Research Methodology
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Lecture - 49
Theoretical Research: Functional Relationships from Experimental Data, Part 01

We have learnt how to do measurements. We have learnt how to use the measurements for hypothesis testing. And now we will take on the problem of Theoretical Research. What does a theorist actually do? Theoretical Research entails a few different things.

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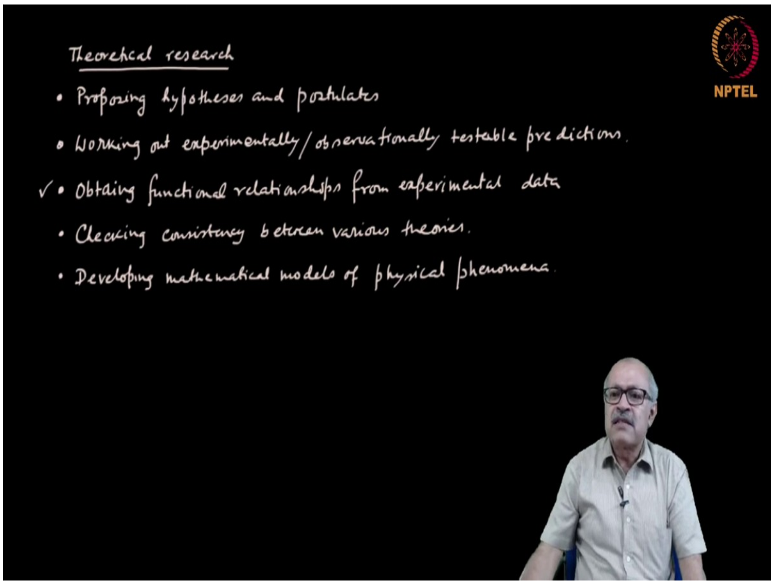

We will talk about theoretical research today. There are a few things that a theorist does. Firstly, proposing hypotheses and postulates to explain various physical phenomena and processes. For example, in order to explain the apparent motion of the planets, Newton proposed the Theory of Universal Gravitation. That is a postulate he proposed, and then he had to show that if this postulate is true then what is observed should be observed.

So, that is the task of a theorist. Encountering a situation, encountering a phenomenon, the theorist tries to figure out why did it happen? How does it happen? And the answer to these questions normally come from a hypothesis or a postulate. So, proposing that, working that out is the task of a theorist.

As a good example of a hypothesis, for example, Laplace's hypothesis on the origin of the solar system that there was a nebula which condensed to form the sun and as it condensed it was spinning fast and so it took a disc shape and the sun formed at the centre, the planets formed at the outer periphery of the disc. So, this was another hypothesis by Laplace. They were theorists trying to propose postulates or hypotheses to explain certain observed phenomena.

Secondly, when one proposes a hypotheses or postulate, one has to work out the experimentally or observationally testable predictions. So, the task of a theorist is not only to propose a hypothesis, but also to work out the experimentally or observationally testable predictions. For example, somebody proposed the Big Bang Theory, but other people worked on the Big Bang Theory and showed that if the Big Bang Theory is true, then the observable ratio of hydrogen and helium today should be this. Then, on that basis, one can go on to check whether the predicted thing is true or not. And if it is not to be found true, then the premise on which it was built should be false. But if it is true, then it will only strengthen our confidence on that particular theory.

This step essentially is related to some numerical values. One has to predict something that is observationally or numerically or experimentally testable means one has to predict a value and that is what is ultimately tested. How to test that, we have already covered in this course.

Now, when a particular phenomenon is encountered an experimentalist normally does some preliminary investigation of that. Identifies what are the independent variables that can be varied independently of everything else. If these are varied, what vary as a result of that—these are the dependent variables. So, one identifies the independent and the dependent variables.

Normally, in order to obtain the initial clues, one performs some experiments where one varies the independent variables and observes the resulting change in the dependent variables. And these are plotted as graph and from there, one is often able to extract some kind of a functional relationship.

