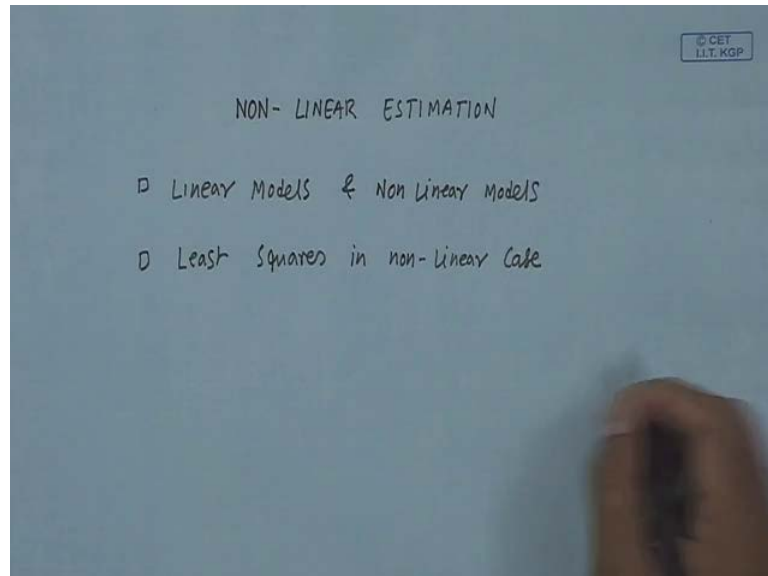


Regression Analysis
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Lecture - 32
Non-Linear Estimation

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Hi, today we will start non-linear estimation, and here is the content of this topic linear models and non-linear models. So, we will give detailed definition of non-linear models and then we will talk about least square in non-linear case, so how to fit non-linear model using least square technique. So, given a set of observation say x_i, y_i , the starting point is that we start with the simple linear regression model or if we have more than one regressor we start with multiple linear regression model. Of course, those models are linear model. Also you must have realized that the polynomial regression is also a linear model. So, let me give the detailed definition of non-linear model and also linear model.

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Linear Models Models that are linear in parameters
are called linear model

$$Y = \beta_0 + \beta_1 Z_1 + \beta_2 Z_2 + \dots + \beta_{k-1} Z_{k-1} + \epsilon$$

where the Z_i is any function of the basic regressors.
 x_1, x_2, \dots, x_{p-1}

$$Y = \beta_0 + \beta_1 (x_1 - x_2) + \beta_2 (x_1 - x_2)^2 + \epsilon$$

is a linear model.

Linear models, models that are linear in parameter are called linear model, this is important linear is in parameters not in the regressor. The model for multiple linear regression is beta naught plus beta 1 z 1 plus beta 2 z 2 plus say beta k minus 1 z k minus 1 plus epsilon. Where, the z i is any function of the basic regressor variables. What I mean by this, the basic regressors are say x 1, x 2 say x p minus 1. Then y is equal to beta naught plus beta 1 into x 1 minus x 2 plus beta 2 into x 1 minus x 2 square plus epsilon. So, this is a linear model. Because here, z 2 could be any function of the basic regressors. But, this model is linear in parameters, the parameters are beta naught, beta 1 and beta 2. So, this model is called linear models.

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Non Linear Models: Models that are non-linear in parameters

$$Y = e^{\theta_1 + \theta_2 t + \epsilon} \quad \text{--- ①}$$
$$Y = \frac{\theta_1}{\theta_1 - \theta_2} [e^{-\theta_2 t} - e^{-\theta_1 t}] + \epsilon \quad \text{--- ②}$$

t: regressor variable
 θ : parameters.

① & ② are non-linear in the sense that they involve θ_1 & θ_2 non-linear way. ① is called intrinsically linear

① can be transformed to $\ln Y = \theta_1 + \theta_2 t + \epsilon$

Non linear models, models that are non-linear in parameters are called non-linear model. Let me give examples, Y is equal to e to the power of theta 1 plus theta 2 into t plus epsilon. So, here y is the response variable and in non-linear case generally we represent the regressor variable by t instead of x. So, this is a non-linear model because it is non-linear in theta 1 and theta 2.

