Research Methodology

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Lecture - 50
Theoretical Research: Functional Relationships from Experimental Data, Part 02

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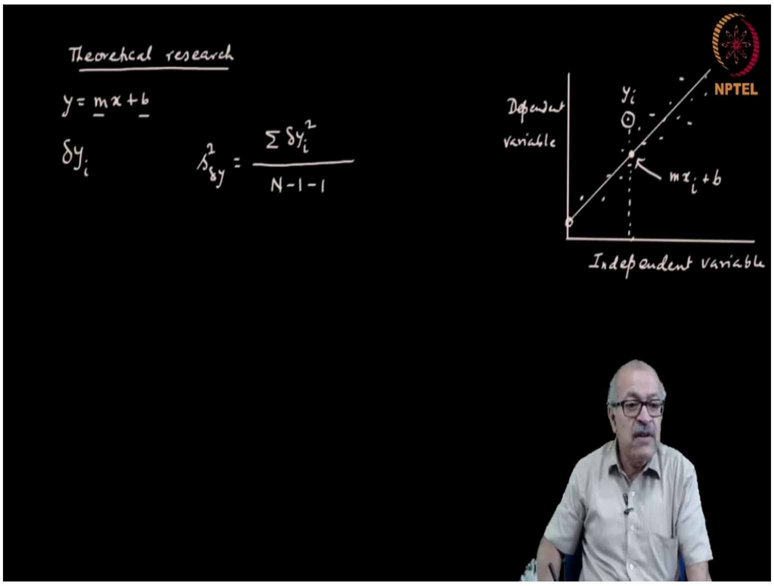

You have to notice one thing: if the data actually do not really fit a straight line and you apply this method, you will still get some value of m and some value of b. That does not mean it will make any sense. So, one has to first ascertain that either from the theory you do expect a straight line fit, or the data when plotted do indicate a straight line fit. Then only you should apply this method to obtain the values of m and b.

Else, what you do where the graph does not indicate a straight line fit, what do you do then, I will come to that later. But obtaining what you have just obtained: we have obtained the value y is equal to m x plus b, we have obtained m, and we have obtained b. This does not suffice.

The reason is that we have obtained some values, but whenever we want to state we always have to state with the error bar. So, we have to obtain the estimated value of m, but there has to be an error bar stated with m, there has to be an error bar stated with b. So, from the data we also have to obtain the standard error in m and the standard error in b. Without that, the scientific enterprise of estimating the straight line fit is not complete.

In order to do that, first let us try to figure out how much would be the deviations. That means, the delta y_i, these are the deviations of the actual data points from the straight line fit. If they have a distribution, then there should be a mean and there should be a standard deviation. Right? How to calculate the standard deviation of this?

How do you calculate the standard deviation of the deviation from the straight line fit? While we do that, we are assuming that we have estimated m and b, thus we have estimated the straight line, and now we are talking about the deviation from that.

So, I will write it as s square which is the variance of delta y. What is that? That will be all these, the various delta y squares. Normally in order to obtain the variance, we divide it by N, the total number of points, minus 1. But here notice that the points are not scattered in any possible way. The points are scattered around an one-dimensional object. It is basically these deviations we are talking about, not just a scatter of points and their standard deviation.

So, because it is now scattered around an one-dimensional object, therefore, the dimension has reduced by another one. So, it is minus another minus 1.

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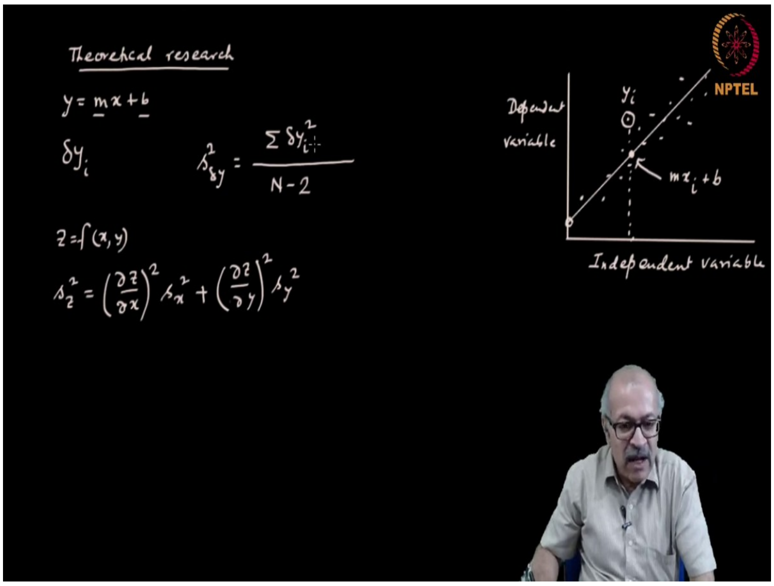

So, effectively it is N minus 2. This is how you have to obtain the standard deviation after you have obtain the m and b, because you have estimated the straight line then these are calculated from that. So, square root of that will be the standard deviation.

