ME 209
Numerical Methods

8. Regression 2

Non-linear Regression

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7.2 Nonlinear Regression

Given n data points $(x_1, y_1), (x_2, y_2), \ldots, (xn, yn)$ best fit $y = f(x)$ to the data, where $f(x)$ is a nonlinear function of x .

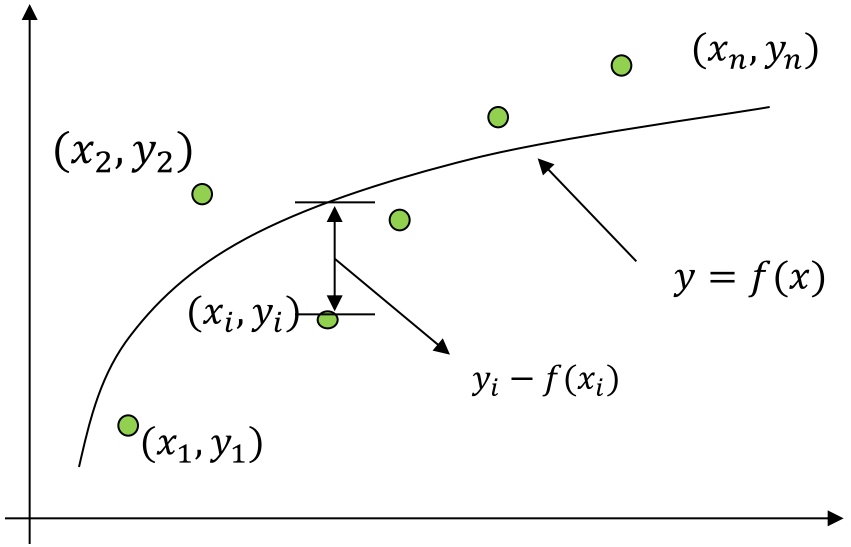


Figure. Nonlinear regression model for discrete y vs. x data

Some popular nonlinear regression models:

1. Exponential model: $(y = ae^{bx})$

2. Power model: $(y = ax^{b})$

3. Saturation growth model: $\left(y = \dfrac{ax}{b + x}\right)$

4. Polynomial model: $(y = a_0 + a_1 x + \ldots + a_n x^{n})$

Exponential Model

Given $(x_1, y_1), (x_2, y_2), \ldots (x_n, y_n)$, best fit $y = ae^{bx}$ to the data. The variables a and b are the constants of the exponential model. The residual at each data point x_i is

