

## 6. Least squares regression

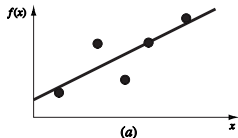
- curve fitting and statistics
- straight line fit to data
- linearization of nonlinear equations
- fitting a polynomial to data
- multiple linear regression
- general linear least squares

# 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**

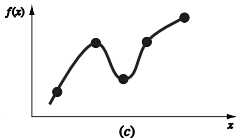
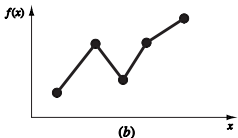
## Regression

- 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



# Engineering practice and curve fitting

- common engineering need: estimating intermediate values
- many properties are not tabulated → must fit your own data
- 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:
  1. model coefficients unknown → determine best-fit values
  2. model coefficients known → 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 [ $\times 10^{-6}$  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  $y_1, \dots, y_n$

### 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  $s_y$ ) 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  $s_y$  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:

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

- coefficient of variation

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

indicates that the data are tightly clustered around the mean



# Outline

- 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

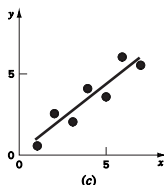
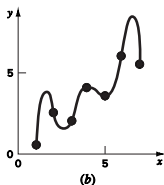
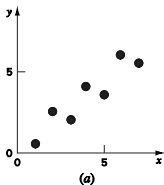
## Straight line data fitting

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

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

**Line model:**  $y = a_0 + a_1x + e$  where  $a_0, a_1$  are to be determined based on data

- $a_0$  is intercept
- $a_1$  is slope
- $e = y - a_0 - a_1x$  is *error* or *residual*
- residual is discrepancy between true value of  $y$  and approximate value  $a_0 + a_1x$



## 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

$$\begin{aligned}-\sum_i y_i + na_0 + a_1 \sum_i x_i &= 0 \\ -\sum_i (y_i x_i) + a_0 \sum_i x_i + a_1 \sum_i x_i^2 &= 0\end{aligned}$$

- 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

$x_i$	1	2	3	4	5	6	7
$y_i$	0.5	2.5	2.0	4.0	3.5	6.0	5.5

- compute the following quantities:

$$n = 7, \quad \sum x_i = 28, \quad \bar{x} = \frac{28}{7} = 4$$

$$\sum y_i = 24, \quad \bar{y} = \frac{24}{7} = 3.428571$$

$$\sum x_i y_i = 119.5, \quad \sum x_i^2 = 140$$

- thus

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

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

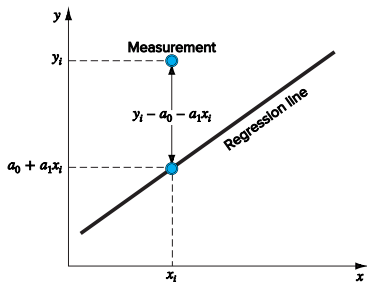
and

$$y = 0.07142857 + 0.8392857x$$

# Residuals and error analysis

## Error for the linear fit

$x_i$	$y_i$	$(y_i - \bar{y})^2$	$(y_i - a_0 - a_1 x_i)^2$
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
$\Sigma$	24.0	22.7143	2.9911



sum of squared residuals:

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

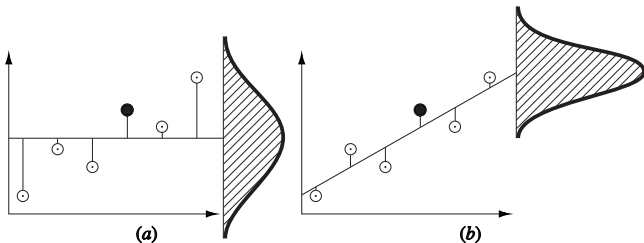
- least squares line is unique: any other line gives a larger  $S_r$
- residuals quantify the vertical discrepancies between observed  $y_i$  and the line

## 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 ( $a_0$  and  $a_1$ ) were used to compute  $S_r$ 
  - 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*



## 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

$$r^2 = \frac{S_t - S_r}{S_t} \implies r = \frac{n \sum x_i y_i - (\sum x_i)(\sum y_i)}{\sqrt{n \sum x_i^2 - (\sum x_i)^2} \sqrt{n \sum y_i^2 - (\sum y_i)^2}}$$