Now, we are actually trying to find out the standard deviation in m and the standard deviation in b. What does it depend on? They depend on these deviations.

Earlier, when we were talking about a variable z depending on x and y, we knew the error standard errors in x, we knew the standard errors in y, then what will be the standard error in z? We had earlier encountered a situation where z was a function of x and y, then we saw that the variance in z is the derivative of z with respect to x square, s_x square plus derivative of z with respect to y square s_y square.

$$s_z^2 = \left(\frac{\partial z}{\partial x}\right)^2 s_x^2 + \left(\frac{\partial z}{\partial y}\right)^2 s_y^2$$

So, this is something that we encountered earlier when we are talking about propagation of errors and this is what we will use. In what sense? In the sense that the deviation the variance in m, the variance in b will be dependent on the variance of these y's, delta y's.

So, that is how you will use it. If I want to write it, it will look something like this.

$$\begin{aligned} s_m^2 &= \left(\frac{\partial m}{\partial y_1}\right)^2 s_{\delta y}^2 + \left(\frac{\partial m}{\partial y_2}\right)^2 s_{\delta y}^2 + \cdots \\ &= s_{\delta y}^2 \left[\left(\frac{\partial m}{\partial y_1}\right)^2 + \left(\frac{\partial m}{\partial y_2}\right)^2 + \cdots\right] \\ &= s_{\delta y}^2 \sum_k \left(\frac{\partial m}{\partial y_k}\right)^2 \end{aligned}$$

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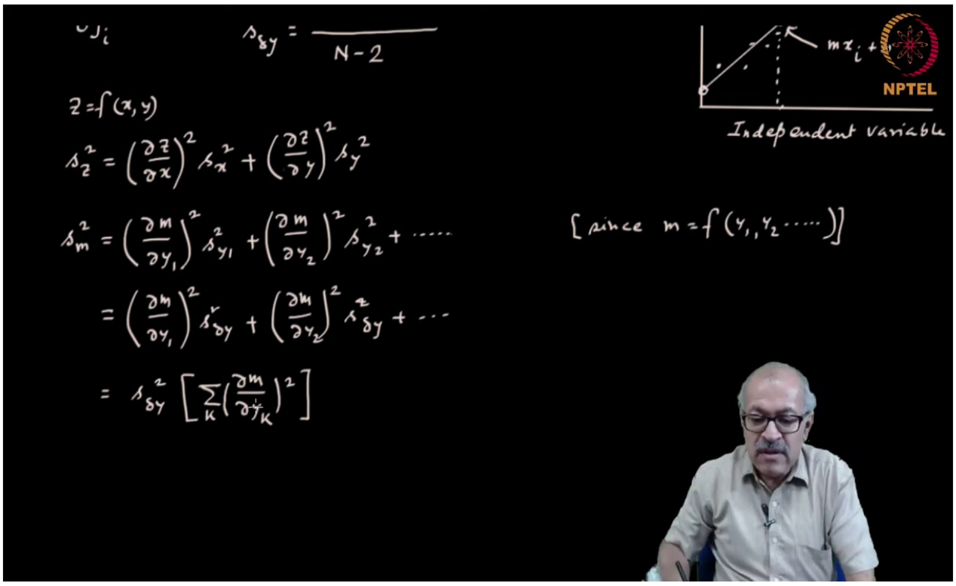

The variance in m will then be dependent on delta m by delta y_1, y_1 is actually the first point, say, here. The delta y_1 is the difference of the first point from the straight line. So, delta y_1 times the variance in y_1 plus delta m delta y_2 square, there is a variance in y_2 plus dot dot dot dot dot. Why? Because m is a function of y 1, y 2, and all that, those data points.

Now, the variance of y_1 and y_2 and y_3, these are not actually different things. These are basically this variance. So, we can simplify that as delta m, delta y_1 times this one is nothing but s square delta y (because this s square delta y is the variance of the data points from the straight line fit and this is just one of them). So, it will have the same character.

