Inverse Methods in Heat Transfer
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Lecture – 58
Physics Informed Neural Networks – An Intuitive Explanation

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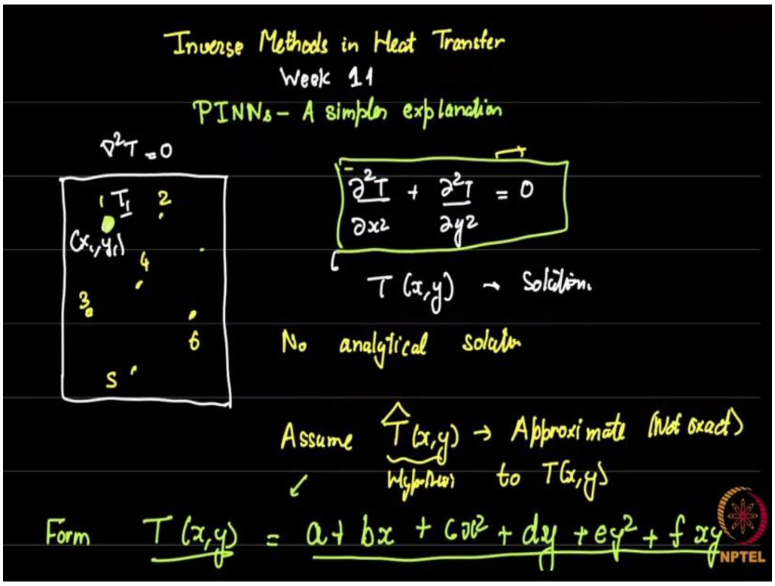

Welcome back we are in week eleven of inverse methods in heat transfer. In the last video I gave you a preliminary explanation of what PINNs are and within that I had just told you about how the loss function for the ODE can be used as ODE or PDE even though I did not talk about PDEs there, can be used as a substitute of having ground truth. in this video I would like to give you a simpler explanation that does not exist within the literature but I would like to give you a simple explanation and a sort of intuitive explanation for how PINNs came about okay and once you understand this video well enough, I think you will be able to see the last video also in a better light and also the upcoming videos within this week clearly.

So let us go back to a simple problem or even a slightly complicated problem. so let us take a 2D problem and let us say we are solving $\frac{\partial^2 T}{\partial x^2} = 0$ which means $\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$. We know that the solution given certain boundary conditions is given by some $T(x, y)$, this is the solution so we know this already unfortunately we cannot find it analytically okay. So, the problem of course is no analytical solution if you were doing CFD the way to solve using CFD would be exactly what I told you before split this into some mesh, read each one of these as an independent unknown, each one of these points as an independent unknown and then turn this into difference equation approximated and then solve it.

We are going to take a slightly different approach now okay so what I call this slightly more intuitive order simpler approach, which will directly lead to PINNs once we use neural networks. so what I am going to do is I am going to assume and this should remind you of the forward models that we did we are going to assume some solution $\hat{T}(x, y)$ which is approximate okay remember it is not exact to $\mathrm{T(x, y)}$ so in this sense this is our hypothesis okay now not only that I am going to give as I would ask you to recollect what I had talked about earlier in machine learning I am going to give a form that this approximation takes. Except now I am going to take a very simple form last time I took a neural network we cannot write or make head or tail of what it is doing.

But here I am going to assume $\mathrm{T(x, y) = \ a + bx + cx^2 + dy + ey^2 + fxy}$. Now instead of that having a, b, c, d, I am going to write $\mathrm{T(x, y) = \ w_0 + w_1x + w_2x^2 + w_3y + w_4y^2 + w_5xy}$. Now this is a function this is obviously a function.

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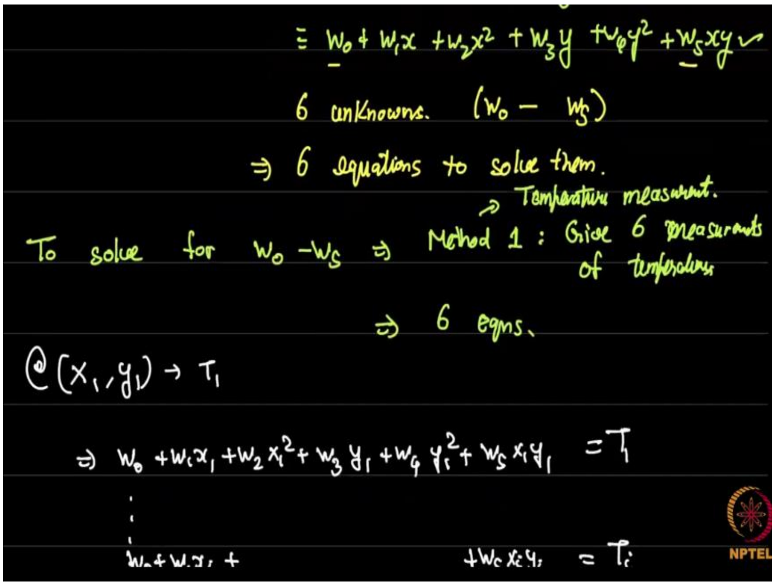

