Surrogates and Approximations in Engineering Design
Prof. Palaniappan Ramu
Department of Engineering Design
Indian Institute of Technology, Madras

Lecture - 01
"Overview and Motivation of Course"

So, welcome to the course on Approximations and Surrogates in Engineering Design that is the title of the course, but the focus of this course is in the context of design. Practically, we will focus on structural design, but it could be on any design, any engineering design. More specifically, we will be looking at the framework of optimization.

Basically, optimization is seen as resource optimization, in structural engineering you would look at minimizing the weight. In such section in such cases, how can you organize this into a nice mathematical structure so, that you can solve it algorithmically is what engineering optimization is about; which we will cover for the first part of the course. It will be introduction to engineering optimization.

As you would have learned are you still most of your research student so, you keep using functions to represent physical characteristics. These functions there is a big assumption that they represent the physical nature or they are expected and we hope that they will represent the physical nature of the problem at hand. Then we deal with these functions to certain types of solutions that we are interested in our quantities that we are interested in deriving from them. The underlying assumption is you have this function that captures your physical characteristic that is what the assumption is.

But this model that we are talking about are the function that we are talking about, need not capture the entire physics ok. There is a little bit of an uncertainty, there is a little bit of an error and it is an approximation. For instance, for you to relate to a finite element model is a representation or it is just a model it is modeling, it is a numerical modeling technique if you think about it.

It just captures how a particular structure deforms, what are the stresses in that. If you change the element the values are likely to change that is why you do grid convergence studies, whether it is finite element or CFD or you can use Simulink to model any characteristic ok. Now, we need to understand what are the limitations of this model, that is also an important part of it. But, why did I talk about models being approximations of the physical characteristic is because, this course deals about such things in the context of optimization.

During optimization you need to have these functions, where you will go find gradients you want to minimize something, you want to maximize something. There are some constraint that you need to satisfy, you should not violate and these functions are not readily available. In a classical course on optimization we will give you the functions take f, g and h and you go and optimize; this is what a classical course on optimization does that is important.

Because you know how to deal with the solution steps in that case, but in reality we would not have these functions in closed form. So, there are many things that we might want to do in that sense, is we need to know how to construct these functions. The moment you say I am going to construct this function, it does not come directly out of physics; sometimes it might, but sometime it does not come out of physics. I give you a complex structure, I give you a complex loading and I ask you can you find out how it is going to deform for this particular load. What might be the way that you would or what is the way that you adopt to find the let us say the stress or the deflection ok.

This is interactive by the sense and they made sure it is interactive right. So, you will have to respond to my questions. So, if I give you a complex structure with the complex loading mechanism and I ask you to find the deflection and stresses, I am interested in the maximum deflection on the stresses. How would you go about doing it?

Student: (Refer Time: 04:16).

Software also in one sense uses mathematics so, the answer was that. So, you would try to use a because, you do not have a closed form solution that is why I put the word complex structure. Most of our solutions, that we have analytical solutions for displacement and stresses are for simple structures is what do you have. When you have a complex structure you do not have that and one way to do that is as he pointed out, it is software is a is what we look at, but software is also an approximation. It tries to approximate the actual displacement and the stresses with the known mathematics that I mean with yeah with the mathematics that we know that is what it tries to do.

So, if you use a software it is an approximation. The moment you say approximation, it captures the physics only partially even the best model there is a little bit of an error. So, this error in modeling will propagate into your analysis also and hence in the result. So, you need to know how this error is propagating and how will that affect my results ok. So, it is important because all these models are associated with some kind of an error or an uncertainty because, practically you cannot use infinite number of elements in a finite element or a CFD model; you need to limit them.

So, it becomes important for an engineer to appreciate this because an engineer is the one who is going to designs any kind of a structure. You are the one who are going to model some kind of functions that will capture the physics of the problem. So, you need to know how these errors in the models will propagate into your analysis and hence, into your results and how will I look at my results accordingly ok.

