ENGR 308 (Fall 2025) S. Alghunaim

# 6. Least squares regression

- curve fitting and statistics
- straight line fit to data
- linearization of nonlinear equations
- fitting a polynomial to data
- multiple linear regression
- general linear least squares

### **Curve fitting: motivation**

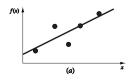
- data are often available only at discrete points along a continuum
- we may need estimates at points between known values
- we can use simple function to approximate complicated data
- this is called curve fitting

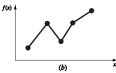
#### Regression

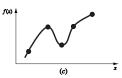
- data contain significant error or noise
- · derive curve representing general trend
- curve does not necessarily pass through all points
- example: least squares regression

#### Interpolation

- data are very accurate
  - fit a curve (or piecewise curves) exactly
  - estimate values between points
  - example: interpolation







curve fitting and statistics SA — ENGR308 6.2

## Engineering practice and curve fitting

- common engineering need: estimating intermediate values
- two main applications: trend analysis and hypothesis testing

#### Trend analysis

- use data patterns for prediction
  - interpolation: within the range of available data
  - extrapolation: outside the available range
- · applications appear in all fields of engineering

#### Hypothesis testing

- compare existing mathematical model with observed data
- two cases:
  - model coefficients unknown → determine best-fit values
  - 2. model coefficients known  $\rightarrow$  check adequacy of predictions
- multiple models may be tested, best selected empirically

### Other uses of curve fitting

- derive simpler functions to approximate complicated ones
- essential tool in numerical methods:
  - numerical integration
  - solution of differential equations
- · provides efficiency and insight into underlying physical systems

### Statistics for experimental data

- engineering measurements often provide limited raw information
- example:

24 readings of coefficient of thermal expansion of structural steel [× $10^{-6}$  in/(in· °F)]

6.495	6.595	6.615	6.635	6.485	6.555
6.665	6.505	6.435	6.625	6.715	6.655
6.755	6.625	6.715	6.575	6.655	6.605
6.565	6.515	6.555	6.395	6.775	6.685

range: 6.395 to 6.775  $\times 10^{-6}$ 

• more insight is obtained by computing descriptive statistics:

1. mean: location of the center of the data

2. standard deviation and variance: spread of the data

#### Mean and standard deviation

given data points  $y_1, \ldots, y_n$ 

#### Arithmetic mean

$$\bar{y} = \frac{\sum_{i=1}^{n} y_i}{n}$$

#### Standard deviation

$$s_y = \sqrt{\frac{S_t}{n-1}}, \quad S_t = \sum_{i=1}^n (y_i - \bar{y})^2$$

- measures the spread of data about mean
- if measurements are spread out widely around the mean,  $S_t$  (and  $S_v$ ) will be large
- if they are grouped tightly, the standard deviation will be small
- the variance is the square of standard deviation:

$$s_y^2 = \frac{\sum_{i=1}^n (y_i - \bar{y})^2}{n-1} = \frac{\sum y_i^2 - (\sum y_i)^2 / n}{n-1}$$

#### Coefficient of variation

#### Coefficient of variation

$$\text{c.v.} = \frac{s_y}{\bar{y}} \times 100\%$$

- · provides a normalized measure of spread
- similar in spirit to relative error

**Remark:**  $S_t$  and  $S_v$  are based on n-1 degrees of freedom

- this nomenclature arises because  $(\bar{y} y_1) + (\bar{y} y_2) + \cdots + (\bar{y} y_n) = 0$
- if  $\bar{y}$  is known and n-1 of the values are specified, the remaining value is fixed
- hence only n-1 of the values are freely determined
- another justification: there is no spread of a single data point
- however, it is also common to be defined by dividing by n instead of n-1

### Example

6.495	6.595	6.615	6.635	6.485	6.555
6.665	6.505	6.435	6.625	6.715	6.655
6.755	6.625	6.715	6.575	6.655	6.605
6.565	6.515	6.555	6.395	6.775	6.685

- n = 24 measurements of coefficient of thermal expansion
- average (mean):

$$\sum y_i = 158.4, \quad \bar{y} = \frac{158.4}{24} = 6.6$$

standard deviation and variance:

$$\sum (y_i - \bar{y})^2 = 0.217$$
,  $s_y = \sqrt{\frac{0.217}{24 - 1}} = 0.097133$ ,  $s_y^2 = 0.009435$ 