$$E_i = y_i - ae^{bx_i}$$

The sum of the square of the residuals is

$$S_r = \sum_{i=1}^{n} E_i^2$$

$$= \sum_{i=1}^{n} \left(y_i - ae^{bx_i}\right)^2$$

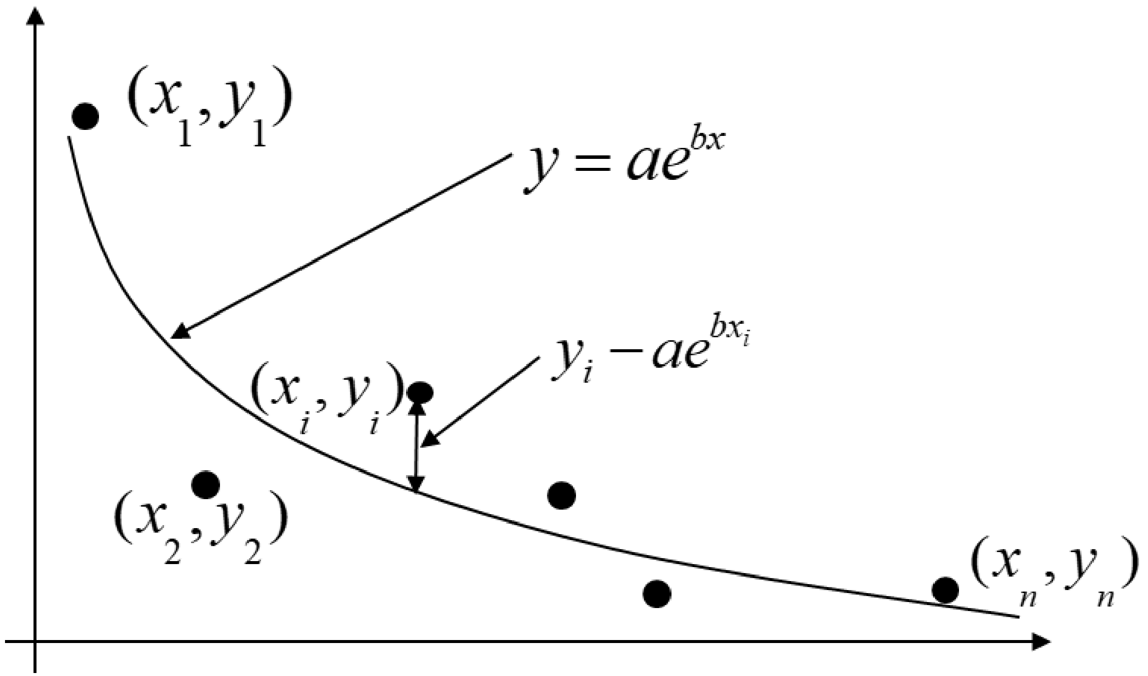


Figure. Exponential model of nonlinear regression for y vs. x data

Finding Constants of Exponential Model

To find the constants a and b of the exponential model, we minimize S_r by differentiating with respect to a and b and equating the resulting equations to *zero*. Rewriting the equations, we obtain

$$-\sum_{i=1}^{n} y_i e^{bx_i} + a\sum_{i=1}^{n} e^{2bx_i} = 0$$

$$\sum_{i=1}^{n} y_i x_i e^{bx_i} - a\sum_{i=1}^{n} x_i e^{2bx_i} = 0$$

Solving the first equation for a yields

$$a = \frac{\sum_{i=1}^{n} y_i e^{bx_i}}{\sum_{i=1}^{n} e^{2bx_i}}$$

Substituting a back into the previous equation

$$\sum_{i=1}^{n} y_i x_i e^{bx_i} - \frac{\sum_{i=1}^{n} y_i e^{bx_i}}{\sum_{i=1}^{n} e^{2bx_i}} \sum_{i=1}^{n} x_i e^{2bx_i} = 0$$

The constant b can be found through numerical methods such as bisection method or the secant method.

Example 1-Exponential Model

Many patients get concerned when a test involves injection of a radioactive material. For example for scanning a gallbladder, a few drops of Technetium-99m isotope is used. Half of the Technetium-99m would be gone in about 6 hours. It, however, takes about 24 hours for the radiation levels to reach what we are exposed to in day-to-day activities. Below is given the relative intensity of radiation as a function of time.

Table. Relative intensity of radiation as a function of time.