Let me give one more example, say y is equal to theta 1 by theta 1 minus theta 2 into e to the power of minus theta 2 t minus e to the power of minus theta 1 t plus epsilon. So, this is very clear that this model is non-linear in parameters, parameters are theta 1 and theta 2. So, these are the non-linear models and here t is regressor variable and theta are parameter. So, let me call it say 1 and 2. 1 and 2 are non-linear, in the sense that they involve the parameters theta 1 and theta 2 in non-linear way. That is why these two models are called non-linear. And now you can see that 1 can be transformed to say log base e, so $\ln y$ is equal to theta 1 plus theta 2 t plus epsilon.

So, once you take this transformation this non-linear model becomes linear, linear on the data $\ln y$ and t. This type of non-linear functions are called intrinsically linear. So, 1 is called intrinsically linear, because you can very easily transform this non-linear model to a linear model by taking some transformation. Well, so we understood what is linear model and what is non-linear model.

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Least Squares in non-linear case

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Standard notations for linear & non-linear Least Squares

Response	Linear Y	non-linear Y
Subscripts	$i=1, 2, \dots, n$	$u=1, 2, \dots, n$
Regressor variables	X_1, X_2, \dots, X_{k-1}	t_1, t_2, \dots, t_{k-1}
parameters	$\beta_0, \beta_1, \dots, \beta_{k-1}$	$\theta_1, \theta_2, \dots, \theta_{k-1}$

And, this is the notation for the linear and the non-linear case. So, given a non-linear model we are going to estimate the parameter of the non-linear model. Here, are some notations, you can see that for response variable in the linear case we represent it by y . So, y generally stands for the response variable and in non-linear case also y stands for response variable, and subscripts for linear case it is i is from 1 to n , and then here you know just notation, and here we will use instead of i , that is instead of calling y_i we will say y_u and u is also from 1 to n , so n observations.

And, in case of linear models we use the regressor variables standard notations x_1, x_2, \dots, x_{k-1} . But, here we will be using t_1, t_2, \dots, t_{k-1} . And in case of linear the parameters are $\beta_0, \beta_1, \dots, \beta_{k-1}$ and in case of non-linear we use $\theta_1, \theta_2, \dots, \theta_{k-1}$, this notation you know and to make your life difficult. Well, now let me start with the non-linear model.

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$$Y = f(t_1, t_2, \dots, t_k, \theta_1, \theta_2, \dots, \theta_p) + \epsilon$$

write $\tilde{t} = (t_1, t_2, \dots, t_k)'$, $\tilde{\theta} = (\theta_1, \theta_2, \dots, \theta_p)'$

$$Y = f(\tilde{t}, \tilde{\theta}) + \epsilon$$

or $E(Y) = f(\tilde{t}, \tilde{\theta})$ if we assume $E(\epsilon) = 0$

we also assume that ϵ are uncorrelated, $V(\epsilon) = \sigma^2$

$$\epsilon \stackrel{\text{ind}}{\sim} N(0, \sigma^2)$$

Suppose we have n observations (Y_u, \tilde{t}_u) , $u = 1(1)n$.

$$Y_u = f(\tilde{t}_u, \theta) + \epsilon_u$$

Say, general model y equal to $f(t_1, t_2, \dots, t_k)$ and $\theta_1, \theta_2, \dots, \theta_p$ plus ϵ . So, this is non-linear model, f is non-linear in the parameters $\theta_1, \theta_2, \dots, \theta_p$, and in vector notation we write t equal to (t_1, t_2, \dots, t_k) and θ vector is $(\theta_1, \theta_2, \dots, \theta_p)$. And then in terms of this vector notation, we can write y equal to $f(t, \theta) + \epsilon$, or also we can write, expectation of y , this is the non-linear model we are talking about. Expectation of y is equal to $f(t, \theta)$, if we assume expectation of ϵ is equal to 0.