· coefficient of variation

c.v. = 
$$\frac{0.097133}{6.6} \times 100\% = 1.47\%$$

indicates that the data are tightly clustered around the mean

#### **Outline**

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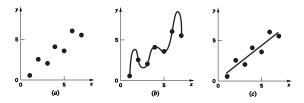
## Straight line data fitting

simplest example of least squares: fitting a straight line to observations

$$(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$$

**Line model:**  $y = a_0 + a_1 x + e$  where  $a_0, a_1$  are to determined based on data

- $a_0$  is intercept
- a<sub>1</sub> is slope
- $e = y a_0 a_1 x$  is error or residual
- residual is discrepancy between true value of y and approximate value  $a_0 + a_1 x$



## Least squares fit of straight line

minimize the sum of squared residuals over data:

$$S_r = \sum_{i=1}^n e_i^2 = \sum_{i=1}^n (y_i - a_0 - a_1 x_i)^2$$

- called linear regression
- to find  $a_0$  and  $a_1$  that minimize  $S_r$ , we set partial derivatives w.r.t.  $a_0, a_1$  to zero:

$$\frac{\partial S_r}{\partial a_0} = -2\sum_i (y_i - a_0 - a_1 x_i) = 0$$

$$\frac{\partial S_r}{\partial a_1} = -2\sum_i (y_i - a_0 - a_1 x_i) x_i = 0$$

yields a unique line for a given data set

#### Solution

rewriting previous equation as

$$-\sum_{i} y_{i} + na_{0} + a_{1} \sum_{i} x_{i} = 0$$
$$-\sum_{i} (y_{i}x_{i}) + a_{0} \sum_{i} x_{i} + a_{1} \sum_{i} x_{i}^{2} = 0$$

which can be written as:

$$\begin{bmatrix} n & \sum_{i} x_{i} \\ \sum_{i} x_{i} & \sum_{i} x_{i}^{2} \end{bmatrix} \begin{bmatrix} a_{0} \\ a_{1} \end{bmatrix} = \begin{bmatrix} \sum_{i} y_{i} \\ \sum_{i} x_{i} y_{i} \end{bmatrix}$$

these are called the *normal equations* 

• solving the normal equations:

$$a_1 = \frac{n \sum x_i y_i - \sum x_i \sum y_i}{n \sum x_i^2 - (\sum x_i)^2}, \quad a_0 = \bar{y} - a_1 \bar{x}$$

where  $\bar{x}$  and  $\bar{y}$  are the sample means of x and y

## **Example**

fit a straight line to the x and y values in the table

· compute the following quantities:

$$n = 7$$
,  $\sum x_i = 28$ ,  $\bar{x} = \frac{28}{7} = 4$   
 $\sum y_i = 24$ ,  $\bar{y} = \frac{24}{7} = 3.428571$   
 $\sum x_i y_i = 119.5$ ,  $\sum x_i^2 = 140$ 

thus

$$a_1 = \frac{n \sum x_i y_i - \sum x_i \sum y_i}{n \sum x_i^2 - (\sum x_i)^2} = \frac{7(119.5) - (28)(24)}{7(140) - (28)^2} = 0.8392857$$

$$a_0 = \bar{y} - a_1 \bar{x} = 3.428571 - (0.8392857)(4) = 0.07142857$$

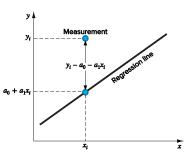
and

$$y = 0.07142857 + 0.8392857x$$

## Residuals and error analysis

#### Error for the linear fit

$x_i$	Уi	$(y_i - \bar{y})^2$	$(y_i - a_0 - a_1 x_i)^2$
1	0.5	8.5765	0.1687
2	2.5	0.8622	0.5625
3	2.0	2.0408	0.3473
4	4.0	0.3265	0.3265
5	3.5	0.0051	0.5896
6	6.0	6.6122	0.7972
7	5.5	4.2908	0.1993
Σ	24.0	22.7143	2.9911



sum of squared residuals:

$$S_r = \sum_{i=1}^n (y_i - a_0 - a_1 x_i)^2 = 2.9911$$

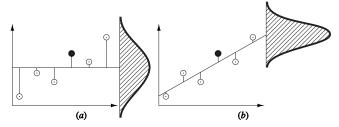
- least squares line is unique: any other line gives a larger  $S_r$
- $\bullet$  residuals quantify the vertical discrepancies between observed  $y_i$  and the line