t(hrs)	0	1	3	5	7	9
γ	1.000	0.891	0.708	0.562	0.447	0.355

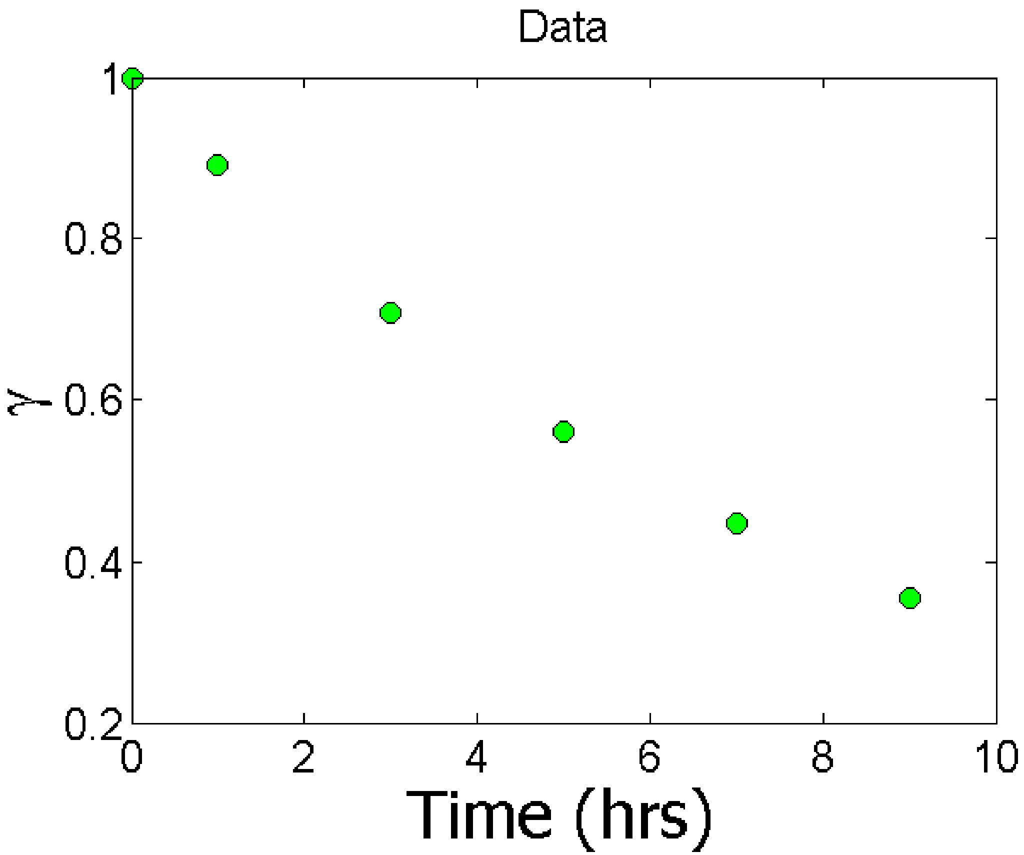
The relative intensity is related to time by the equation $\gamma = Ae^{\lambda t}$

Find:

a) The value of the regression constants A and λ

b) The half-life of Technetium-99m

c) Radiation intensity after 24 hours



Plot of data

a) The value of λ is given by solving the nonlinear Equation

$$\sum_{i=1}^{n} y_i x_i e^{bx_i} - \frac{\sum_{i=1}^{n} y_i e^{bx_i}}{\sum_{i=1}^{n} e^{2bx_i}} \sum_{i=1}^{n} x_i e^{2bx_i} = 0 \longrightarrow f(\lambda) = \sum_{i=1}^{n} \gamma_i t_i e^{\lambda t_i} - \frac{\sum_{i=1}^{n} \gamma_i e^{\lambda t_i}}{\sum_{i=1}^{n} e^{2\lambda t_i}} \sum_{i=1}^{n} t_i e^{2\lambda t_i} = 0$$

Equation above can be solved for λ using bisection method. To estimate the initial guesses, we assume λ = –0.120 and λ = –0.110 . We need to check whether these values first bracket the root of f (λ) = 0 . At λ = −0.120 , the table below shows the evaluation of f (− 0.120).

Table 2 Summation value for calculation of constants of model

i	t_i	γ_i	$\gamma_i t_i e^{\lambda t_i}$	$\gamma_i e^{\lambda t_i}$	$e^{2\lambda t_i}$	$t_i e^{2\lambda t_i}$
1	0	1	0.00000	1.00000	1.00000	0.00000
2	1	0.891	0.79205	0.79205	0.78663	0.78663
3	3	0.708	1.4819	0.49395	0.48675	1.4603
4	5	0.562	1.5422	0.30843	0.30119	1.5060
5	7	0.447	1.3508	0.19297	0.18637	1.3046
6	9	0.355	1.0850	0.12056	0.11533	1.0379
$\sum_{i=1}^{6}$			6.2501	2.9062	2.8763	6.0954

