MA2252 Introduction to Computing

Lecture 13
Least Squares Regression

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Learning outcomes

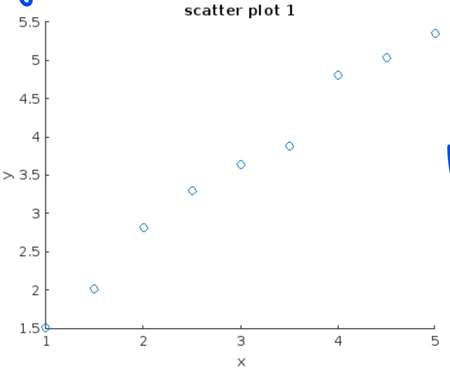
At the end of lecture, students will be able to

- understand scatter plot and regression
- understand theory of Least Squares Regression
- solve basic regression problems in MATLAB

Scatter plot

A **scatter plot** plots two different sets of data using dots. Unlike line plot, the dots are not connected by a curve.

2D scatterplot plots data of two different variables as dots.



plot(x,y)

scatter(x,y)

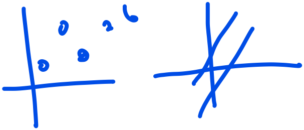
plot(x,y,'o')

Scatter plot (contd.)

MATLAB's scatter() function can be used to create a scatter plot.

Example: The code below creates the scatter plot shown earlier.


```
x=1:0.5:5; %create data for vector x
s=size(x); %find size of vector x
y=x+rand(s); %create a vector y=x+'some random values'
scatter(x,y) %create scatter plot
title('scatter plot 1')
xlabel('x')
ylabel('y')
```



Scatter plot (contd.)

Demo

Regression

Regression is a statistical technique used to find the 'best-fit curve' that describes a scatter plot.

curve which is closest approximation to the data

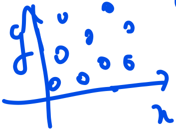
Depending on the data trend in a scatter plot, one may use

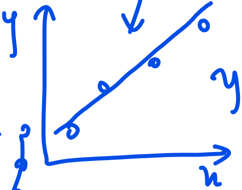
- ~~Linear Regression~~

Linear Regression curve

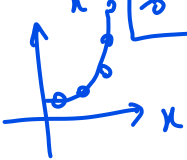
- ~~Non-linear Regression~~

Non-linear Regression curve





$y = mx + c$



curve

Linear Regression example

regression line

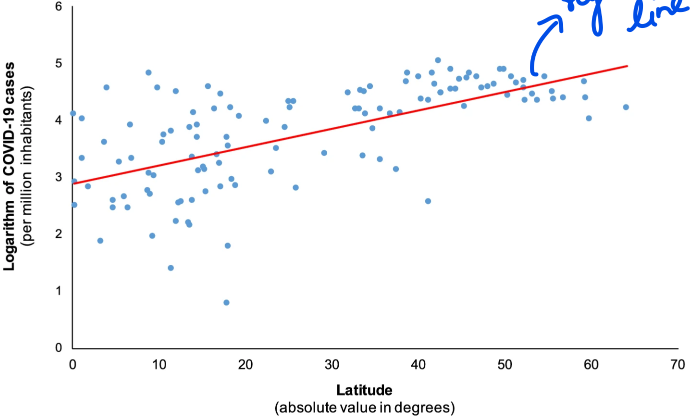


Figure: Scatter plot showing linear trend [1]

Non-linear Regression curve example

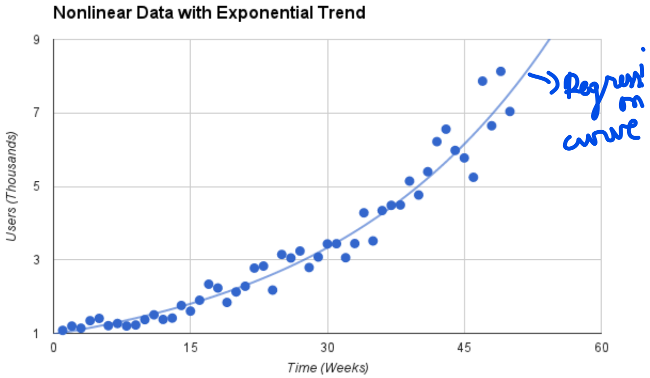


Figure: Data showing number of active users on a website with time [2]

[1] Chen, S., Prettner, K., Kuhn, M. et al. Climate and the spread of COVID-19. Sci Rep 11, 9042 (2021). https://doi.org/10.1038/s41598-021-87692-z

[2] http://sam-koblenski.blogspot.com

Regression model

linear function
or nonlinear
function

A regression model provides a function to describe the relationship between one (or more) independent variables and a dependent variable.

A basic regression model is the 'Least Squares Regression model'.

$m >> n$

Here, the relationship between dependent data points $y_i (i = 1, 2, ...m)$ and independent data points x_i is modelled as

For m data points,

$$\hat{y}(x) = \sum_{i=1}^{n} \alpha_i f_i(x) \tag{1}$$

$\alpha_1 f_1(x) + \alpha_2 f_2(x) + \cdots f_n(x)$

will give m eqns.

plot your regression curve

n parameters

$\hat{y}(x_1) = \sum_{i=1}^{n} \alpha_i f_i(x_1)$

$\hat{y}(x_2) = \cdots f_i(x_2)$

$\vdots$

$\hat{y}(x_m) \cdots$

where

- $\hat{y}(x)$ is an estimation function
- α_i are parameters of estimation function
- $f_i(x)$ are linearly independent basis functions

The parameters are then found by minimising the total squared error E.

$$E = \sum_{i=1}^{m} (\hat{y} - y_i)^2 \tag{2}$$

Substituting (1) in (2) gives

$$E = \sum_{i=1}^{m} \left(\sum_{j=1}^{n} \alpha_j f_j(x_i) - y_i \right)^2 \tag{3}$$

E is a function of n variables namely $\alpha_j (j = 1, 2, \cdots, n)$.

$$\frac{\partial E}{\partial \alpha_j} = 0$$

Least Squares Regression (contd.)