#### Standard error of the estimate

a "standard deviation" for the regression line can be defined as

$$s_{y/x} = \sqrt{\frac{S_r}{n-2}}$$

- $s_{y/x}$  is called the *standard error of the estimate*
- we divide by n 2 since two estimates (a<sub>0</sub> and a<sub>1</sub>) were used to compute S<sub>r</sub>
   there is no such thing as the "spread of data" around a straight line connecting two points
- $s_{y/x}$  quantifies spread of data around the regression line



straight line fit to data SA — ENGR308 6.14

#### Coefficient of determination

- $S_t$ : total sum of squares around the mean (before regression)
- $S_r$ : sum of squares of residuals around regression line (unexplained error)
- $S_t S_r$ : improvement of straight line fit compared with average value

#### Normalized improvement

$$r^{2} = \frac{S_{t} - S_{r}}{S_{t}} \implies r = \frac{n \sum x_{i} y_{i} - (\sum x_{i})(\sum y_{i})}{\sqrt{n \sum x_{i}^{2} - (\sum x_{i})^{2}} \sqrt{n \sum y_{i}^{2} - (\sum y_{i})^{2}}}$$

- r<sup>2</sup>: coefficient of determination
- r: correlation coefficient
- $r^2 = 1$ : perfect fit ( $S_r = 0$ )
- $r^2 = 0$ : no improvement  $(S_r = S_t)$

### **Example**

compute total standard deviation, standard error of estimate, and correlation coefficient for data in last example

· standard deviation:

$$s_y = \sqrt{\frac{22.7143}{7 - 1}} = 1.9457$$

standard error of the estimate:

$$s_{y/x} = \sqrt{\frac{2.9911}{7 - 2}} = 0.7735$$

since  $s_{y/x} < s_y$ , the linear regression model has merit

extent of improvement is quantified by

$$r^2 = \frac{22.7143 - 2.9911}{22.7143} = 0.868 \quad \text{or} \quad r = \sqrt{0.868} = 0.932$$

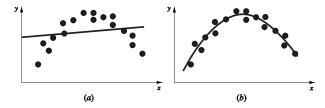
• interpretation: 86.8% of original uncertainty has been explained by linear model – caution: high r does not always imply a good fit

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#### **Linear transformation**

- line fitting assumes linear relation between dep. and indep. variables
- always begin regression analysis by plotting the data
- for nonlinear data, other approaches are required such as polynomial regression



- nonlinear models can sometime be transformed into linear form
  - linear regression can then be applied to estimate coefficients
  - results must be transformed back for predictive use

## **Exponential model**

$$y=\alpha_1 e^{\beta_1 x}$$

- $\alpha_1, \beta_1$  are constants
- models growth or decay (population, radioactive decay)
- nonlinear for  $\beta_1 \neq 0$

Linearization: take natural log:

$$\ln y = \ln \alpha_1 + \beta_1 x$$

- plot  $\ln y \text{ vs } x$
- slope =  $\beta_1$ , intercept =  $\ln \alpha_1$

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#### Power model

$$y = \alpha_2 x^{\beta_2}$$

- $\alpha_2, \beta_2$  are constants
- widely used in engineering (e.g., scaling laws)

Linearization: take base-10 log:

$$\log y = \beta_2 \log x + \log \alpha_2$$

- plot  $\log y$  vs  $\log x$
- slope =  $\beta_2$ , intercept =  $\log \alpha_2$

## Saturation-growth-rate model

$$y = \frac{\alpha_3 x}{\beta_3 + x}$$

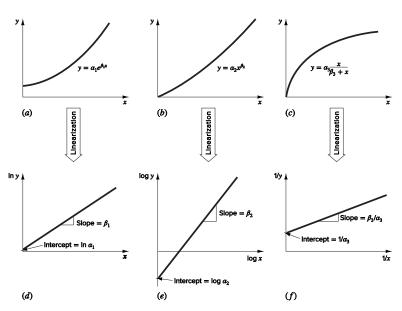
- used for population growth under limiting conditions
- levels off (saturates) as x increases

Linearization: invert the equation:

$$\frac{1}{y} = \frac{\beta_3}{\alpha_3} \frac{1}{x} + \frac{1}{\alpha_3}$$

- plot 1/y vs 1/x
- slope =  $\beta_3/\alpha_3$ , intercept =  $1/\alpha_3$

# **Summary**



### **Example**

we fit data to the model  $y = \alpha_2 x^{\beta_2}$ 

x	у	$\log x$	$\log y$
1	0.5	0.000	-0.301
2	1.7	0.301	0.226
3	3.4	0.477	0.534
4	5.7	0.602	0.753
5	8.4	0.699	0.922