Now the number of unknowns here are six unknowns. we have $\mathrm{w_0}$ through $\mathrm{w_5}$ which are not known which would mean we need six equations to solve them okay. Now if you need six equations to solve them there are several ways of doing so one method could have been you give you actually have an experiment and you make let us say six measurements so let us call these points one two three four five six.

To solve for w_0 through w_5 so remember the moment you solve for w_0 through w_5 you know the temperature at every point here because I have written temperature as an expression okay so if I solve for w_0 through w_5 you can use method one, which is give six measurements of temperatures. So, the moment I give six measurements if temperatures what happens I will have six equations.

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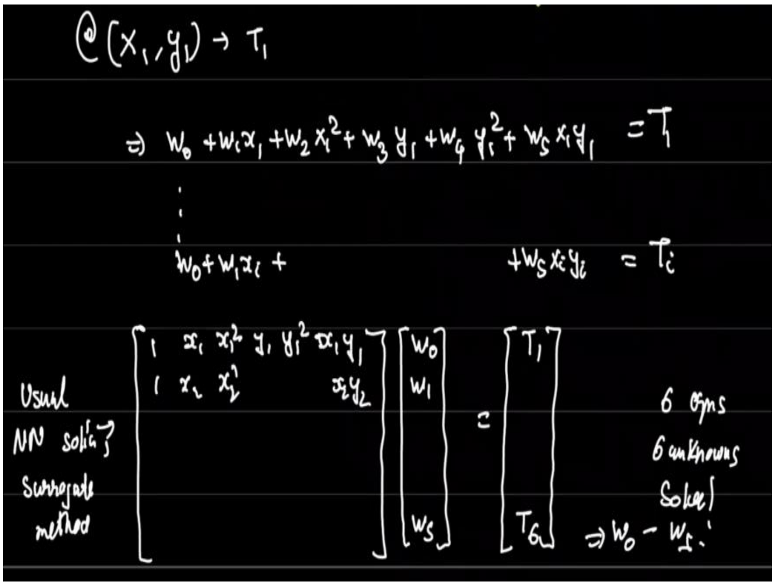

How so? for example let us say that at this point this point let us say the source location x_1, y_1 the temperature was measured to be T_1 either through some prior simulation or through an experiment you know this so you will say that at x_1, y_1 temperature was T_1 so this will say $w_0 + w_1x + w_2x^2 + w_3y + w_4y^2 + w_5xy = T_1$.

You can write equations such as this in general you will have $w_0 + w_1x_i + w_2{x_i}^2 + w_3y_i + w_4{y_i}^2 + w_5x_iy_i = T_i$. If you write this as a matrix the unknowns remember are w_0, w_1, w_2, w_3, w_4, w_5 on the right hand side you will have T_1 through T_6 and here you will have x_1, ${x_1}^2$, y_1, ${y_1}^2$ sorry there will be a constant term which is one then x_1, ${x_1}^2$, y_1, ${y_1}^2$ and then x_1y_1 similarly 1 x_2, ${x_2}^2$ so on and so forth until x_2y_2 so you have six equations, six unknowns solve and there you have your temperatures okay so sorry there you have w_0 to be w_5.

But suppose I do not have these I do not have $T_1, T_2, T_3, T_4, T_5, T_6$, now this would be comparable to usual NN solutions or the surrogate method okay I will explain the connection later on, but this is similar to the surrogate solution.