We also assume that ϵ are uncorrelated and also variance of ϵ is equal to σ^2 , and ϵ vector follows normal $N(0, \sigma^2)$ so independent. So, these are the basic assumption we do in case of simple linear regression model, simple or multiple regression model also, we are making the same assumption for the non-linear model. And suppose we have n observations like (y_u, \tilde{t}_u) , like we had before you know y_i, x_i for i equal to 1 to n . Here, notation difference is u from 1 to n . Then we can write y_u for the u th observation is equal to $f(\tilde{t}_u, \theta) + \epsilon_u$.

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$y_u = f(t_u, \theta) + \epsilon_u$
Error / Residual Sum of Squares $S(\theta) = \sum (y_u - f(t_u, \hat{\theta}))^2$
To find LSE, $\hat{\theta}$, we need to differentiate $S(\theta)$ w.r.t. $\hat{\theta}$
p normal equations are:
$$\sum (y_u - f(t_u, \hat{\theta})) \left. \frac{\partial f(t_u, \hat{\theta})}{\partial \theta_i} \right|_{\theta = \hat{\theta}} = 0$$

When $f(t_u, \hat{\theta})$ is linear $\frac{\partial f(t_u, \hat{\theta})}{\partial \theta_i}$ is a fun of t_u only & independent of $\hat{\theta}$.
When the model is non-linear in θ 's, $\frac{\partial f(t_u, \hat{\theta})}{\partial \theta_i}$ will be the normal equation

Now, we have the model say y_u equal to $f(t_u, \theta)$ plus ϵ_u and we have to fit this model. Fitting this model means you are given a set of observations 1 to n and you have to estimate the regression coefficients. So, by using the least squared techniques we consider the residual or error sum of squares, call it, $S(\theta)$ is equal to y_u minus $f(t_u, \theta)$ whole square, basically you know if you put hat here this becomes the observed response and this is the estimated response. So, this is the u th residual and residual square is $S(\theta)$, so this is the quantity you want to minimize in order to find the least squared estimates.

To find least squared estimates $\hat{\theta}$, we need to differentiate $S(\theta)$ with respect to θ , θ is a vector, it has p components. If you differentiate with respect to $\theta_1, \theta_2, \dots, \theta_p$, from there you will get p normal equations, p normal equations are summation y_u minus $f(t_u, \theta)$. Differentiating this function with respect to θ_i and then the partial derivative, this involves θ_i , so the partial derivative of this one $f(t_u, \theta)$ with respect to θ_i and that at the point θ equal to $\hat{\theta}$.

This is the point you want to estimate so this equal to 0. This is the i th normal equation and if you differentiate with respect to θ_j you will get the j th normal equation, this way you will get p normal equations. And now you should realize that when $f(t_u, \theta)$ is linear then this partial derivative $f(t_u, \theta)$ by $\Delta \theta_i$ is a function of t_u only. If it is

linear in t_i then when you differentiate it does not involve θ_i . So, it is a function of regressors only and independent of θ or specifically independent of θ_i .

When this model is non-linear, means f is non-linear. When the model is non-linear in θ , so will be the normal equations. If the model is linear then the partial derivatives are independent of θ but if the model is non-linear then the partial normal equations are also non-linear.

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Example $Y = f(\theta, t) + \epsilon$ where $f(\theta, t) = e^{-\theta t}$

$$Y = e^{-\theta t} + \epsilon, \quad S(\theta) = \sum_u (Y_u - e^{-\theta t_u})^2$$