• take logarithm:

$$\log y = \beta_2 \log x + \log \alpha_2$$

- this is a linear equation in  $\log x$  and  $\log y$
- ullet apply linear regression to the transformed data to find  $eta_2$  and  $\loglpha_2$

## **Example**

linear regression of the log-transformed data yields:

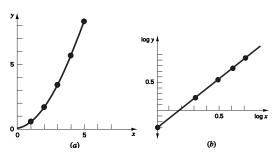
$$\log y = 1.75 \, \log x - 0.300$$

• slope:  $\beta_2 = 1.75$ 

• intercept:  $\log \alpha_2 = -0.300 \Longrightarrow \alpha_2 = 10^{-0.300} \approx 0.501$ 

• final model:

$$y = 0.501 \, x^{1.75}$$



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## Quadratic model and least squares objective

suppose data are related by a quadratic model:

$$y = a_0 + a_1 x + a_2 x^2 + e$$

- $(a_0, a_1, a_2)$  are model parameters to be determined
- given data  $(x_1, y_1), \ldots, (x_n, y_n)$ , the residual sum of squares is

$$S_r = \sum_{i=1}^n (y_i - a_0 - a_1 x_i - a_2 x_i^2)^2$$

• we minimize  $S_r$  by setting partial derivatives to zero

$$\frac{\partial S_r}{\partial a_0} = -2\sum (y_i - a_0 - a_1 x_i - a_2 x_i^2) = 0$$

$$\frac{\partial S_r}{\partial a_1} = -2\sum x_i (y_i - a_0 - a_1 x_i - a_2 x_i^2) = 0$$

$$\frac{\partial S_r}{\partial a_2} = -2\sum x_i^2 (y_i - a_0 - a_1 x_i - a_2 x_i^2) = 0$$

## Normal equations for the quadratic

collecting terms yields a 3 × 3 linear system:

$$na_0 + (\sum x_i)a_1 + (\sum x_i^2)a_2 = \sum y_i$$

$$(\sum x_i)a_0 + (\sum x_i^2)a_1 + (\sum x_i^3)a_2 = \sum x_i y_i$$

$$(\sum x_i^2)a_0 + (\sum x_i^3)a_1 + (\sum x_i^4)a_2 = \sum x_i^2 y_i$$

in matrix form:

$$\begin{bmatrix} n & \sum x_i & \sum x_i^2 \\ \sum x_i & \sum x_i^2 & \sum x_i^3 \\ \sum x_i^2 & \sum x_i^3 & \sum x_i^4 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \sum y_i \\ \sum x_i y_i \\ \sum x_i^2 y_i \end{bmatrix}$$

• solve for  $(a_0, a_1, a_2)$  with any linear solver

### General mth-order polynomial regression

$$y = a_0 + a_1 x + a_2 x^2 + \dots + a_m x^m + e$$

• minimize  $S_r = \sum_{i=1}^n (y_i - \sum_{k=0}^m a_k x_i^k)^2$  by setting partial derivatives to zero:

$$\begin{bmatrix} n & \sum x_i & \cdots & \sum x_i^m \\ \sum x_i & \sum x_i^2 & \cdots & \sum x_i^{m+1} \\ \vdots & \vdots & \ddots & \vdots \\ \sum x_i^m & \sum x_i^{m+1} & \cdots & \sum x_i^{2m} \end{bmatrix} \begin{bmatrix} a_0 \\ a_0 \\ \vdots \\ a_m \end{bmatrix} = \begin{bmatrix} \sum y_i \\ \sum x_i y_i \\ \vdots \\ \sum x_i^m y_i \end{bmatrix}$$

• results in *m*+1 normal equations in *m*+1 unknowns

#### Standard error of the estimate

$$s_{y/x} = \sqrt{\frac{S_r}{n - (m+1)}}$$

#### Coefficient of determination

$$r^2 = \frac{S_t - S_r}{S_t}, \qquad S_t = \sum_{i=1}^n (y_i - \bar{y})^2$$

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## Example: fit a quadratic

fit quadratic  $y = a_0 + a_1x + a_2x^2 + e$  model to data

we have

$$n = 6$$
,  $\sum x_i = 15$ ,  $\sum x_i^2 = 55$ ,  $\sum x_i^3 = 225$ ,  $\sum x_i^4 = 979$ ,  
 $\sum y_i = 152.6$ ,  $\sum x_i y_i = 585.6$ ,  $\sum x_i^2 y_i = 2488.8$ 