The solution for n parameters α_j which minimise the total squared error E is given as

$$\beta = pinv(A) * Y \tag{4}$$

Here,

- β is a column vector with n entries α_j
- A is a mxn matrix with entries $A(i,j) = f_j(x_i)$
- $pinv(A)$ is the pseudo-inverse of A
- Y is a column vector with m entries y_i

Least Squares Regression (contd.)

Derivation of (4)**:** Please refer book and lecture recording

Example: Perform a least squares regression for the scatter plot created before using estimation function $\hat{y}(x) = \alpha_1 x + \alpha_2$.

$f_1(x) = x \quad , \quad f_2(x) = 1$

handle

```
openfig('scatter_plot_1.fig') %opens figure scatter_plot_1.fig
a = get(gca,'Children');
x = get(a, 'XData'); %extract x-data points
y = get(a, 'YData'); %extract y-data points
A=[x',ones(size(x'))]; %create the matrix A of basis functions
beta=pinv(A)*y'; %evaluate vector beta containing values of parameters

%plot the regression line
hold on
plot(x,beta(1)*x+beta(2))
```

$$\begin{array}{cc} F_1(x) & \\ \end{array}$$

$$A = \begin{bmatrix} x_1 & 1 \\ x_2 & \vdots \\ \vdots & \vdots \\ x_m & 1 \end{bmatrix}_{m \times 2} \qquad \beta = \mathrm{pinv}(A) * Y$$

$$\beta = \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix}$$

$\alpha_1 = \mathrm{Beta}(1) \; , \; \alpha_2 = \mathrm{Beta}(2)$

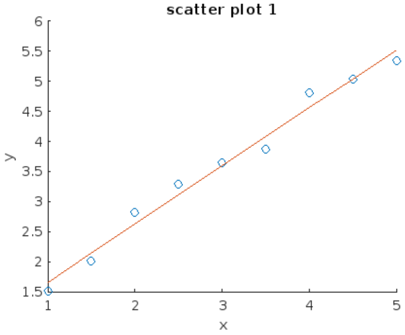


Figure: Regression line

polyfit and polyval functions

When the estimation function $\hat{y}(x)$ is a polynomial, MATLAB's polyfit and polyval functions can be used.

For vectors x and y containing x-data and y-data points respectively,

- p=polyfit(x,y,n) creates a vector p of the coefficients of regression polynomial p(x) of degree n
- polyval(p,x) calculates the values of p(x)

$y = \alpha_1 x + \alpha_2$

$n = 1$

$p = \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix}$ $p = \text{polyfit}(x, y, 1)$

polyfit and polyval functions (contd.)

Example: This code creates the same regression line as was shown before.

```
openfig('scatter_plot_1.fig') %opens figure scatter_plot_1.fig
a = get(gca,'Children');
x = get(a, 'XData'); %extract x-data points
y = get(a, 'YData'); %extract y-data points

p= polyfit(x,y,1); %creates coefficients of regression polynomial of degree 1
Y=polyval(p,x); %evaluates the value of polynomial at x-data points
hold on
plot(x,polyval(p,x)) %plot the regression polynomial
```

polyfit and polyval functions (contd.)

Demo

$\frac{1}{\alpha x+\beta}$

Sometimes, a nonlinear estimation function provides the best fit for a scatter plot. This means we require

non-linear in α_j

$y = \frac{1}{x}$, $\sin x$, $\log x$, 2^x

$$\hat{y}(x) = g(\alpha_1, \alpha_2, \cdots, \alpha_n, x) \tag{5}$$

$\cancel{\hat{y} = \sum_{i=1}^{m} \alpha_j f_j(x_i)}$

where g is some nonlinear function.

In some special cases, a transformation such as

$$\tilde{y}(x) = h(\hat{y}(x)) \tag{6}$$

$\hat{y} = \alpha_1 x^2 + \alpha_2 x + \alpha_3$

$f_1(x) = x^2$, $f_2(x) = x$, $f_3(x) = 1$

can linearise the equation (5) into (1).

h is a clever transformation

$\alpha_1(\quad) + \alpha_2(\quad)$

Example: Consider the estimation function

$\beta = \text{pinv}A \cdot Y$

$$\hat{y}(x) = \alpha_1 e^{\alpha_2 x} \tag{7}$$

$\log \hat{y} = \log(\alpha_1 e^{\alpha_2 x})$

Applying the transformation

$\beta = \begin{bmatrix} \tilde{\alpha}_1 \\ \alpha_2 \end{bmatrix}$

$$\tilde{y}(x) = log(\hat{y}(x)) \tag{8}$$

$= \log \alpha_1 + \log(e^{\alpha_2 x})$

converts (7) into

$$\tilde{y}(x) = \tilde{\alpha_1} + \alpha_2 x \tag{9}$$

$= \log \alpha_1 + \alpha_2 x$

where we define $\tilde{\alpha_1} = log(\alpha_1)$. Now, least squares regression can be applied to equation (9). The parameter α_1 can be found using $\alpha_1 = e^{\tilde{\alpha_1}}$.

$\alpha_1 = e^{\tilde{\alpha}_1}$

$f_1(x) = 1, \quad f_2(x) = x$

End of Lecture 13

Please provide your feedback here