Similarly, delta m delta y_2 times s square delta y plus and all that. So, effectively then this will get the s square delta y square common. And what remains inside is nothing but these individual ones, which can be written as sum over delta m delta y_k, its square and sum over k.

So, all I have done is to take these common. What remains are these terms. I have expressed that as a sum; that is what I have done. So, now, we need to find out these values.

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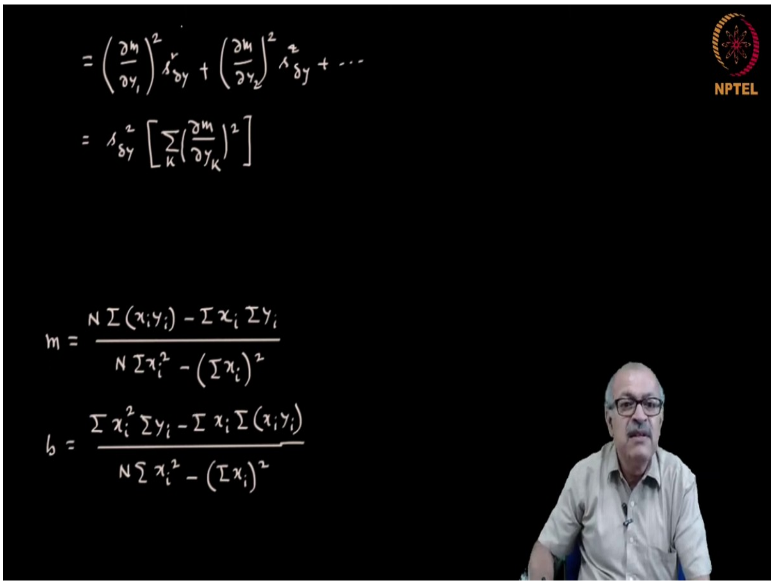

In order to find these values, I will use whatever we had earlier calculated as the m and b. So, s_m square, the variance in m is given by this.

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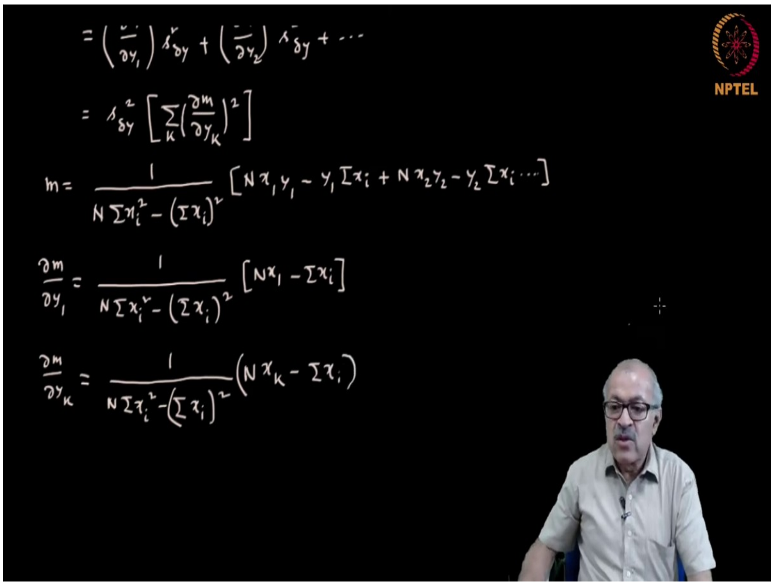

Now, we have already seen that m was two separate quantities. The denominator first: that was N sum over x_i square minus sum over x_i whole square. That was the denominator. The numerator was: N x_1 y_1, I am breaking apart in form of 1, 2 and all that. So, it will be N x_1 y_1 minus it was y_1 sum over x_i. So, that was the first term.

Similarly, there would be similar terms for 2. So, plus N x_2 y_2 minus y_2 sum over x_i dot dot and that continues.

$$m = \frac{1}{N\sum x_i^2 - (\sum x_i)^2}\left[N x_1 y_1 - y_1 \sum x_i + N x_2 y_2 - y_2 \sum x_i + \cdots\right]$$

Now we are to find the derivatives. So, we have to differentiate m with respect to delta y 1, the first one. And that will indicate what will happen for the general case k.

$$\frac{\partial m}{\partial y_1} = \frac{1}{N\sum x_i^2 - (\sum x_i)^2}\left[N x_1 - \sum x_i\right]$$

So, if I take the derivative, the denominator remains the same. So, denominator is N sum x_i square minus sigma x_i whole square. Now, the first one yields only N x_1. This one is minus sum over x_i and the rest will disappear. Similarly for y_2. It will have the similar terms, only 2 here.