From Table 2 $n = 6$

$$\sum_{i=1}^{6} \gamma_i t_i e^{-0.120 t_i} = 6.2501$$

$$\sum_{i=1}^{6} \gamma_i e^{-0.120 t_i} = 2.9062$$

$$\sum_{i=1}^{6} e^{2(-0.120) t_i} = 2.8763$$

$$\sum_{i=1}^{6} t_i e^{2(-0.120) t_i} = 6.0954$$

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i	t_i	γ_i	$\gamma_i t_i e^{\lambda t_i}$	$\gamma_i e^{\lambda t_i}$	$e^{2\lambda t_i}$	$t_i e^{2\lambda t_i}$
1	0	1	0.00000	1.00000	1.00000	0.00000
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5	7	0.447	1.3508	0.19297	0.18637	1.3046
6	9	0.355	1.0850	0.12056	0.11533	1.0379
$\sum_{i=1}^{6}$			6.2501	2.9062	2.8763	6.0954

$$f(-0.120) = (6.2501) - \frac{2.9062}{2.8763}(6.0954) = 0.091357$$

Similarly (At λ = −0.110)

$$f(-0.110) = -0.10099$$

Since $f(-0.120)\times f(-0.110)<0$, the value of λ falls in the bracket of $[-0.120,-0.110]$.

The next guess of the root then is

$$\lambda = \frac{-0.120+(-0.110)}{2} = -0.115$$

Continuing with the bisection method, the root of $f(\lambda)=0$ is found as $\lambda = -0.11508$.

and the value of A

$$A = \frac{\sum_{i=1}^{n} \gamma_i e^{\lambda t_i}}{\sum_{i=1}^{n} e^{2\lambda t_i}} = \frac{\begin{array}{c} 1\times e^{-0.11508(0)} + 0.891\times e^{-0.11508(1)} + 0.708\times e^{-0.11508(3)} + \\ 0.562\times e^{-0.11508(5)} + 0.447\times e^{-0.11508(7)} + 0.355\times e^{-0.11508(9)} \end{array}}{\begin{array}{c} e^{2(-0.11508)(0)} + e^{2(-0.11508)(1)} + e^{2(-0.11508)(3)} + \\ e^{2(-0.11508)(5)} + e^{2(-0.11508)(7)} + e^{2(-0.11508)(9)} \end{array}} \begin{array}{l} = \dfrac{2.9373}{2.9378} \\ = 0.99983 \end{array}$$

The regression formula is hence given by

$$\gamma = 0.99983\, e^{-0.11508t}$$

b) Half life of Technetium-99m is when $\gamma = \frac{1}{2}\gamma\Big|_{t=0}$

$$0.99983 \times e^{-0.11508t} = \frac{1}{2}(0.99983)e^{-0.11508(0)}$$

$$e^{-0.11508t} = 0.5$$

$$-0.11508t = \ln(0.5)$$

$$t = 6.0232 \text{ hours}$$

c) The relative intensity of the radiation after 24 hrs is

$$\gamma = 0.99983 \times e^{-0.11508(24)}$$

$$= 6.3160 \times 10^{-2}$$

This result implies that only

$$\frac{6.316 \times 10^{-2}}{0.9998} \times 100 = 6.317\%$$ radioactive intensity is left after 24 hours.

Polynomial Model

Given n data points $(x_1, y_1), (x_2, y_2), \ldots\ldots, (x_n, y_n)$ use least squares method to regress the data to an m^{th} order polynomial. $y = a_0 + a_1 x + a_2 x^2 + \cdots\cdots + a_m x^m, m < n$