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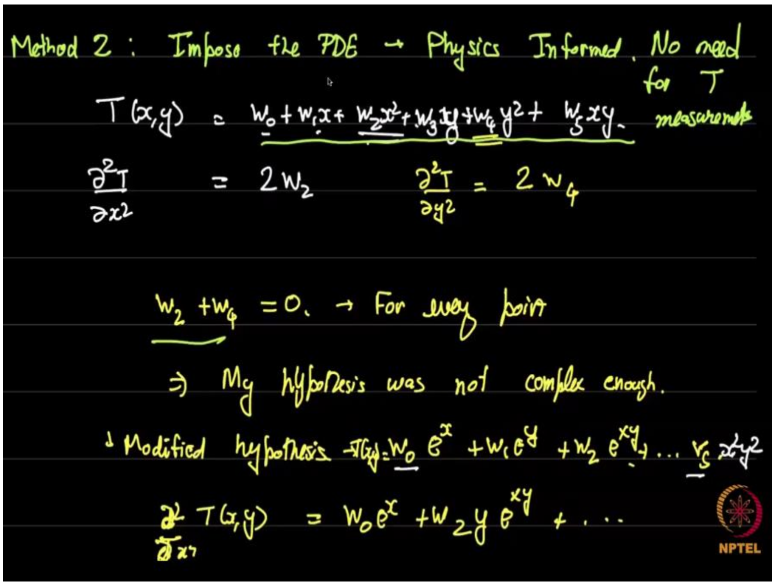

But there is an alternate method so let me call this the second method let us give a name to method one which is through temperature measurement. Now let us look at method two method two says impose the PDE now even though I do not know the temperature at this point I do have one piece of information what is that I know this, I know that $\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$ at these points what does that lead to okay impose the PDE how do I impose the PDE I already know the temperature expression w zero plus etcetera up till w five xy then I can find out what del square t del x square is.

Now $\frac{\partial^2 T}{\partial x^2}$ let us write this out just for our reference $\frac{\partial^2 T}{\partial x^2}$ will have $2w_2$ okay this term this term and all the other terms actually go to zero okay so w zero w one did take simply differentiate the expression for t and you get this expression. what about $\frac{\partial^2 T}{\partial y^2}$? $\frac{\partial^2 T}{\partial y^2}$ will give you $2w_4$ so we now get the equation that $w_2 + w_4 = 0$. Now unfortunately for the function that I took if our $\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$ I will get this value for every point

This will tell me that my hypothesis was not complex enough or complicated enough. So, I can modify my hypothesis. so let me use a simpler function something like $w_0 e^x + w_1 e^y + w_2 e^{xy}$ etcetera and let us say I take some w five terms so when I take t of xy is something of this sort and I do $\frac{\partial^2 T}{\partial x^2}$ or $\frac{\partial^2 T}{\partial x^2}$, this will give me $w_0 e^x$ plus let us say in this case $w_2 y e^{xy}$ so on and so forth I will have an analytical expression.

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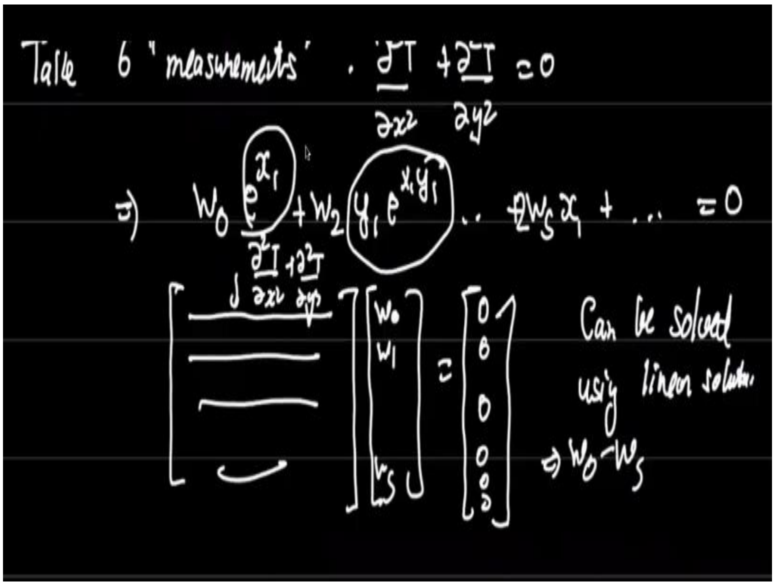

Now once again say I have only five or six unknowns take six measurements. These measurements all say the same thing $\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$. so for example I could get something like $w_0 e^{x_1} + w_2 y_1 e^{x_1 y_1} + \ldots + 2w_5 x_1 \ldots$ then if you differentiate it with respect to x you will have something like two x plus some derivative due to y is equal to zero once you write this this will again look like a matrix except this will be a little bit more complicated this will represent $\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}$ all the coefficients like $e^{x_1}, e^{y_1}, e^{x_1 y_1}$ so on and so forth and you will have w_0, w_1, w_5 equal to on the right hand side will be zero zero zero zero zero zero okay.