So, this course overall will talk about such things, but to be more specific bullet point wise we will the first part of the course will introduce you to basic engineering optimization. So, we will talk about how what basic problem formulation is, what is the the general structure of an optimization problem is. We will discuss very simple iso contour kind of objective functions and constraints and how to find the minima's or the maxima's. We will talk about sufficiency condition necessary conditions we will touch upon a little bit on Karush-Kuhn-Tucker conditions ok. And Lagrangian multiplier we will introduce, we will not go into the concept discussion and all that we will introduce Karush-Kuhn-Tucker condition.

Of course, I assume that you all be in graduate students you know what a gradient is, you know slope and 1D becomes gradient in 2D and higher dimensions. Because that so, those kind of normal vector and all that is some information that you already know about. So, we will skip the most elementary part of it, we will focus on the elementary part of the engineering part not on the math part; on the engineering part we will focus on the elementary elements that will be for the first part. Then the second part what I will do is I will introduce something called the design of experiments ok. Whenever, we are interested in such approximations basically, you need to have some values of the response that you are interested in, otherwise you cannot go and approximate you need to have some feel.

So, where and how do I within the design space where and how do I get these responses is what design of experiments is all about. So, classically people like Taguchi and all that proposed techniques like orthogonal array which is which has its own advantages and limitations, but those are focused mostly on the manufacturing sector ok. How to reduce the variation in the manufactured components and all that but later when what we call as the design and analysis of computer experiments called DACE's; DACE's stands for Design and Analysis of Computer Experiments.

When computer models try to replace your experimental models people try to use design of experiments in a computational sense, not on the physical sense. Then they were able to come up with a space filling techniques it is called space filling means, there is you have a design space and then you want to maximize the information in the design space. So, you can from my information theory perspective also you can do a design of experiment. You can do from a game theory perspective you can do a design of experiment.

So, we will look at something called a space filling technique primarily, we will look at something called a LHS; Latin Hypercube Samples in that. And after that so, this will be the second part that will focus and once you have the design of experiments you have the design points then you can go and generate the responses and those points. Then you will have to fit a surface or a line depending on what dimension it is; that will eventually become the functions for you to optimize.

So, this is how we will proceed. So, first we look at basic optimization, then we look at design of experiments, then at those design of experimented points you will run the simulations and you will have a set of responses. Using those responses you will fit some surfaces which will be used in the optimization so, you will get some results. But, you know that there are some errors in this approximations that you built. You need to see how those errors will propagate in the optimization solution that you have ok, this is what.

So, if I remove the optimization part from the discussion, this still exists as a separate discussion. If I remove the doe part from the discussion it still exists as a metamodel. So, if you look at it each part of what we are going to discuss is independent in themselves ok. You do not need to know where these points came from, I can just give you a bunch of data and say can you tell me for this x 1 x 2 x 3; what is going to be my y, that is that that is an independent problem by itself ok. However, if you are trying to do an optimization you would like to have a functional relationship between x and y and you want to find a good combination of x or y or given a target why you want to find the x and all that ok.

So, in that case then you need to know you let us start asking these questions like at what is in the design space at what points did you generate these ok. What happens if I use some other set of points that is what is the design of experiments ok. And the design of experiment influences your meta model ok, the meta model will influence your optimization result. So, it is a cyclic problem.

So, hence it is good to set it in the context of design and analyze it ok. Today people are talking about big data analysis and all that yes. So, there if you see there is no scarce it is always, it is usually big; people do not know what to do with a lot of information ok. But, design problems are not like that, but in design problems you do not have data that is where the problem is ok.

When you are trying to design something, if you are a wise engineer if you know you get something for free in a technical sense, what you would ask for god comes up to you and then says I will give you one wish, what do you want ok. Of course, you cannot ask for monetary benefits. What you should ask for is, what do you will ask for. Let us say that you are trying to design, all of your you are trying to design an offshore structure.

Student: Data.

Sorry.

Student: Data.

Can you give me design data not general data, can you give me design data ok. So, this question will get repeated during the course multiple times ok. And your answer also should get upgraded because, the course will get slowly upgraded in the version that we are talking about ok. So, I will keep asking this question if god appears to you what will you ask, at this point with your learning from optimization what will you ask. With your learning from design of experiment what will you ask, with your learning from metamodel what will you ask?