And once these functional relationships are obtained, then that provides the clue to the theorist. So, obtaining functional relationships from experimental data is an important activity. For example, when we encountered for the first time the issue of black body radiation, then the black body radiation was experimentally tested. That means, the quantity of radiation in different wavelengths was plotted and from there obtained a graph like this. From there people tried to extract some kind of a functional relationship, one for this part and another for that part. So, we had a functional relationship and then the task of the theorist was to answer why is this particular relationship.

But, the first step was to obtain some kind of a functional relationship. If something is exponentially related to another variable, then one has to explain why is this exponential relationship true.

The fourth thing that a theorist does is a bit subtle. The point is that, all the different theories in a particular branch of science should be consistent with each other. That means, if this is true, this cannot be true—that kind of situation should not prevail. If there are two theories they should not contradict each other, at least they should be consistent with each other.

Across the disciplines also, for example, if something is a theory in physics, that should not be at odds with a theory in chemistry; or if this theory is true, then that should not be observed in chemistry which is actually observed. So, this should not be the situation. That means, there has to be, both within the discipline as well as across discipline, consistency between theories, and that is what a theorist always has to check.

For example, Einstein noticed that there is a inconsistency between Newton’s laws of motion and Maxwell’s laws of electromagnetism. There is a basic inconsistency between them. If this is true, there is a difficulty in accepting that. So, there is an inconsistency, and in order to resolve that inconsistency, Einstein developed his theory of relativity.

So, two theories have to be consistent, checking consistency between various theories is an important activity. One cannot develop a theory in, for example, particle physics or condensed matter physics that will be at odds with what is known in, say, relativity. So, one has to be consistent. One has to check for consistency.

A theorist has to develop mathematical models of physical phenomena, because, if you have a mathematical model, with that you can understand why a certain thing happens, why a certain thing behaves the way it does or you can also predict what will be the behaviour of a system under certain specific circumstances.

So, these are essentially the things that a theorist does. But, at the base of it, anything that a theorist does, should have explanatory power. It should explain something, and it should explain more than what it was initially proposed to explain. So, it has to have a broader explanatory power.

Take any good theory: theory of electromagnetism by Maxwell, theory of motion by Newton, the theory of relativity by Einstein, theory of biological evolution by Darwin—all these have great explanatory power. So, that is another thing that a theorist tries to achieve to explain something.

We have already done the ‘proposing hypothesis and postulate’ part. Working out the experimentally or observational testable predictions is something that we will do. But let us first take this particular part: Obtaining functional relationship from experimental data.

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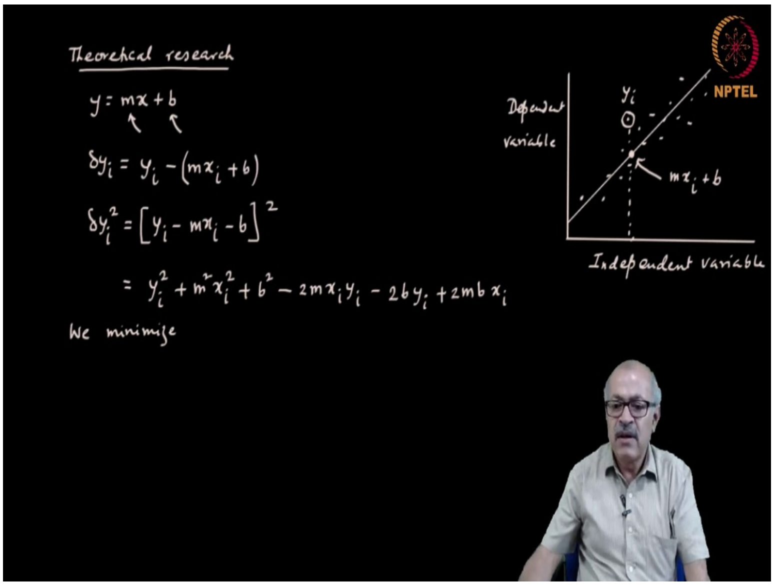

When you have plotted some experimental result, then it is often depicted like this. Here, for example, it could be the independent variable and here is the dependent variable. And you can have points something like this, scattered for different values. A scatter of points like this would essentially indicate that there is a straight line passing through it.