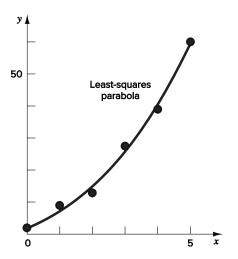
· normal equations:

$$\begin{bmatrix} 6 & 15 & 55 \\ 15 & 55 & 225 \\ 55 & 225 & 979 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 152.6 \\ 585.6 \\ 2488.8 \end{bmatrix}$$

- solution:  $a_0 = 2.47857$ ,  $a_1 = 2.35929$ ,  $a_2 = 1.86071$
- quadratic fit:

$$y = 2.47857 + 2.35929 x + 1.86071 x^2$$

# Example: fit a quadratic



## Example: fit a quadratic

$x_i$	$y_i$	$(y_i - \bar{y})^2$	$(y_i - a_0 - a_1 x_i - a_2 x_i^2)^2$
0	2.1	544.44	0.14332
1	7.7	314.47	1.00286
2	13.6	140.03	1.08158
3	27.2	3.12	0.80491
4	40.9	239.22	0.61951
5	61.1	1272.11	0.09439
Σ	152.6	2513.39	3.74657

- from the residuals table:  $S_r = 3.74657$ ,  $S_t = 2513.39$
- standard error (quadratic, m+1=3 parameters):

$$s_{y/x} = \sqrt{\frac{S_r}{n - (m+1)}} = \sqrt{\frac{3.74657}{6-3}} = 1.12$$

coefficient of determination:

$$r^2 = \frac{S_t - S_r}{S_t} = \frac{2513.39 - 3.74657}{2513.39} = 0.99851, \qquad r = 0.99925$$

so 99.851% of original variability is explained by quadratic model; fit is excellent

#### **Outline**

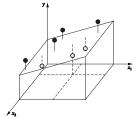
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## Multiple linear regression

linear model with multiple predictors:

$$y = a_0 + a_1 x_1 + a_2 x_2 + \dots + a_m x_m + e$$

- in data-fitting, y is called *outcome* and  $x_1, \ldots, x_m$  are called *features*
- for two predictors, the best-fit "line" becomes a plane in  $(x_1, x_2, y)$



• choose coefficients  $\{a_j\}_{j=0}^m$  that minimize the sum of squared residuals

$$S_r = \sum_{i=1}^n (y_i - a_0 - a_1 x_{1i} - \dots - a_m x_{mi})^2$$

over data  $(x_i, y_i)$  for  $i = 1, \dots, n$  where  $x_i = (x_{1i}, \dots, x_{mi})$  is an m-vector

## Least squares plane fit

for m=2

$$S_r = \sum_{i=1}^n (y_i - a_0 - a_1 x_{1i} - a_2 x_{2i})^2$$

take partial derivatives and set to zero:

$$\frac{\partial S_r}{\partial a_0} = -2 \sum (y_i - a_0 - a_1 x_{1i} - a_2 x_{2i}) = 0$$

$$\frac{\partial S_r}{\partial a_1} = -2 \sum x_{1i} (y_i - a_0 - a_1 x_{1i} - a_2 x_{2i}) = 0$$

$$\frac{\partial S_r}{\partial a_2} = -2 \sum x_{2i} (y_i - a_0 - a_1 x_{1i} - a_2 x_{2i}) = 0$$

matrix (normal equations) form:

$$\begin{bmatrix} n & \sum x_{1i} & \sum x_{2i} \\ \sum x_{1i} & \sum x_{1i}^2 & \sum x_{1i}x_{2i} \\ \sum x_{2i} & \sum x_{1i}x_{2i} & \sum x_{2i}^2 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \sum y_i \\ \sum x_{1i}y_i \\ \sum x_{2i}y_i \end{bmatrix}$$

### Example

data (generated by  $y = 5 + 4x_1 - 3x_2$ )

у	$x_1$	$x_2$	$x_1^2$	$x_{2}^{2}$	$x_1x_2$	$x_1y$	$x_2y$
5	0	0	0	0	0	0	0
10	2	1	4	1	2	20	10
9	2.5	2	6.25	4	5	22.5	18
0	1	3	1	9	3	0	0
3	4	6	16	36	24	12	18
27	7	2	49	4	14	189	54
Σ	54	16.5	76.25	54	48	243.5	100

$$\sum y = 54, \quad \sum x_1 = 16.5, \quad \sum x_2 = 14$$
$$\sum x_1^2 = 76.25, \quad \sum x_2^2 = 54, \quad \sum x_1 x_2 = 48$$
$$\sum x_1 y = 243.5, \quad \sum x_2 y = 100$$

normal equations:

$$\begin{bmatrix} 6 & 16.5 & 14 \\ 16.5 & 76.25 & 48 \\ 14 & 48 & 54 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 54 \\ 243.5 \\ 100 \end{bmatrix} \Rightarrow a_0 = 5, a_1 = 4, a_2 = -3$$