So, your answer to that this will reflect what you understand out of the course that we are talking about, anyway. So, you want more data but, in design you do not have more data, when you are trying to do a new product development ok. So, right now we are looking at a product biomedical device ok. So, the other day what happened is we called some guy who manufactures this kind of devices and we ask he here is a technology, we would like to give it off ok. So, he said oh this is an excellent technology ok, but the problem is I really do not know what the market for this is ok.

Let us say that you developed an ultrasound machine which is of low cost. Today only I will do with the MOU and take it from you, because I know that there is a market for an ultrasound machine. This is a very good product I understand, but I really do not know what the market is. So, it is possible for us to create the market, but that is a different ballgame. So, that is the data for instance ok.

So, like that if you take a device for instance and then it is working ok, but if you want to understand the characteristics of that ok. If I ask you what happens if you are going to increase the thickness or decrease the thickness or you are going to strengthen this, there are correlations between these stuff, you do not know. You will have to run some simulations or you will have to run some experiments which is going to cost you in terms of time, energy, money ok. Because, when I said why energy and time is because you cannot just give in a model, you cannot just go and build a finite element model; you need to know what it does ok. Material models we do not have today ok, it is all approximate only.

How do you get the approximations? Have anyone does non-linear finite element here? When I say non-linear is the material non-linearity I am talking about. Anything not even material non-linearity, plasticity someone does? How many of you use finite element? No one uses finite element, is it fine ok. So, but do you know what final element is right, finite element methods you know. So, for instance if you take ok, we will come to that a little no we will do this maybe I will add and delete later.

Many things we use in real life are actually approximations which we do not look it up from that front. So, look at it why is this course so important is. If you want to know the stress or a strain ok; what is the basic knowledge that you need to know, you need to have about it or in a simple strength of materials course which is the first element that has taught that relate stress and strain.

Student: Elasticity modulus.

Elastic modulus ok, but elastic modulus also comes in form of what, some law that does expose.

Student: Hooke's law.

Hooke's law.

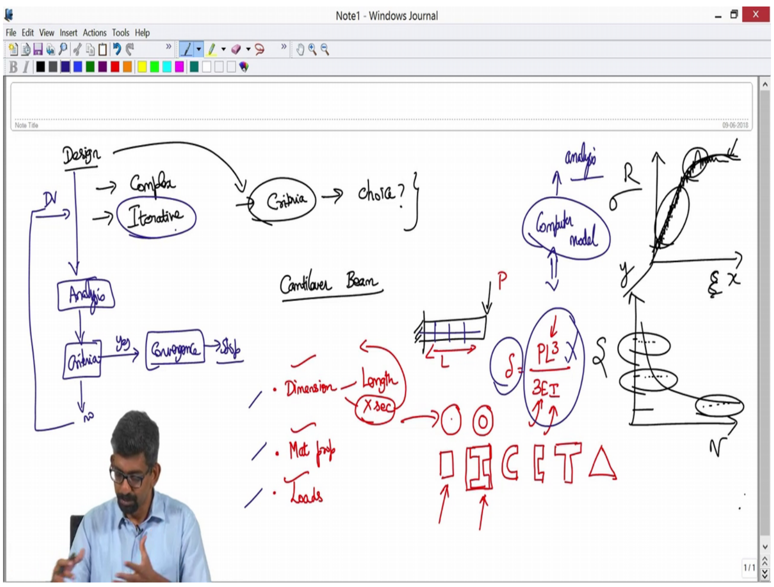
Student: (Refer Time: 14:53).

So, what Hooke's law says is theoretical; it says within the elastic zone your stress and strain are.

Student: (Refer Time: 15:00).

So, from that relation from whatever that theory says you get a quantity which is what he said; elastic modulus I will get ok. What that says is this course, goes like this right.

(Refer Slide Time: 15:16)



How and where did you get this graph from? Because, whatever the graphs that you have in those textbooks are all.

Student: Expensive.

These are all called the fitted graphs. In reality what happened, but in no textbook you would see then you would get a graph like that. So, be it for at each site you have to go and do few samples, at each site you have to go and do few samples. Then you will have that is what the ASTM standard says, it is not a single point and then you do it. So, all these are also data driven, if you would like to call it.

