finite dimensional space. So you have taken the problem and then transformed it. Okay. For example, finite difference method. You are not able to force residual to equal to 0 at all the points. You know you have to take two finite grid points or to save it that is = 0.

So actually this problem is an approximation of the original problem, this is an (()) (41:52), this is not a true problem, this is just you know, this just look like this but not this is not equal to this. Okay. And further, see how many errors we complete. First of all, we are not able to solve the original problem, we transformed it into some computable. Then you know, you say that this is belongs to some Rl, let us say this, give the transform problem in n dimensions.

And this is in some m dimensions, so let us say this is Rn to Rn okay and equations in unknown you have got. And this T cap is a different operator all together. We saw the differential operator. These are algebraic equations; you know something else. Now when you go to computer okay, you cannot solve using real numbers. You have finite precision; you do everything using rational numbers okay. And then—

See, non-linear different—non-linear algebraic equations, you cannot solve them exactly. You use Newton-Raphson, so you further approximate this. See, you started from her, you approximated this. From here you again approximate because you know Newton-Raphson is required Newton-Raphson requires Taylor series approximation again, okay. So there are series of approximations. Just imagine, so what you get finally okay. So there is an approximation for,

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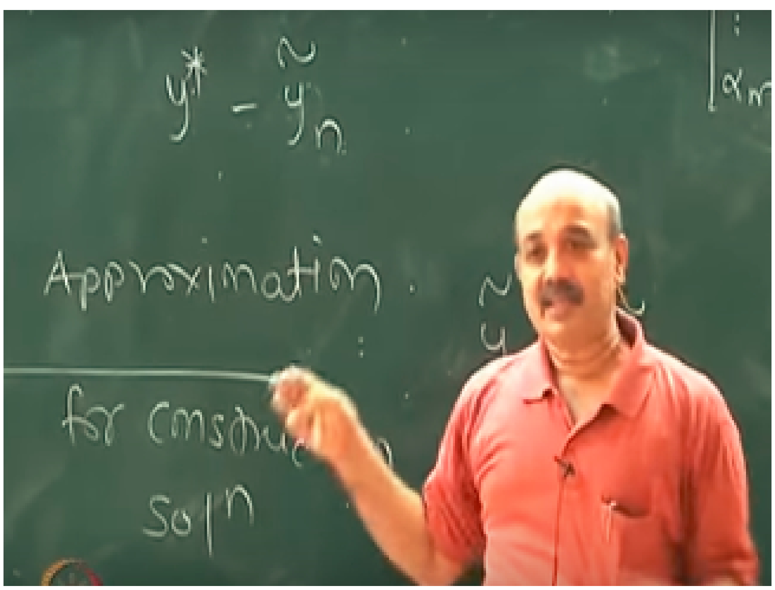

Okay. You end up with, Yn tilde Xn tilde. Suppose the true solution of this, this problem transform problem was actually y* y* or let us say yn* xn* and then true solution here is y* x*.

So a true, true solution is y* x*. Then you have a transform problem which has a true solution. Suppose you forget where it came from, okay that is a true solution, so that will be yn* xn*. Okay. But non-linear algebraic equations suppose you get, you are not able to solve them again.

So you get a approximation to this, so that is yn tilde xn tilde. Okay. What would be interest you is, what is the difference between y*- yn tilde. Well, first of all, can I compute this? Sometimes in many cases you just cannot actually define this, because you know you a true solution will be a continuous function and this finite element method, finite difference method, you got some finite points, so what is the error between this and this?

This is defined only at finite points, this is defined everywhere in the domain so you know, this animal is difficult to even thing about. Okay, so this you start with something, you want to solve something you actually transform it that also you cannot solve then you re-transform it okay. What you will see that when you go from here to here.

Now this lecture I will start post mid-sem. When I go from here to here again I have to use approximation. Again when I solve this problem I am going to again go back to Taylor series, I am going to go back to (()) (45:20), polynomial approximations, interpolation, same idea. So Taylor series and you know interpolation again with this, but again I am not able to solve this. So again Taylor series, again you know, the interpolation kind of approximations and then solve that problem. Okay. So finally what we get and what we intend to do is completely different.

Hopefully, you know they are close and that is where your insight as an engineer comes into picture. Are these numbers which computerized, does it make sense? Is this close to this? Well, in many situations you do not know what is 2y or you do not know what is 2x. But as an engineer you have gut feeling that what is true what should true x look like. Okay. You know that, you know if there is a PFR the concentration of the reacting species will reduce as z.

You know this, okay. So if that is not happening here okay you know there is something wrong. Computer is giving me garbage. Okay. So that is where in spite of all these you know advanced techniques in spite of availability of very, very powerful computing tools we are still in business because your intuition as chemical engineer is required, otherwise compute will do everything, you and me will not be required. But fortunately that is not the case, okay.

We still get our job because you have to make a comment whether this, though you cannot find the difference whether this yn tilde which you get finally. Does it make sense? Okay, is it a good solution? So that is where we come into picture. Now to do all these business you have to solve everything approximately. To solve approximately you have to give an initial guess, how do you give initial guess? Only if you are a good physicist, engineer, chemist, chemical engineer.

You can generate a good reasonable initial guess and then you can solve the problem, otherwise you will not be able to solve the problems. Okay. So this brings us to end of problem discretization. So what we have seen till now is that first of all, we have seen that a problem can be represented most of the problems in chemical engineering or engineering represented by this generic form where y, they are inverse problems, they are given y and y we have to find out x.

We cannot solve them in most of the cases, so we transform them into this problem, so we have come up to this point. Okay. Now post mid-sem, I will begin how to go from here to here and how to compute the solution. Okay. So now I will get into solving tools like solving linear algebraic equation, solving sparse matrix equation, solving them using some iterative methods all kinds of things.

Non-linear algebraic equations, we have look at one method Newton-Raphson, there are very tricks enhancements. How do you do those enhancements? And then second thing which we have look at is ODE initial problem because many problems get transformed to ODE initial problems. So how do you integrate differential equations subject to initial conditions, all those Runge–Kutta methods, Predictor–corrector method, Euler integration everything will come in that, so post mid-sem, we will look at tools, till now we have look at problem transformations.