Once again this can be solved, I am explicitly avoiding boundary conditions which I will talk about later can be solved using simple linear solutions. This gives us w zero through w five it is the same as before. Now notice what we have done here is we do not need, this is completely physics informed, no need for t measurements. Now why is there no need for t measurements? All we did is we have simply said that at each of these six points the physics of the problem which is $\partial^2 T$ equal to zero is imposed and all we had was a hypothesis function, it could be quadratic like this it turns out it is a bad function because nothing is left.

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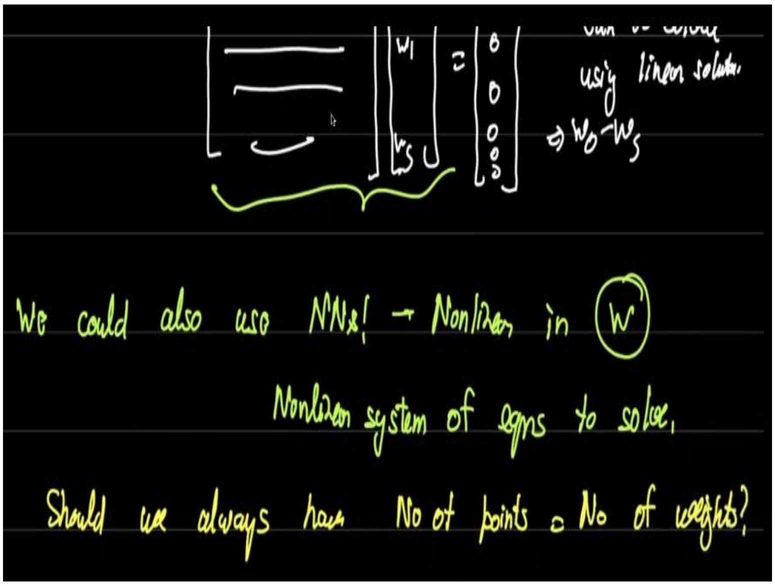

You can now add cubic quartic power four sine cos whatever you have or we could also use neural networks. So, if I use six measurements and the only number of parameters in my neural Network are six you could solve it except there is one difference this is a linear system, because my hypothesis was linear in w, whereas a neural network is nonlinear as we have seen in the last three four weeks in w. So instead of getting a linear system we will get a nonlinear system of equations to solve. Now again you can solve this using gauss newton or you can use Levenberg Marquardt or you can use gradient descent. Now the question is this should we always have number of points equal to number of weights okay. So, for example let us go back to the very first case that we took. we took six measurements here one two three four five six are these six thermocouple locations let us say and we also had exactly six unknowns w zero through w five.

Is it required that the number of thermocouple measurements should be exactly the same as the number of unknowns? The answer is no because we have been doing this throughout this course. what do we do? If let us say I have only this but I have more points let us say I keep on adding more thermocouple measurements and I go till let us say hundred thermocouples now, what do I do? I do not have to increase the complexity of my function all I need to do is instead of solving this system of equations I solve the equation in least square sets why is that? so let us come back here.

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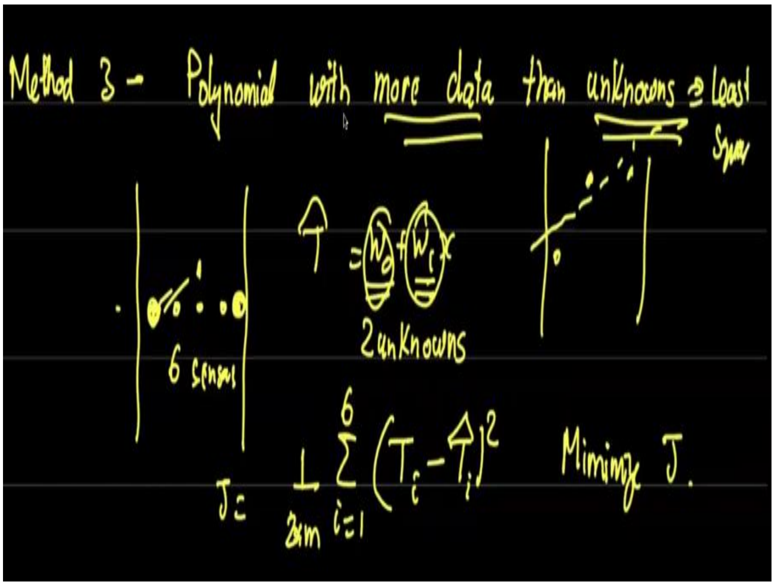