Because, we assume that these functions this is the way that it is start to us ok. But what is happening here is, there is a bit of approximation that goes into it ok. So, usually when you come here also in the yielder quantity that you want; we do not get too much into the details. But, if you are a material science engineer they will ask for an upper limit and the lower limit because, if I do another test for the same type of specimen this one is likely to vary ok. So, it could be an experimental error, it could be a material defect from the manufacturing sense. You can never have a deterministic material ok, but that takes the discussion slightly in a different sense, it becomes a uncertainties ok. How to quantify the uncertainties and propagate that is not what we are going to talk about.

What we are saying is even this is a material model; we just say Young's modulus, but that Young's modulus is over years and years of experience and people get those information ok. But there is always an uncertainty that is associated with it, one of the reason for that uncertainty is also your modeling error ok. For a simple cantilever beam you need to use a highly refined mesh to get the exact value that you will get, but in reality you will not get that value.

Because, in reality you cannot mimic what you do on the computer and what you do in the closed form solution ok. There is always be manufacturing issues ok, your boundary condition you will not get the exact boundary condition as modeled in the computer model ok. It is all it is a vicious cycle, if you see we usually teach it the other way. In reality it is like this your computer cannot catch, but it can also be seen this way ok, this is what your computer models, but in reality it is not that ok.

So, there is limitations on both sides. So, this is for instance this is a data driven approximation it is very similar, it is very similar as what we will do, but we will look it up from a response perspective. In this case this is a response that is of interest, but the variable need not be I mean it is really not a variable in this case. But let us say this was x and not epsilon and then I can have y ok, then it becomes a surface here that is what we. So, to put the context we are going to talk about design in general.

So, the design itself is complex in nature and one thing that you have to understand about design in general is, it is iterative and it is also iterative. Why it is iterative? It is because, usually you have alternatives and what is your interest the moment you have alternatives. When you have multiple alternatives, you want to buy a cell phone this can be casted as a design problem ok; not making the cell phone that is also a design problem. So, let us say that you are interested in buying a cell phone, do you think then there is only one cell phone. So, there are lot of cell phones today which means each one of them is an alternative for you, but not all of them is an alternative for you. Why?

Student: Specific needs.

You have some specific needs, specific needs, specific limitations those become your objectives and your constraints ok. So, design always the moment you say design it means that there are alternatives and when you have alternatives, what would be your goal. So, you go to a company today.

Student: Company.

So, you go to a cell phone shop you say I want a cell phone or you even go to a hotel, you say I want [FL]. You go to a good hotel let us say ok, do not ask me what hotel, but you go to a good hotel. So, you go there and then you say I want a [FL], you think the guy will go and bring [FL] directly or what is the servers response is going to be when you say.

Student: (Refer Time: 20:36).

[FL].

Student: Quantity, different (Refer Time: 20:38) quantity they will ask.

Yeah, quantity is one thing yeah true.

Student: There are varieties, variety.

So, is he is gonna ask do you want plain [FL], do you want [FL], do you want that [FL], do you want mini [FL], do you want macro [FL], whatever that is right. So, there are alternatives ok. Now, the moment there are alternatives ok, leave your [FL] example come back to your cell phone example. The moment you have alternatives, what would govern your choice.

Student: Cost.

Cost is one thing that will govern your choice, but let us say that your again swift back to the your [FL] example. So, there are multiple choices right. So, what do you think is going to govern your.

Student: Best suited, best suited, best taste, best taste, depends on your hunger.

Depends on your what is your appetite at that point in time. If you know the cost and if you worry about the cost for [FL] yes ok, but [FL] are like 10's of rupees right. For a cell phone cost makes lot of sense like 8000, 20000, 30000. So, for cell phone cost makes sense, but for [FL] it is really not at this point right. So, appetite at that point in time, taste could be one thing, what is served in the next table also might influence your decision. So, the why I left out the social I mean left out the [FL] example is because, there are lot of social factors. In a cell phone also there is a social factor called the you know it is.

Student: (Refer Time: 22:02).

It is seen ourselves status symbol and you want to have peer pressure and all that but we are not talking about that. But, if you look at it people we call like social scientists ok. Today we use abstract mathematics to represent certain things in social sciences; there we will capture all these things. Like why an interior of a house should not be painted red, for instance this is a social factor that is involved with that.