So, on visual inspection, we might guess that there is a straight line fit, something like this. But, a visual inspection does not always give accurate results, so we have to get a good fit of this graph. In some cases the data plotted might not indicate a straight line relationship, or a background theory might not indicate a straight line relationship. It might be a curve or something like that.

We will deal with these cases later. But most important is that, this has to be fit in some kind of a functional form. And the simplest functional form is the straight line form. So, let us first deal with that.

Wherever there is a possibility of fitting into a straight line, then we will try to fit that and here the expression that we have to obtain is y is equal to m x plus some constant b.

$$y = mx + b$$

So, b is here, m is the slope of this line. So, when you have a situation like this, these are the individual points. For example, let us assume that this point is the ith point.

For this value of the independent variable, if the straight line fit says this point and the actual point is out there, so, there is a gap. There is a difference between them. So, let us call that y and this is the ith point. Here, this particular point: at the same value of the independent variable x, this is m x_i plus b. The ith point. We are trying to fit as good as possible.

So, how do we do that? Effectively, we are trying to estimate the values of m and b and that should be the best possible estimate. How do you judge if something is the best possible estimate? The difference of the points on this line and the actual points observed in the experiment should be the minimum. But we see that there are differences.

So, if you draw different lines at different slope and different values of b, you will find that the on an average the difference between the points on the line and the actual points that are obtained will be different, and this is what we need to minimize. So, we are actually talking about the difference delta y_i. At the ith point, delta y_i is the difference: y_i - (m x_i + b).

And for every point there will be such a delta y_i and overall that has to be minimized. But this will lead to positive values as well as negative values. If at some place it is positively deviated and at some place it is negatively deviated, they might cancel each other. To avoid that, we take a square of this.

So, what we try to do is to take a square of that. y_i square is equal to this whole thing square. This whole thing square is y_i minus m x_i minus b square which we can expand as

$$
\begin{aligned}
(\delta y_i)^2 &= \left[y_i - (mx_i + b)\right]^2 \\
&= y_i^2 + m^2 x_i^2 + b^2 + 2mx_i b - 2mx_i y_i - 2y_i b
\end{aligned}
$$

So, that is what happens when we expand it.

Now, this is what we will try to minimize. What we minimize is the summation of all these values for all these points.

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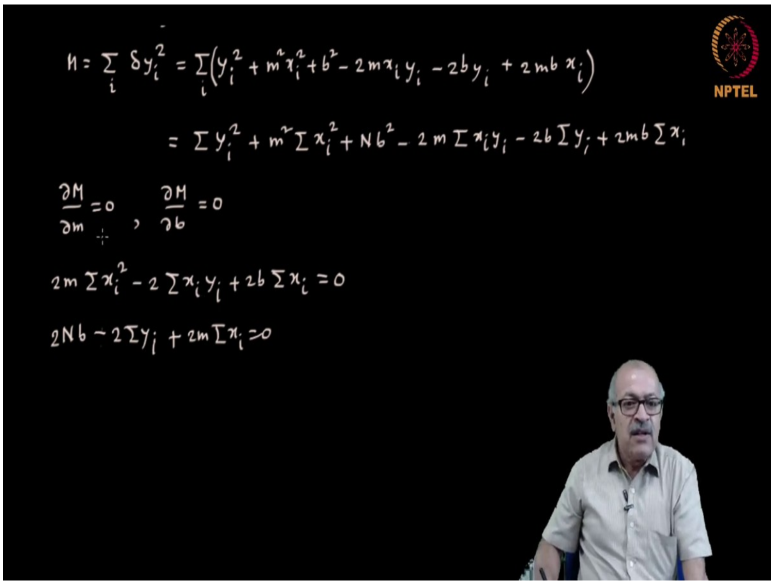

So, we are actually trying to we minimize: let us call it M is equal to summation of all the delta y_i squares summation over i. And then if we substitute it here, we get summation over i. Summation i of what? This is

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\begin{aligned}
M &= \sum(\delta y_i)^2 \\
&= \sum y_i^2 + m^2\sum x_i^2 + Nb^2 + 2mb\sum x_i - 2m\sum x_i y_i - 2b\sum y_i
\end{aligned}
$$

This whole thing will be summed with respect to i. And if we now expand it then we find that.