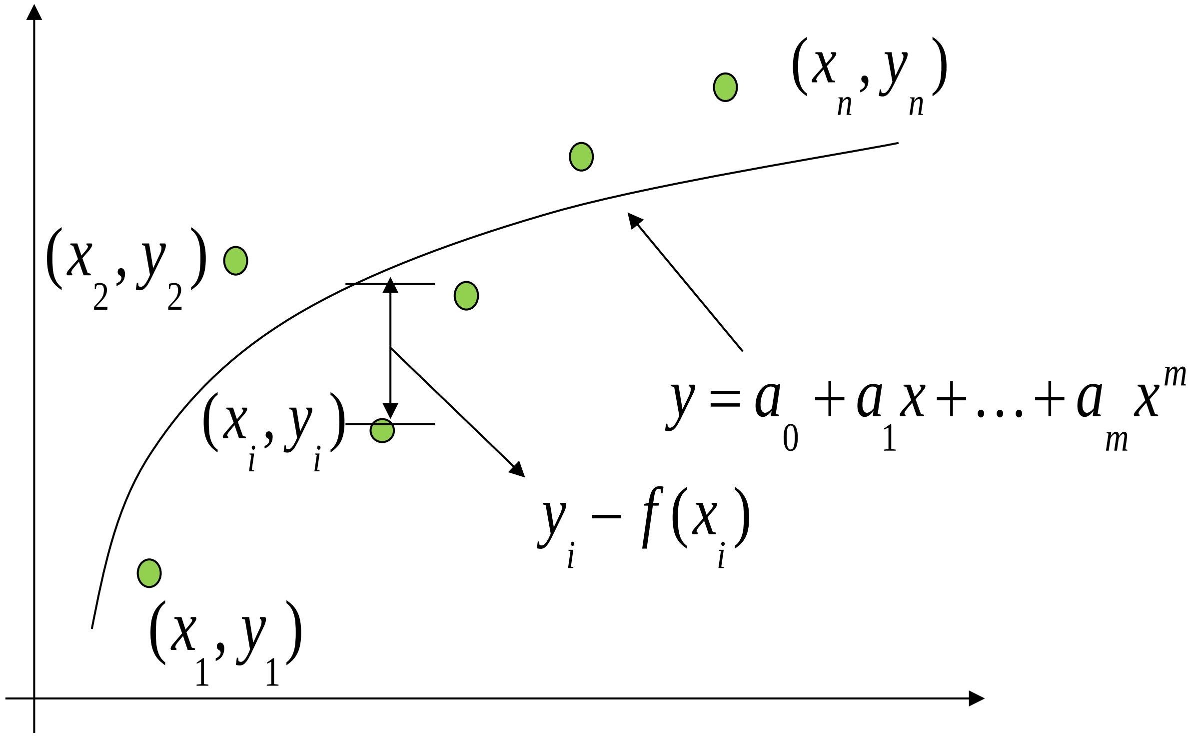

Figure. Polynomial model for nonlinear regression of y vs. x data

The residual at each data point is given by

$$E_i = y_i - a_0 - a_1 x_i - \ldots - a_m x_i^m$$

The sum of the square of the residuals is given by

$$S_r = \sum_{i=1}^{n} E_i^2$$

$$= \sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i - \ldots - a_m x_i^m\right)^2$$

To find the constants of the polynomial regression model, we put the derivatives with respect to a_i to zero, that is,

$$\frac{\partial S_r}{\partial a_0} = \sum_{i=1}^{n} 2\left(y_i - a_0 - a_1 x_i \;-\;.\;.\;.-a_m x_i^m\right)(-1) = 0$$

$$\frac{\partial S_r}{\partial a_1} = \sum_{i=1}^{n} 2\left(y_i - a_0 - a_1 x_i \;-\;.\;.\;.-a_m x_i^m\right)(-x_i) = 0$$

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$$\frac{\partial S_r}{\partial a_m} = \sum_{i=1}^{n} 2\left(y_i - a_0 - a_1 x_i \;-\;.\;.\;.-a_m x_i^m\right)(-x_i^m) = 0$$