Single normal equation:

$$\frac{\partial S(\hat{\theta})}{\partial \theta} = 0 \Rightarrow \sum_u (y_u - e^{-\theta t_u}) t_u e^{-\theta t_u} = 0$$

$$\Rightarrow \sum y_u t_u e^{-\theta t_u} - \sum t_u e^{-2\theta t_u} = 0$$

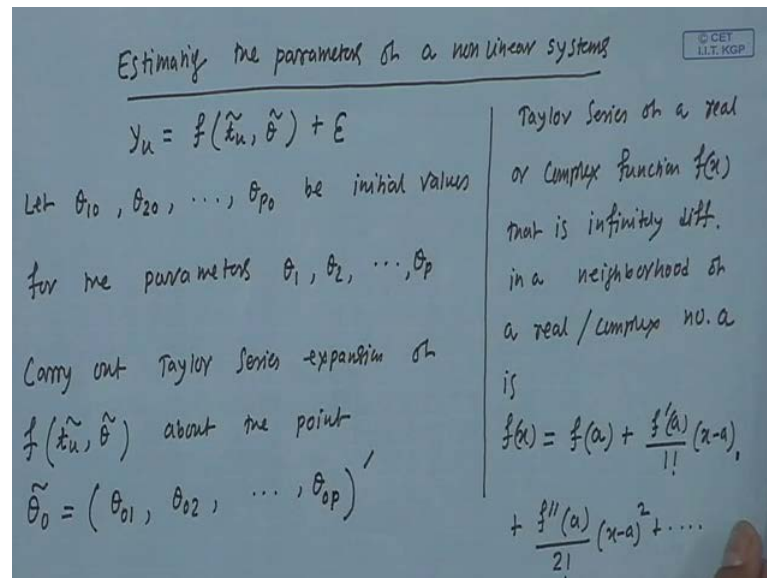
\rightarrow Finding $\hat{\theta}$ is not easy.

Let me give you an example, consider this model, say y equal to f theta t plus epsilon, where f theta t is equal to e to the power of minus theta t . That means we are considering the model e to the power of minus theta t plus epsilon, so this is the model. So, what is my s theta here, my s theta is equal to y_u minus e to the power of minus theta t_u , its only one regressor say t , this is whole square sum over u , this is my s theta and we want to minimize, we want to estimate theta in such a way that this is minimum.

That means, the single normal equation is obtained by differentiating s theta with respect to theta this equal to 0, implies summation y_u minus e to the power of minus theta t_u and then the derivative of this one with respect to theta, so this is t_u into e to the power of minus theta t_u , this is equal to 0 and sum over u . So, this gives that you know, your normal equation is $y_u t_u e$ to the power of minus theta t_u minus $t_u e$ to the power of minus twice theta t_u equal to 0.

So, what I want to say here is that if the model is non-linear and the normal equations are also non-linear, this is considered a normal equation and it is non-linear in theta. So, finding theta which satisfy this equation is not easy. So, finding theta hat, means you know you solve this the theta you got is the theta hat, so this is not easy here. Now, how to estimate the parameters of non-linear systems.

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Estimating the parameters of a non-linear systems, Notation ally it may look very difficult but the idea is simple here. So, I am given a model like this, what I am given is that, I am given the model y_u equal to $f t u$ theta plus epsilon. This is non-linear in theta and the idea here is that to estimate the parameter, as you must have observed that if the model is non-linear then the normal equations are also non-linear and then solving the non-linear systems equations are difficult.

So, what we will do is that we will approximate this non-linear function by linear functions using Taylor series. This is non-linear and we will approximate this one by a linear function, for that let me talk about the Taylor series. As you know Taylor series of real or complex function $f x$ that is infinitely differentiable in a neighborhood of real or complex number a is $f x$ equal to $f a$ plus f prime a by 1 factorial into x minus a plus f double prime a by 2 factorial into x minus a square. So, here you are expressing a function, any function in terms of polynomial.

So, here what we will do is that, similarly we will approximate this non-linear function by a linear function, so we will take up to this term using the Taylor series. Let θ_1^0 , θ_2^0 and θ_p^0 be initial values for the parameters θ_1 , θ_2 , θ_p , and then we carry out this Taylor series expansion about this initial value. So, you carry out Taylor series expansion of this non-linear function $f(t, u, \theta)$ in the neighborhood of this point, about the point say θ^0 , which is equal to θ_1^0 , θ_2^0 , θ_p^0 . We will carry out the Taylor series expansion of this non-linear function about the point or in the neighborhood of this point. So, we will take up to this term because we are looking for a linear approximation for this non-linear term of this non-linear function.