So, this is this whole thing. This whole thing is summed over i. Now if you now expand it, term by term sum over y i square plus m square sum over x i square plus b square it has to be counted n times because it is summed. So, it is the n total number of points times b square plus twice m sum minus sum over x i y i minus twice b sum over y i and this is plus twice m b sum over x i. So, we have this situation.

Now, this is what we are trying to minimize. For all minimization problems we are trying to minimize it, and thereby we are trying to obtain the best values of m and b. So, we will need to obtain the derivative of capital M with respect to small m and we have to equate it to 0 and then we have to take the derivative of capital M with respect to b and again equate it to 0.

$$
\frac{\partial M}{\partial m} = 0 \ \text{ and } \ \frac{\partial M}{\partial b} = 0
$$

So, these are the two things we need to obtain and equate to 0. Now, if you take a derivative of capital M with respect to small m the first one yields, this one will yield nothing, this one will yield twice m this so it is twice m sigma x i square, this will yield nothing because it is differentiation with respect to m, this one will yield minus twice sum x i y i, this one will yield nothing, this one plus twice b sum x i that should be equal to 0.

$$2m\sum x_i^2 + 2b\sum x_i - 2\sum (x_i y_i) = 0$$

Similarly, if you take a derivative with respect to b then we get first one will yield nothing, second one will yield nothing, this is N twice N b plus this will yield nothing, this will yield sorry minus twice sum over y i and this is plus twice m sum over x i equal to 0.

$$2Nb + 2m\sum x_i - 2\sum y_i = 0$$

Now, these are two simultaneous equations with two variables m and b and it can be easily solved. I will not go into the trouble of actually solving it, because it is somewhat longish algebraic procedure which is conceptually trivial.

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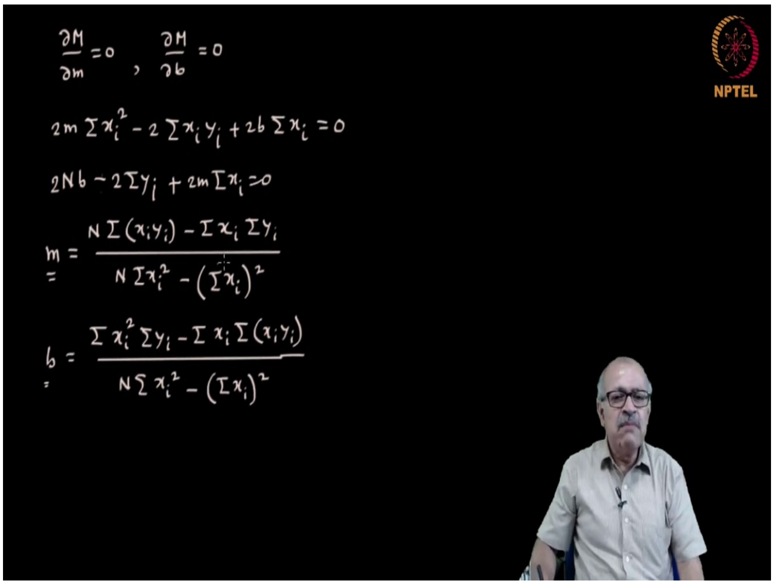

So, I will just write down the results:

$$m = \frac{N\sum(x_i y_i) - \sum x_i \sum y_i}{N\sum x_i^2 - (\sum x_i)^2}$$

Well this is the expression for the m and the similar expression for b we can obtain as conceptually obtaining this expressions are rather simple. So, I am not going into the details of that. It is actually trivial.

$$b = \frac{\sum x_i^2 \sum y_i - \sum x_i \sum (x_i y_i)}{N\sum x_i^2 - (\sum x_i)^2}$$

So, these are the values of m and b. You notice that the right hand side each term in the right hand side are known.

So, if the data are known, all you need to do is to put the things in the right hand side and then calculate the values of m and b. So, this is how we actually obtain the slope and the value of b from the data. This is called the least square fit, because you see that here we are taking the square of the differences and its sum is something that we are minimizing. It is least of the squares. So, this is called the least square fit. There are many programs in which these expressions are already input. So, all you need to do is to feed in the data it will give you the expression for the straight line.