Setting those equations in matrix form gives

$$\begin{bmatrix} n & \left(\sum_{i=1}^{n} x_i\right) & . & . & . \left(\sum_{i=1}^{n} x_i^m\right) \\ \left(\sum_{i=1}^{n} x_i\right) & \left(\sum_{i=1}^{n} x_i^2\right) & . & . & . \left(\sum_{i=1}^{n} x_i^{m+1}\right) \\ . & . & . & . & . \\ \left(\sum_{i=1}^{n} x_i^m\right) & \left(\sum_{i=1}^{n} x_i^{m+1}\right) & . & . & . \left(\sum_{i=1}^{n} x_i^{2m}\right) \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ . \; . \; . \\ a_m \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} x_i \, y_i \\ . \quad . \quad . \\ \sum_{i=1}^{n} x_i^m y_i \end{bmatrix}$$

The above are solved for $a_0, a_1, \ldots, a_m$

Example

Regress (fit) the thermal expansion coefficient vs. temperature data to a second order polynomial.

Table. The thermal expansion coefficient at given different temperatures

Temperature, T (ºF)	Coefficient of thermal expansion, α (in/in/ºF)
80	6.47×10^{-6}
40	6.24×10^{-6}
−40	5.72×10^{-6}
−120	5.09×10^{-6}
−200	4.30×10^{-6}
−280	3.33×10^{-6}
−340	2.45×10^{-6}

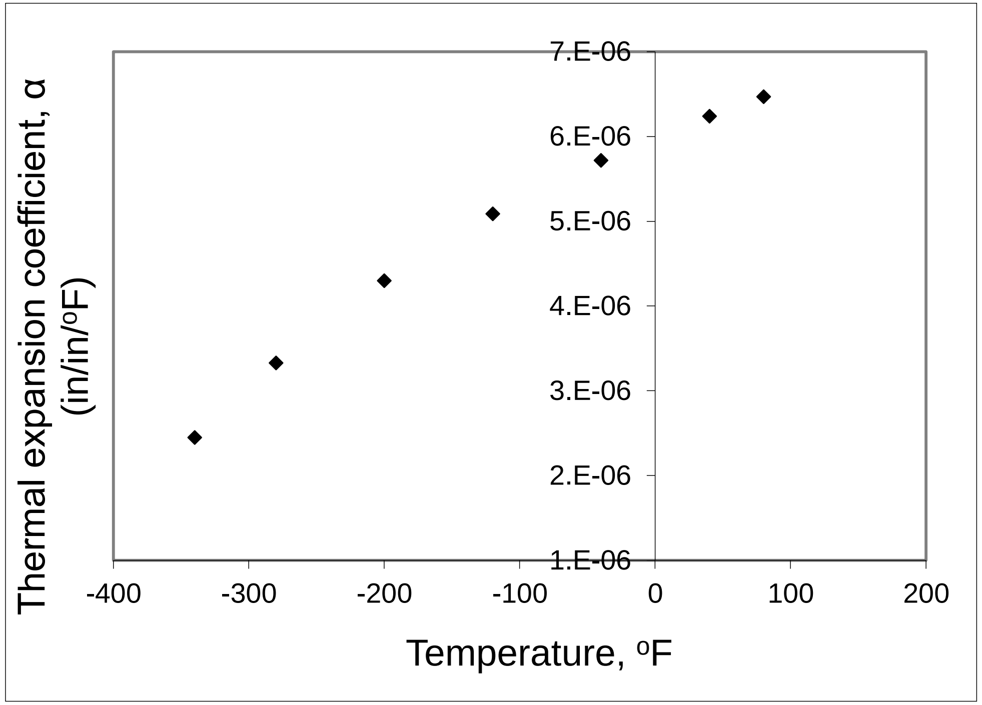

Figure. Data points for thermal expansion coefficient vs temperature.