- $r^2$ : *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

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

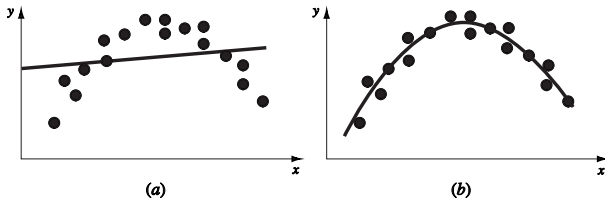
- interpretation: 86.8% of original uncertainty has been explained by linear model
  - caution: high  $r$  does not always imply a good fit

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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  $\ln y$  vs  $x$
- slope =  $\beta_1$ , intercept =  $\ln \alpha_1$

## 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

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

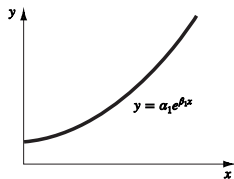
- used for population growth under limiting conditions
- levels off (saturates) as  $x$  increases

**Linearization:** invert the equation:

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

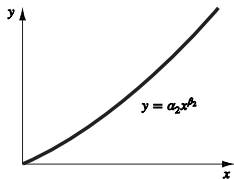
- plot  $1/y$  vs  $1/x$
- slope =  $\beta_3/\alpha_3$ , intercept =  $1/\alpha_3$

# Summary



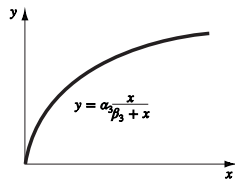
(a)

Linearization



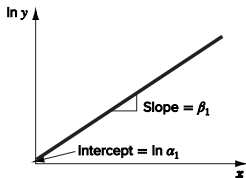
(b)

Linearization

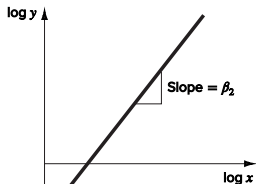


(c)

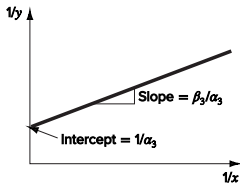
Linearization



(d)



(e)



(f)

## Example

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

$x$	$y$	$\log x$	$\log y$
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  $\log y$
- apply linear regression to the transformed data to find  $\beta_2$  and  $\log \alpha_2$



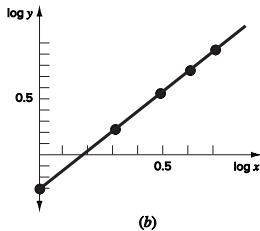
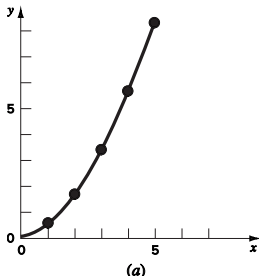
## Example

linear regression of the log-transformed data yields:

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

- slope:  $\beta_2 = 1.75$
- intercept:  $\log \alpha_2 = -0.300 \implies \alpha_2 = 10^{-0.300} \approx 0.501$
- 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:

$$y = a_0 + a_1x + a_2x^2 + e$$

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

$$S_r = \sum_{i=1}^n (y_i - a_0 - a_1x_i - a_2x_i^2)^2$$

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

$$\frac{\partial S_r}{\partial a_0} = -2 \sum (y_i - a_0 - a_1x_i - a_2x_i^2) = 0$$

$$\frac{\partial S_r}{\partial a_1} = -2 \sum x_i (y_i - a_0 - a_1x_i - a_2x_i^2) = 0$$

$$\frac{\partial S_r}{\partial a_2} = -2 \sum x_i^2 (y_i - a_0 - a_1x_i - a_2x_i^2) = 0$$

## Normal equations for the quadratic

- collecting terms yields a  $3 \times 3$  linear system:

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

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

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

- 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 $m$ th-order polynomial regression

$$y = a_0 + a_1x + a_2x^2 + \cdots + a_mx^m + e$$

- 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:

$$\begin{bmatrix} n & \sum x_i & \cdots & \sum x_i^m \\ \sum x_i & \sum x_i^2 & \cdots & \sum x_i^{m+1} \\ \vdots & \vdots & \ddots & \vdots \\ \sum x_i^m & \sum x_i^{m+1} & \cdots & \sum x_i^{2m} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_m \end{bmatrix} = \begin{bmatrix} \sum y_i \\ \sum x_i y_i \\ \vdots \\ \sum x_i^m y_i \end{bmatrix}$$