So, now what happens is when you have an alternative; why I gave all these examples at the moment you have multiple alternatives, what is going to govern your choice ok.

Which [FL] are you going to order? Which cell phone are you going to get? Even when you filter it down based on the cost, based on your needs you are still going to have alternatives. You are saying my cost is 10000 rupees, I need a good battery backup, I need a good selfie camera kind of a stuff, it should have a high mega everything; then you still have alternatives ok. So, but for you to come from this much different cell phones to this much there were some criteria that made things for you like.

So, that let you make so, this criteria becomes important. What is the criteria that will govern my choice? So, for the same product he is going to ask for a battery backup, meaning for the same price for instance he is going to ask for a battery backup. He might ask for a selfie camera, he might ask for larger data capability, someone might ask for a good audio stuff in that and there are n number of features right For the same product same type of product meaning the choices might differ. So, is the case with an automobile for instance, if you take an automobile there are multiple alternatives; for the same cost you have a width of stuff.

Someone is focused on the efficiency of fuel, someone is considered on very good in aesthetics, someone is covered on power, but if you look at it many of these are conflicting ok. The idea is you want to have as many packed into the same stuff, but usually these are conflicting. If you want a very good power then you might not have efficiency in it. If you have a very good aesthetics maybe you might not have a power in that maybe. So, but we would like to bring this trade off together, that is why it is called a tradeoff. I would like to have as much as possible in the same system that is also the overall idea of optimization.

So, but coming back to the even the criteria; if you look at it from a design perspective there is one basic question that people usually ask is, what is the difference between design and analysis; is there a difference at all, is there a difference between design and analysis? The very fact that you have two different words tells you that they are different. What are the difference between design and analysis?

Student: (Refer Time: 25:10) after design analysis (Refer Time: 25:12).

After design analysis comes. So, after analysis there is no design.

Student: Analysis makes sure that design works.

Analysis makes sure that design works, to be more.

Student: Design.

Politically correct, analysis not make sure analysis says how a particular design.

Student: Works, works.

Works or what is the quantity of interest correct. Now, I ask you to design a cantilever beam ok. So, cantilever beam means tip load because, this is what we have understood from interviews. The moment you say draw a cantilever beam immediately we will go draw a cantilever beam and put it tip load ok. So, let us take that assumption there is a tip load there is a cantilever beam ok. What are the logical question that you are expected to answer I mean expected to ask me?

Student: (Refer Time: 26:14).

Sorry.

Student: Dimension.

Dimension of the beam ok. So, we will go to the cantilever beam problem. So, you are going to ask for dimension. So, in dimension what all will you ask?

Student: (Refer Time: 26:44) cross section.

Cross section dimensions, you will ask cross section dimensions. Someone said length then.

Student: Material, material, material properties material.

Material properties.

Student: (Refer Time: 27:04).

Sorry.

Student: Load, load.

Load yeah, load good. Yes, it is dependent on load.

Student: Section for the (Refer Time: 27:13).

So, this guy.

Student: (Refer Time: 27:18).

But did you differ did you decide did I tell you that it is a square, it is hollow. So, basically there is, but is it gonna affect.

Student: Yes.

Yes provided.

Student: (Refer Time: 27:33).

This is what we are talking about then ok. So,.

Student: (Refer Time: 27:42).

This is affected by your.

Student: Cross section.

Cross section right, so, then of course, your material property is this guy, then L is given ok. So, now the question is this is an alternative. Am I going to have a circular cross section? Am I going to have a hollow cross section? Am I going to have a square cross section? Am I going to have a I beam.

Student: I beam.

Can I have a C beam ok, or rather not like this that is the C not a C beam; should I have something like this. There are so many options, can I have a triangular cross section. The one classical stuff that we use is this and this or rather this also. There is a need why will you use an I beam of course, it there is some specific reasons where you will use an I beam. Any column in our buildings are also load carrying structures ok, but this is rectangular in cross section and that is I beam in cross section. What is the difference?

Student: Transverse load (Refer Time: 28:52).

Transverse load ok.

Student: Why to load carrying capacity.

Sorry.

Student: Why to load carrying capacity.

Why to weight to load carrying capacity, sorry always weight is less for the given outer dimension the I beam always saves.