We want to fit the data to the polynomial regression model $\alpha = a_0 + a_1 T + a_2 T^2$

The coefficients a_0, a_1, a_2 are found by differentiating the sum of the square of the residuals with respect to each variable and setting the values equal to zero to obtain

$$\begin{bmatrix} n & \left(\sum_{i=1}^{n} T_i\right) & \left(\sum_{i=1}^{n} T_i^2\right) \\ \left(\sum_{i=1}^{n} T_i\right) & \left(\sum_{i=1}^{n} T_i^2\right) & \left(\sum_{i=1}^{n} T_i^3\right) \\ \left(\sum_{i=1}^{n} T_i^2\right) & \left(\sum_{i=1}^{n} T_i^3\right) & \left(\sum_{i=1}^{n} T_i^4\right) \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} \alpha_i \\ \sum_{i=1}^{n} T_i \, \alpha_i \\ \sum_{i=1}^{n} T_i^2 \alpha_i \end{bmatrix}$$

Table 5 Summations for calculating constants of model

i	$T(^\circ F)$	α (in/in/°F)	T^2	T^3	T^4	$T\times\alpha$	$T^2\times\alpha$
1	80	6.4700×10^{-6}	6.4000×10^{3}	5.1200×10^{5}	4.0960×10^{7}	5.1760×10^{-4}	4.1408×10^{-2}
2	40	6.2400×10^{-6}	1.6000×10^{3}	6.4000×10^{4}	2.5600×10^{6}	2.4960×10^{-4}	9.9840×10^{-3}
3	-40	5.7200×10^{-6}	1.6000×10^{3}	-6.4000×10^{4}	2.5600×10^{6}	-2.2880×10^{-4}	9.1520×10^{-3}
4	-120	5.0900×10^{-6}	1.4400×10^{4}	-1.7280×10^{6}	2.0736×10^{8}	-6.1080×10^{-4}	7.3296×10^{-2}
5	-200	4.3000×10^{-6}	4.0000×10^{4}	-8.0000×10^{6}	1.6000×10^{9}	-8.6000×10^{-4}	1.7200×10^{-1}
6	-280	3.3300×10^{-6}	7.8400×10^{4}	-2.1952×10^{7}	6.1466×10^{9}	-9.3240×10^{-4}	2.6107×10^{-1}
7	-340	2.4500×10^{-6}	1.1560×10^{5}	-3.9304×10^{7}	1.3363×10^{10}	-8.3300×10^{-4}	2.8322×10^{-1}
$\sum_{i=1}^{7}$	-8.6000×10^{2}	3.3600×10^{-5}	2.5800×10^{5}	-7.0472×10^{7}	2.1363×10^{10}	-2.6978×10^{-3}	8.5013×10^{-1}

$n = 7$

$$\sum_{i=1}^{7} T_i^2 = 2.5580\times10^5$$

$$\sum_{i=1}^{7} T_i^3 = -7.0472\times10^7$$

$$\sum_{i=1}^{7} T_i^4 = 2.1363\times10^{10}$$

$$\sum_{i=1}^{7} \alpha_i = 3.3600\times10^{-5}$$

$$\sum_{i=1}^{7} T_i\alpha_i = -2.6978\times10^{-3}$$

$$\sum_{i=1}^{7} T_i^2\alpha_i = 8.5013\times10^{-1}$$

Using these summations, we can now calculate a_0, a_1, a_2

$$\begin{bmatrix} 7.0000 & -8.6000\times10^2 & 2.5800\times10^5 \\ -8.600\times10^2 & 2.5800\times10^5 & -7.0472\times10^7 \\ 2.5800\times10^5 & -7.0472\times10^7 & 2.1363\times10^{10} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 3.3600\times10^{-5} \\ -2.6978\times10^{-3} \\ 8.5013\times10^{-1} \end{bmatrix}$$

Solving the above system of simultaneous linear equations we have

$$\begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 6.0217\times10^{-6} \\ 6.2782\times10^{-9} \\ -1.2218\times10^{-11} \end{bmatrix}$$

The polynomial regression model is then

$$\alpha = a_0 + a_1T + a_2T^2$$

$$= 6.0217\times10^{-6} + 6.2782\times10^{-9}\,\mathrm{T} - 1.2218\times10^{-11}\,\mathrm{T}^2$$

NEXT LECTURE
Numerical Differentiation