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$$f(\tilde{x}_u, \tilde{\theta}) = f(\tilde{x}_u, \tilde{\theta}^0) + \sum_{i=1}^p \left. \frac{\partial f(\tilde{x}_u, \tilde{\theta})}{\partial \theta_i} \right|_{\theta_i = \theta_i^0} (\theta_i - \theta_i^0)$$

Set $f_u^0 = f(\tilde{x}_u, \tilde{\theta}^0)$

$\beta_i^0 = (\theta_i - \theta_i^0)$

$z_{iu}^0 = \left. \frac{\partial f(\tilde{x}_u, \tilde{\theta})}{\partial \theta_i} \right|_{\theta_i = \theta_i^0}$

$$f(\tilde{x}_u, \tilde{\theta}) = f_u^0 + \sum_{i=1}^p z_{iu}^0 \beta_i^0$$

$$Y_u = f(\tilde{x}_u, \tilde{\theta}) + \epsilon_u$$

$$Y_u - f_u^0 = \sum z_{iu}^0 \beta_i^0 + \epsilon_u$$

We can now estimate β_i^0 , $i=1, 2, \dots, p$, by applying least

So, here is the Taylor series expansion, $f(t, u, \theta)$ is equal to $f(t, u, \theta^0)$ plus the partial derivative of this $f(t, u, \theta)$ by $\Delta \theta_i$, θ_i minus θ_i^0 and this derivative at the point θ_i is equal to θ_i^0 , and this i is from 1 to p . You must have understood that this is the Taylor series expansion of this non-linear function up to the first of the second term, linear term.

Now, let me use some more notations, set f_u^0 is equal to $f(t, u, \theta^0)$, and this term we will denote by β_i^0 which is equal to $\theta_i - \theta_i^0$, and then this term we will denote by z_{iu}^0 , so that is nothing but partial derivative of this one θ_i at the point $\theta_i = \theta_i^0$.

Now, if you use all this notations in this linear approximation you can write this one as say, $f(u; \theta)$, so non-linear function is equal to $f(u; \theta)$ because $f(u; \theta)$ is this plus $z_i(u; \theta) \beta_i$ and i is from 1 to p . So, this is the linear approximation of the non-linear function in θ so here it is in terms of β . So, y_u this is the model we started with, y_u was $f(u; \theta) + \epsilon_u$, now if I plug this linear approximation of this non-linear function here, what I will get is that, I will get $y_u - f(u; \theta)$ is equal to $z_i(u; \theta) \beta_i + \epsilon_u$.

Now, you can see that this is a linear model in β , this is same as multiple linear regression model. So, in this model we can estimate this parameter, the transformed parameter β_i using the least squared technique. So, we can now estimate this β_i for i equal to 1 to p by applying least square technique. So, let see how to do this thing.

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The image shows a handwritten derivation on a blue background. At the top, the equation is written as $y_u - f_u^0 = \sum_{i=1}^p z_{iu}^0 \beta_i^0 + \epsilon_u$. Below this, it says "if we write" and defines three matrices: $Z_0 = \begin{bmatrix} z_{11}^0 & \dots & z_{p1}^0 \\ \dots & \dots & \dots \\ z_{1n}^0 & \dots & z_{pn}^0 \end{bmatrix}$, $\tilde{\beta}_0 = \begin{pmatrix} \beta_1^0 \\ \beta_2^0 \\ \vdots \\ \beta_p^0 \end{pmatrix}$, and $\tilde{y}_0 = \begin{pmatrix} y_1 - f_1^0 \\ \vdots \\ y_n - f_n^0 \end{pmatrix}$. The next line shows the matrix equation $\tilde{y}_0 = Z_0 \tilde{\beta}_0 + \epsilon$ with the note "then we estimate $\tilde{\beta}_0$ ". The final line states that $\tilde{\beta}_0$ is given by $\hat{\tilde{\beta}}_0 = (Z_0' Z_0)^{-1} Z_0' y_0$.