Similarly, for y_k, it will be k here.

$$\frac{\partial m}{\partial y_k} = \frac{1}{N\sum x_i^2 - (\sum x_i)^2}\left[N x_k - \sum x_i\right]$$

So, we can in general write the delta m delta y the kth term is, the denominator remains the same, N sum over x_i square minus x_i whole square. Here it will be N x_k minus x_i. So, in general, we can write this. If we can write this, then we can also write its square that is what we need ultimately because we are interested in the terms like this square.

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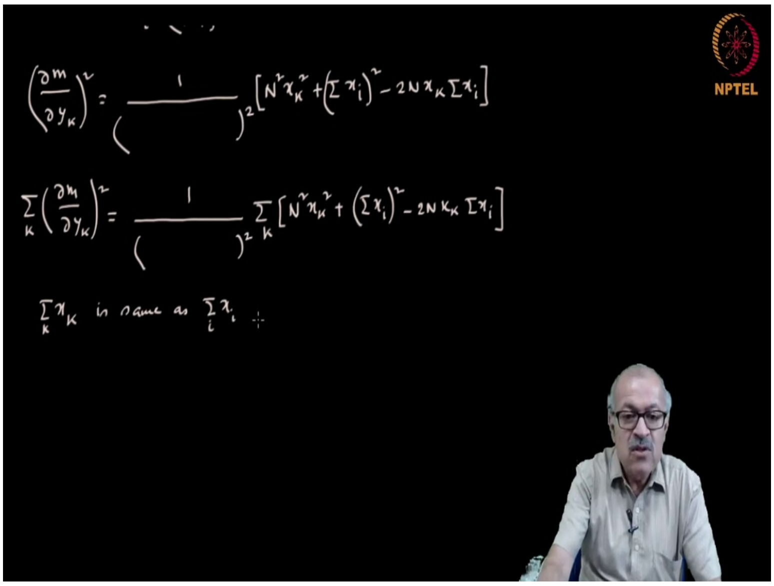

$$\left(\frac{\partial m}{\partial y_k}\right)^2 = \frac{1}{\left[N\sum x_i^2 - (\sum x_i)^2\right]^2}\left[N^2x_k^2 + (\sum x_i)^2 - 2Nx_k\sum x_i\right]$$

So, delta m delta y k, its square will be this term squared is equal to 1 by this term squared this whole term squared. In the numerator, it will be N square x_k square plus sigma x_i whole square minus twice N x_k sigma x_i.

Now, what we need is sum over all k. This has to be summed over all k.

$$\sum_k\left(\frac{\partial m}{\partial y_k}\right)^2 = \frac{1}{\left[N\sum x_i^2 - (\sum x_i)^2\right]^2}\sum_k\left[N^2x_k^2 + (\sum x_i)^2 - 2Nx_k\sum x_i\right]$$

So, sum over k of this fellow, delta m, delta y_k whole square. The denominator did not contain any k term, so that will remain as it is. So, I will just write 1 by whatever it was square; I am not writing every time because it will only consume time. And here we have sum over k of this term.

So, let me just write N square x_k square plus sum over x_i whole square minus twice N x_k sum over x_i. This is what we have to calculate.

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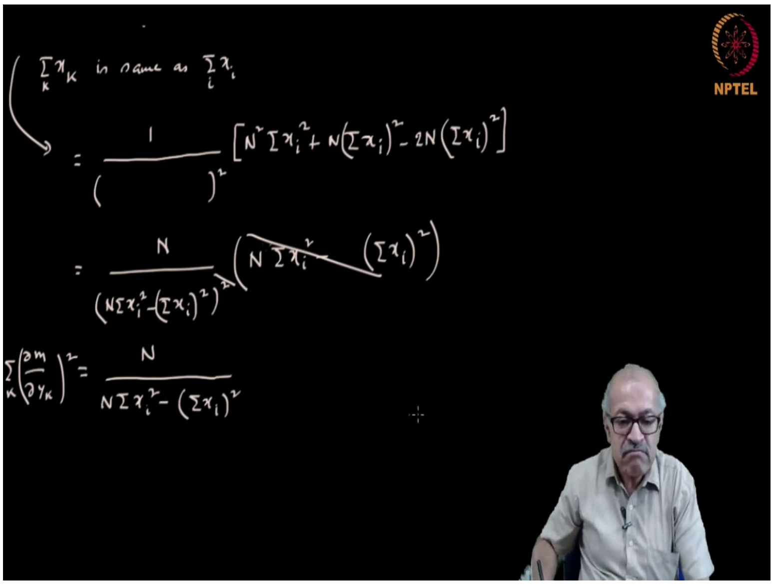