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

## Example: fit a quadratic

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

$x_i$	0	1	2	3	4	5
$y_i$	2.1	7.7	13.6	27.2	40.9	61.1

- we have

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

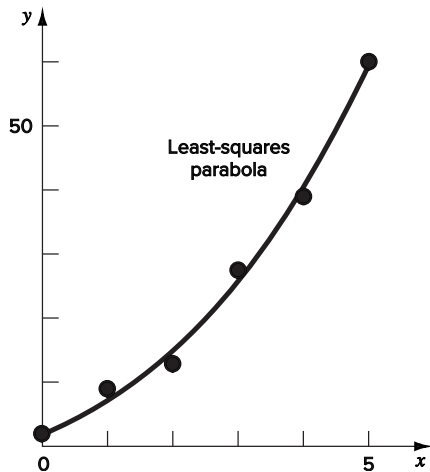
- normal equations:

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

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

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

## Example: fit a quadratic



## Example: fit a quadratic

$x_i$	$y_i$	$(y_i - \bar{y})^2$	$(y_i - a_0 - a_1x_i - a_2x_i^2)^2$
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
$\Sigma$	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:

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

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



# Outline

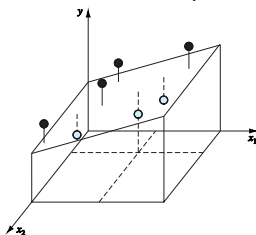
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# Multiple linear regression

linear model with multiple predictors:

$$y = a_0 + a_1x_1 + a_2x_2 + \cdots + a_mx_m + e$$

- in data-fitting,  $y$  is *outcome* and  $x_1, \dots, x_m$  are *features* or *regressors*
- 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

$$S_r = \sum_{i=1}^n (y_i - a_0 - a_1x_{1i} - \cdots - a_mx_{mi})^2$$

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

find model,  $y = a_0 + a_1x_1 + a_2x_2$ , that fits the data:

	$y$	$x_1$	$x_2$	$x_1^2$	$x_2^2$	$x_1x_2$	$x_1y$	$x_2y$
	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
$\Sigma$	54	16.5	14	76.25	54	48	243.5	100

$$\Sigma y = 54, \quad \Sigma x_1 = 16.5, \quad \Sigma x_2 = 14$$

$$\Sigma x_1^2 = 76.25, \quad \Sigma x_2^2 = 54, \quad \Sigma x_1x_2 = 48$$

$$\Sigma x_1y = 243.5, \quad \Sigma x_2y = 100$$

normal equations:

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

## Goodness of fit and uncertainty

- residual sum of squares

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

- 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)

$$r^2 = \frac{S_t - S_r}{S_t}, \quad 0 \leq r^2 \leq 1$$

## 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:

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

- 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

# Outline

- 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**

# Linear-in-parameters model

model is *linear-in-parameter*

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

- $z_0, \dots, z_m$  are *basis functions/feature mapping* that we choose;  $e$  is residual
- the term “linear” refers only to linearity in the parameters  $a_j$
- 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*:  $z_0 = 1, z_1 = x, z_2 = x^2, \dots, z_m = x^m$
- *multiple linear regression*:  $z_0 = 1, z_1 = x_1, z_2 = x_2, \dots$
- $y = a_0 + a_1 \cos(\omega t) + a_2 \sin(\omega t), z_0 = 1, z_1 = \cos(\omega t), z_2 = \sin(\omega t)$



## Normal equations

given data  $(z_i, y_i)_{i=1}^n$  with  $z_i = (z_{0i}, \dots, z_{mi})$ , the least squares criterion minimizes

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

- called *linear regression* or *least squares regression*
- differentiating w.r.t. each  $a_j$  and setting to zero yields the **normal equations**:

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

$$Z = \begin{bmatrix} z_{01} & z_{11} & \cdots & z_{m1} \\ z_{02} & z_{12} & \cdots & z_{m2} \\ \vdots & \vdots & \ddots & \vdots \\ z_{0n} & z_{1n} & \cdots & z_{mn} \end{bmatrix} \in \mathbb{R}^{n \times (m+1)}, \quad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \quad a = \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_m \end{bmatrix}$$

if  $Z^T Z$  is invertible, then the solution is unique  $a = (Z^T Z)^{-1} Z^T y$

– in MATLAB:  $a = Z \backslash y$ , which is called least squares *approximate* solution to  $Za = y$

- this unifies linear, polynomial, and multiple regression under one framework

## 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)