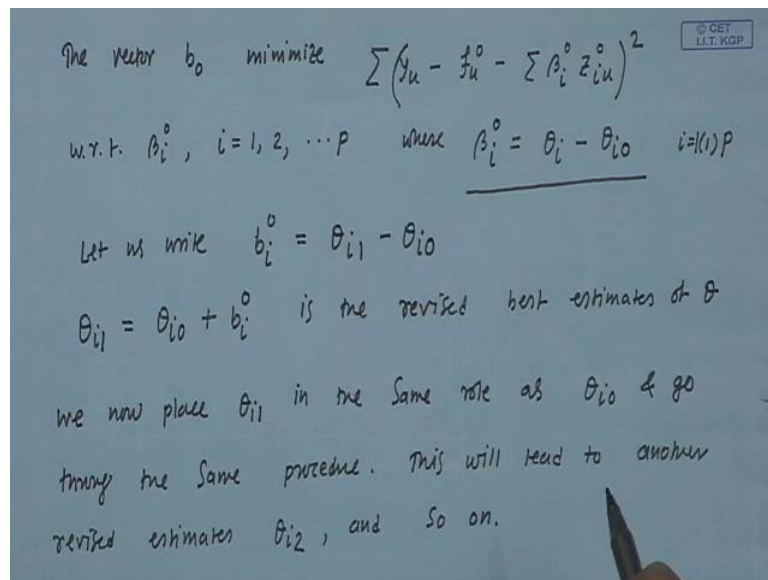
We have the linear model $y_u - f(u; \theta)$ equal to $z_i(u; \theta) \beta_i$, i is from 1 to p plus ϵ_u . So, we started with the non-linear model and then we have a linear model by using the Taylor series approximation. And we are trying to solve this linear model now, so we can write in matrix form, if we write my coefficient matrix Z which is equal to say z_{11} to z_{pn} and then y which is equal to $y_1 - f_1^0$ to $y_n - f_n^0$, so this is my coefficient matrix, and β is my coefficient vector, that is β_1

naught beta 2 naught and beta p naught and let me write my response as y vector, so y vector is y_1 minus f_1 naught and then y_n minus f_n naught.

So, using this matrix notations I can write my simple linear, I mean this basically is a multiple linear regression model. Now, I can write it in the form y naught is equal to z naught beta naught plus epsilon, then the estimate of this beta naught, we know, now we can apply a least squared technique of this one is given by beta naught, which is equal to basically beta naught hat is equal to z naught prime z naught x prime x inverse, x prime y . So, here z naught is nothing but x in the multiple linear regression model so z naught prime y naught.

So, what we have now is that, we have the, let me write these in the vector notation only. We have the fitted model, so the fitted model is, I mean. Of course, this is not the final estimate, we wanted to estimate theta and now we are estimating beta, where beta is sort of theta minus theta naught. And what we will do is that we will improve this estimate iteratively.

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The vector beta naught, which is estimate of b naught, which is estimate of beta naught, this minimize y_u minus f_u naught minus beta i naught z_{iu} naught square. This is nothing but s theta basically with respect to beta i naught, so i is from 1 to p . Where, this beta i naught is equal to theta i minus theta i naught.

We need to understand this part, we want to estimate θ_i 's or $\theta_1 \theta_2 \dots \theta_p$, so this i is from 1 to p . We started with some θ_{naught} , we want to estimate θ_i , and then we have used this Taylor expansion about this point θ_{naught} to make the non-linear function linear. And after making the function, from non-linear to linear, we have estimated this difference, so we have estimated this β_i and that is nothing but β_i .

So, let us write β_i is equal to θ_i minus θ_{naught} . We started with θ_{naught} as a estimate of θ_i and then we see that this quantity, this difference which is nothing but β_i and we have estimated this difference. Now, what I am trying to say is that, you know we started with the initial point and then we will try to improve this estimate iteratively. So, let me put a 1 here, this keeps my estimate of θ_i at the first iteration, so $\theta_{i,1}$ is equal to θ_{naught} plus β_i . We started with θ_{naught} then we improved this θ_{naught} by $\theta_{i,1}$ and this is the revised best estimates of θ_i .