## Goodness of fit and uncertainty

residual sum of squares

$$S_r = \sum_{i=1}^n (y_i - \hat{y}_i)^2, \quad \hat{y}_i = a_0 + a_1 x_{1i} + a_2 x_{2i}$$

• total sum of squares about the mean  $\bar{y}$ :

$$S_t = \sum_{i=1}^n (y_i - \bar{y})^2$$

• standard error of the estimate (multiple regression with *m* predictors)

$$s_{y/x} = \sqrt{\frac{S_r}{n - (m+1)}}$$

• coefficient of determination (explained variance fraction)

$$r^2 = \frac{S_t - S_r}{S_t}, \qquad 0 \le r^2 \le 1$$

### Power-law via multiple linear regression

many engineering relations are multiplicative:

$$y = a_0 \, x_1^{a_1} \, x_2^{a_2} \cdots x_m^{a_m}$$

• take logarithms to linearize:

$$\log y = \log a_0 + a_1 \log x_1 + \dots + a_m \log x_m$$

- perform multiple linear regression with response  $\log y$  and predictors  $\log x_k$
- recover coefficients via  $a_0 = 10^{\text{intercept}}$ , exponents  $a_k$  are the slopes

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### Linear-in-parameters model

model is *linear-in-parameter* 

$$y = a_0 z_0 + a_1 z_1 + a_2 z_2 + \dots + a_m z_m + e$$

- $z_0, \ldots, z_m$  are basis functions/feature mapping that we choose; e is residual
- the term "linear" refers only to linearity in the parameters  $a_i$
- basis functions  $z_j$  may be nonlinear (e.g.,  $z_j = \sin(\omega t)$ )

#### **Examples**

- simple linear regression (line model):  $z_0 = 1$ ,  $z_1 = x$
- polynomial regression:  $z_0 = 1$ ,  $z_1 = x$ ,  $z_2 = x^2$ , ...,  $z_m = x^m$
- multiple linear regression:  $z_0 = 1$ ,  $z_1 = x_1$ ,  $z_2 = x_2$ , ...
- $y = a_0 + a_1 \cos(\omega t) + a_2 \sin(\omega t), z_0 = 1, z_1 = \cos(\omega t), z_2 = \sin(\omega t)$

#### **Matrix formulation**

given data  $(z_i, y_i)_{i=1}^n$  with  $z_i = (z_{0i}, \dots, z_{mi})$ , model can be written as

$$y = Za + E$$

where

$$Z = \begin{bmatrix} z_{01} & z_{11} & \cdots & z_{m1} \\ z_{02} & z_{12} & \cdots & z_{m2} \\ \vdots & \vdots & \ddots & \vdots \\ z_{0n} & z_{1n} & \cdots & z_{mn} \end{bmatrix}$$

is an  $n \times m$  matrix and

$$y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \quad a = \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_m \end{bmatrix}, \quad E = \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{bmatrix}$$

### **Normal equations**

the least squares criterion minimizes

$$S_r = \sum_{i=1}^{n} (y_i - \sum_{j=0}^{m} z_{ji} a_j)^2$$

- called linear regression or least squares regression
- differentiating w.r.t. each a<sub>i</sub> and setting to zero yields the normal equations:

$$Z^T Z a = Z^T y$$

• if  $Z^TZ$  is invertible, then the solution is unique

$$a = (Z^T Z)^{-1} Z^T y$$

- this unifies linear, polynomial, and multiple regression under one framework
- in MATLAB: a=Z\y

#### Remarks

- true nonlinear models, e.g.,  $y = a_0(1 e^{-a_1x})$ , cannot be put into the linear form
- nonlinear models require nonlinear regression

## References and further readings

- S. C. Chapra and R. P. Canale. Numerical Methods for Engineers (8th edition). McGraw Hill, 2021. (Ch.17)
- S. C. Chapra. Applied Numerical Methods with MATLAB for Engineers and Scientists (5th edition).
   McGraw Hill, 2023. (Ch.14, 15)

references SA\_ENGR308 6.38