I am going to revisit I will call this method three which is polynomial with more measurements more data than unknowns where we see this before in the slab problem in the slab problem, we had six sensors but our $\hat{T}$ was simply $w_0 + w_1x$ only two unknowns. so instead of trying to satisfy every single thing all I say is okay you have a prediction, this is the prediction, you try to minimize T-$\hat{T}$ square at all these points are equal to one to six one by two times number of points minimize J. so notice how this comes naturally, let us say the number of points was only two like I made only two measurements, then I have one exact value of w_0 and w_1, if I now make three measurements it is not always certain that the same w_0 and w_1 will satisfy these three and all we do is okay instead of satisfying these three I will have something that goes in the middle.

So, let us say temperature like this you have something of this sort, this will be my hypothesis function. So, if I have more data than the number of unknowns you simply do a least square.

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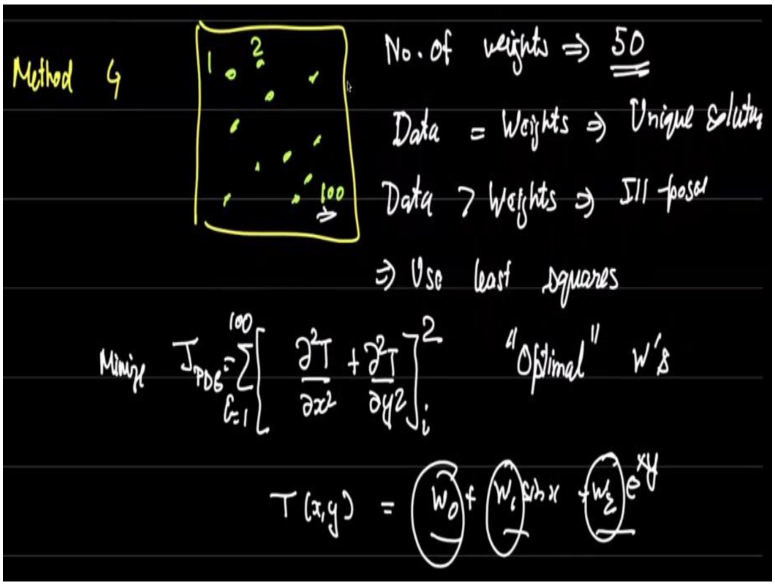

We can do the same thing with method four. method four suppose I have a neural network and I have hundred data points once again, one two three up till hundred and let us say number of weights in the neural network or in the hypothesis function I chose was let us say only fifty, then if it was exactly fifty and exactly fifty here I would have if data equal to weights plus we have unique solution in fact this as you know is the nature of inverse problems but if data is greater than weights we have an ill posed problem and all we need to do is use least square.

So, instead of solving the nonlinear system of equations exactly all you need to do is to minimize J PDE. J PDE simply says $\frac{\partial^2 T}{\partial x^2}$ whatever expression we get plus $\frac{\partial^2 T}{\partial y^2}$ instead of being zero, I will minimize the square of this summed over all the individual points. this is a very simple idea okay so J PDE simply minimizes the sum of these squares over how many other points this is so this is hundred then basically get optimal w's okay. I will re-emphasize this point notice that if I had exactly fifty points there is no optimal w the thing that minimizes this will be such that at each point, I can actually satisfy this exactly equal to zero.

But the moment I increase the data points you have a regularization effect you add more and more points you actually have multiple Choices of w which would have satisfied this but what you want to do is to find that which minimizes $[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}]^2$. now this actually gives you a root breaker for what we were doing in the neural network method whenever you get confused about using a neural network you can think of a normal function you can just think of $T(x, y)$ or $T(x, y, z)$ is an actual function like w zero plus w one sine x plus w two it is some hypothesis function it really does not matter what that function is once you give that since we know that neural networks can approximate everything rather than giving functions handcrafted functions like this we give a general neural network.

So that once We solve w zero w one and w two we know it can approximate the function that we are looking for okay now I hope that this made the idea behind PINNs a little bit clearer in the next video we will see how we can actually incorporate boundary conditions in two different ways one is the one that was pioneered by Lagaris and the next is what was the modification by Raissi and we will see how the modification by Raissi actually enables us to solve inverse problems very elegantly. So, I will see you in the next video thank you.