$$\begin{aligned}
\sum_k \left(\frac{\partial m}{\partial y_k}\right)^2 &= \frac{1}{[N\sum x_i^2 - (\sum x_i)^2]^2}\,[N^2\sum x_i^2 \\
&\quad + N(\sum x_i)^2 - 2N(\sum x_i)^2] \\
&= \frac{1}{[N\sum x_i^2 - (\sum x_i)^2]^2}\,[N^2\sum x_i^2 - N(\sum x_i)^2] \\
&= \frac{N}{N\sum x_i^2 - (\sum x_i)^2}
\end{aligned}$$

Now, notice that the sum over k x_k, is same as sum over i x_i, because this i and k are just dummy variables. So, we can proceed by expressing this as this can be written as equal to; I will keep the denominator as it is 1 by this square. In the numerator, this will become sum over, I will change k to i, it is N square it would be sum over x_i square.

This one is repeated N times, so you will have N plus N sum over x_i this is whole square, whole square minus twice N, this one will be x k sum over, this will result in the same as sum over x i. So, this will be sum over x_i whole square because this sum over k x_k and sum over i x_i are the same things. So, this is basically sum over i x_i twice, so it has become square; is equal to again 1 by whatever it was in the denominator, square.

Now, notice that this and that are the same, this is only twice of that, so we get simply N square sum over x i square minus again N whole sum over x_i whole square. Now, notice what was here you can now take N common, so, this one disappears, square is not necessary, and this one is also appearing.

So, let it remain as it is. So, you have this. What was in this bracket? You notice that it was this. So, now, let me write it: N sigma x_i square, N sigma x_i square minus sigma x_i whole square minus x_i whole square. Notice that this is exactly the same and here is a square. So, this will cancel off with the square, leading to a simpler expression N divided by N sigma x_i square minus x_i whole square.

So, the left hand side was this. Let me write this as sum over k it is delta m delta y_k whole square was this.

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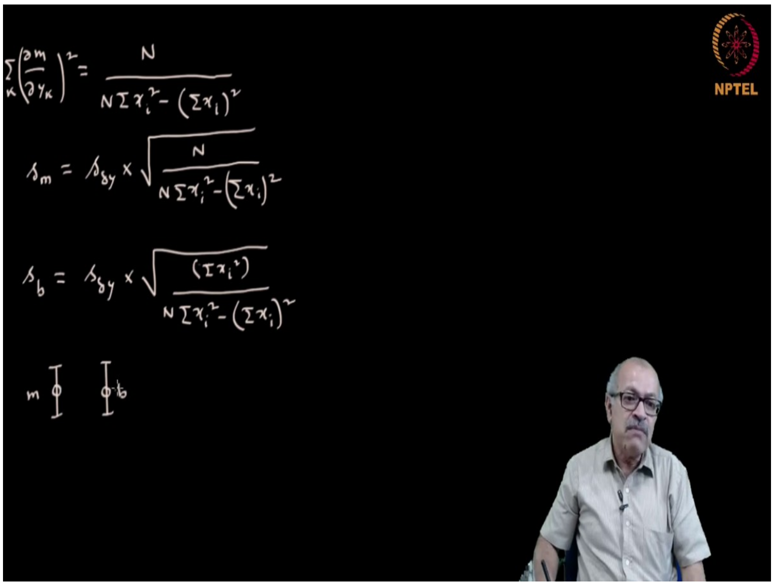

$$s_m = s_{\delta y} \times \sqrt{\frac{N}{N\sum x_i^2 - (\sum x_i)^2}}$$

So, we can now express s_m, the standard deviation in m as standard deviation in delta y, which we have we have already calculated, times the square root of this, square root of N by N sum over x_i square minus x_i whole square. So, this is the standard deviation in m.

And in quite that the similar way we can calculate this standard deviation over b. The method is the same, but it will again be a repetition of the same method of calculation. So, we will not do that. We will simply write the result. It is again the square root of sum over x_i square divided by the same thing: N sigma x_i square minus sigma x_i whole square.

$$s_b = s_{\delta y} \times \sqrt{\frac{\sum x_i^2}{N\sum x_i^2 - (\sum x_i)^2}}$$

So, we have been able then to obtain the value of m with an error bar, and the value of b with an error bar. This is what is needed. That means, when we talk about a straight line fitting, we essentially estimate the values of m and b. But at the same time we have to estimate what could be the error, what could be the standard error for m and b.