Now, again we will place $\theta_{i,1}$ in the same role as θ_{naught} and go through the same procedure. So, this will lead to another revised estimate, $\theta_{i,2}$ and so on. So, we started with θ_{naught} . Let me just give little idea about what I am doing here, is that, we have a non-linear model and that is a non-linear in θ_i . First, what we do is that we take initial estimate of θ_i , that is, θ_{naught} and then we consider the Taylor series expansion of the non-linear function about θ_{naught} and we approximate the non-linear function by a linear function.

And once we have the transformation from non-linear to linear, we can use the result of simple linear regression model. And we estimate the linear model and from that estimate of linear model using the least squared technique, what we get is that from θ_{naught} we get $\theta_{i,1}$. Now, we put this $\theta_{i,1}$, the revised estimate in the same role as θ_{naught} was initially. So, we will do the same thing again, we take the Taylor series expansion of the non-linear function about $\theta_{i,1}$. And then once you have the linear function, once you transform the non-linear model to linear model, we can apply the results of linear regression and from θ_{naught} from $\theta_{i,1}$ you will get $\theta_{i,2}$ and so on.

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$$\theta_{j+1} = \theta_j + b_j$$

$$= \theta_j + (Z_j' Z_j)^{-1} Z_j' (Y - f^j)$$

where $Z_j' = \begin{pmatrix} Z_{1j}^j \\ Z_{2j}^j \\ \dots \\ Z_{nj}^j \end{pmatrix}$ $Z_{iu} = \left. \frac{\partial f(\tilde{x}_u, \tilde{\theta})}{\partial \theta_i} \right|_{\theta = \theta_j}$

$$f^j = (f_1^j, f_2^j, \dots, f_n^j)'$$

$$\theta_j = (\theta_{1j}, \theta_{2j}, \dots, \theta_{pj})'$$

this iterative process continue until

$$|\theta_{i(j+1)} - \theta_{i(j)}| < \delta = \text{some pre specified value} = .00001$$

At some point after the j th iteration, what we will get is, that we will get θ_{j+1} equal to $\theta_j + b_j$. So, in the $j+1$ iteration we improved θ_j by using the same technique and improved on other revised one is that θ_{j+1} . So, this one is nothing but $\theta_j + b_j$, we know what is this b_j , b_j is $(Z_j' Z_j)^{-1} Z_j' (Y - f^j)$. Where, this Z_j' is equal to Z_{iu} to the power of j , I mean the notation not to the power of j . I am sure that you understand what is this, this one is Z_{iu} is the derivative of that non-linear function t_u with respect to θ_i and θ equal to θ_j . So, j result of the j th iteration.

And my f^j is equal to $(f_1^j, f_2^j, \dots, f_n^j)'$ and my θ_j is equal to $(\theta_{1j}, \theta_{2j}, \dots, \theta_{pj})'$. So, you understood from every iteration we are improving the estimation and there should be some stopping criteria, so when the result of j th iteration is not much different from the $j+1$ th iteration we stop there. This iterative process continue until this difference is i , this is the result of $j+1$ th iteration minus $\theta_{i,j}$, j th iteration, when this is less than some δ which is a small quantity, some pre specified value say for example, 0.00001.

So, when you see that the difference between the result obtained from $j+1$ th iteration and the j th iteration is very small, very significant difference. That means you can stop there. This is about the non-linear estimation. So, you understood what is the non-linear model, non-linear means non-linear in parameters $\theta_1, \theta_2, \dots, \theta_p$ and

given a non-linear model, you now know how to approximate that non-linear model by a linear model using the Taylor series expansion. And you also know how to estimate the parameters of non-linear estimation, non-linear model, using the least squared technique. That is all for today.

Thank you.