Student: Weight.

Weight compared; obviously, because if I put a rectangle like this outside that I beam always I am carving out the information right. So, not a strength of material course, but we will tell. So, the deal is under certain conditions I works better ok. So, in any of the structures that you go and see in the workshop for instance any of the rails that you have it will only be I beam ok, it works good under.

Student: Bending.

Bending conditions it is very good ok. So but, why not for our column structures then.

Student: (Refer Time: 29:54).

It might also have other types of, it is not only bending I could just have some kind of a compressive load for instance ok. Buckling could be a situation that could happen and of course, there are also seismic loads if you think about it which we do not worry too much, but that is also there. So, in such situations we do not choose it, but what I am saying is for the same type of cantilever beam, depending on what your application is you would choose the different things. So, that criteria could be your application ok, could be what your goal is ok. I want to reduce weight and I will have the criteria as my constraint as well. So, the criteria is the one that lets you choose which one of this I am going to take.

So, now that process is called design and it is iterative. Please understand you did this you will figure out that it is not and then you go back and then change a little bit in the design ok. That but, that you need to know whether you have rights on changing L, you have rights on changing E, you have rights on changing I. So, then what is analysis?

Student: (Refer Time: 31:06).

So, deciding what these are.

Student: (Refer Time: 31:12).

Is your design, when I put that into the equation what will my displacement b is called analysis. Sir, what is the big deal we know PL cube by 3 EI. Let us say that I am lazy I do not even want to calculate this I put in a excel sheet, you just give me what E IR, is it will give me delta what is the analysis. True putting it in excel sheet is a analysis ok. Now, the moment I make this cantilever beam slightly complex, you cannot use this equation anymore.

Immediately what you will do that was the first question that I asked you, you take the help of a software which essentially divides this into multiple elements; uses some partial differential equation to solve that. So, this part an are an equivalent of this in a computer model and solving it is what is we call as analysis. So, if you look at it analysis is a step in design. For a given combination of dimension material property and loads, you go and plug that into your computer model it will tell you what your responses. So, that is one analysis.

So, for you to have an idea of for a given length, for a given cross section, for a given load I need to know what my displacement is; where I do not have my explicit equation. If you do not have this you need to run a computer model, then only the analysis will say oh this stress is too large. Sorry this displacement is too large, that is not that is much more than my allowable displacement. So, immediately you can just use your simple commonsense to say probably I need to reduce my length or I need to let us say that it is more. Then you need to reduce your length, one way to do that would be to reduce your length or you need to.

Student: (Refer Time: 33:31).

Change your material property accordingly or play around with your I, depending on what you have where you have controlled, what you can change. So, these are sometimes in some text these are called control variables. In the context of optimization, these are called what variables?

Student: (Refer Time: 33:48).

They are called design variables because, they govern the design, they tell you these guys so, they are called the design variables. When you modify the design variable the responses likely to change ok, that is called analysis. For each combination of my design variables, what is my response value is called an analysis and multiple analysis is typically encompasses a design.

Because, every time what happens is under the context of design you will have to have an analysis done and you will have a design variable. For a particular design variable I do this analysis, I check whether my criteria is and then yes, no. If it is no, it goes back changes my design variable, comes back in this. If it is yes, look for convergence that we will talk stop.

So, in this whole stuff this analysis is an iterative thing that is what I told that design itself is an iterative stuff ok. We are not even going into a new product development or a new product design because, then you will have to go into user requirement analysis and then choose the material. After doing an analysis you will figure out that this is not what it is, you go back and change the entire design that is not what we are talking about. We know that you need a cantilever beam, we know that you are going to do a electric scooter, you are doing to do a crankshaft for a particular automobile. So, we know all that in that specifically what or how you are going to change the design is what the question is ok.

So, if you look at it people talk this is also what you call like inter disciplinary ok. So, one requires a mechanical background, the other one would require a civil background, someone something might require an electronics background. But, the technology for you to let you or the algorithms that allow you to make this decision is the same in terms of optimization ok. So, this is just to tell you what an analysis is, what criteria is and what is a design; these are all subsets of a design. But, why are we desired talking this in the context of optimization. This whole stuff that I am talking about, can be cast into an optimization problem which is what we are interested.