And this is what we have been able to calculate by calculating the standard deviation s_m and standard deviation s_b. So, this way we have been able to calculate the standard errors in the value of m the value of b.

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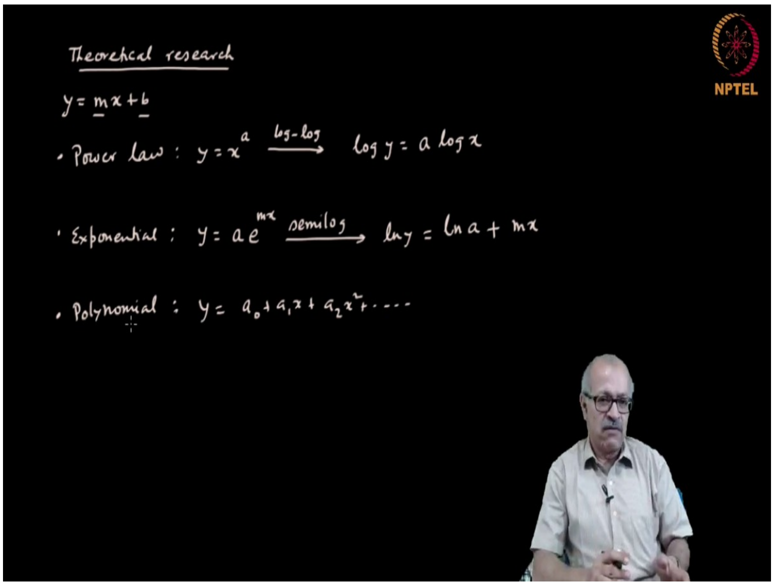

This was where you are trying to fit into a straight line. But as I said, all fitting need not be fit into a straight line. There are other situations where some non-linear fit is necessary. But in that we have to be bit careful because there are certain non-linear functions that are more prevalent, common, in physical sciences, and there are some which do not really yield much insight. The ones that are really important are the exponential function and the power law.

So, first the power law and second the exponential. These two the functional forms yield some physical insight and that is why physicists are often interested in these.

$$y = x^a$$

For power law it is y is equal to x to the power some constant a and this is y is equal to e to the power x or let me write this rather general form, one can write it as e to the power some m x and there is a coefficient a. That is a general form of the exponential function.

$$y = ae^{mx}$$

How do you do that? We extract this by actually reducing to the linear form. How? If you plot that in a log graph, then you actually do this a log of y is equal to a log of x.

$$\log y = a \log x$$

So, this is a straight line relationship between two logs and the log could be with the base of anything, it could be 10, it could be 2, it could be e, whatever.

So, in this case, we simply plot the same data on a log graph and if it now approximates a straight line, then it is a power law. And this straight line fit can be can be found exactly the way I have just shown.

In case of the exponential graph, we plot it on a semi log graph. Well, this will be in the ln and this will be just plotted. So, this will be ln y is equal to, this will be ln a plus this will be just m x.

$$\ln y = \ln a + mx$$

Now, because it is e to the power m x, this has to be only to the natural logarithm. This will be in the natural logarithm form. If you do that, then you will get again a straight line fit with this representing b. So, in both these cases it can be cast in the form of a straight line fit and the straight line fit can be obtained by the least square method that I have just shown. So, all these forms then can be extracted from the same method that I have already illustrated.

If there is some data which cannot be cast into either of these forms, but it is apparent that it is a non-linear data, then we try to express it as a polynomial fit. Polynomial fit, which is basically y is equal to sum a0 plus a1 x plus a2 x square plus dot dot dot. Any graph can be fit into this form. But let me tell you that it does not really yield any physical insight.

Having expressed a graph in this form is essentially admission to the fact that, you are saying ‘I do not know what the functional form is’. So, this will not help the theorist to obtain a reason why it should be so. If it is a form like this, then a theorist can try to find out why it should be so. If the it is like this then also the physicist can try to find out why it should be so. But if it is like this, one cannot.

So, in general, even though any graph can be fit into the polynomial form, it does not really lead to much insight and therefore, we normally do not do it. So, effectively, meaningful curve fitting are obtained in the form of the linear fit or the power law fit or the exponential fit. The others really do not yield much insight and therefore, I will not cover that in this course.