

## 6. Linear Regression

- linear least-squares/regression
- solving linear least-squares
- BLUE property
- distribution of LS estimators
- weighted least-squares and other variants

# Linear regression

- a linear relationship between variables  $y$  and  $x_k$  using a linear function:

$$y = \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_n x_n \triangleq x^T \beta$$

where  $y \in \mathbf{R}^m$ ,  $x \in \mathbf{R}^{m \times n}$ ,  $\beta \in \mathbf{R}^n$

- $y$  contains the measurement variables and is often called the *regressed/response/explained/dependent variable*
- $x_k$ 's are the input variables that explain the behavior of  $y$ ; called the *predictor/explanatory/independent variables*
- $\beta$  is the *regression coefficient*
- example: product sale amount (unit) is explained by advertising costs (USD)

$$\text{Sales} = \beta_1 \cdot \text{TV} + \beta_2 \cdot \text{Radio} + \beta_3 \cdot \text{News paper}$$

$\beta_1$  gives the average sale increase for one unit increase in TV ads (others fixed)

- given a data set:  $\{(x_i, y_i)\}_{i=1}^m$  we can form a matrix form

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{m1} & x_{m2} & \cdots & x_{mn} \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_n \end{bmatrix} \triangleq y = X\beta$$

- the matrix  $X$  is sometimes called *the design/regressor matrix*
- given  $y$  and  $X$ , one would like to estimate  $\beta$  that gives the linear model output match best with  $y$
- in practice, in the presence of noise and disturbance, more data should be collected in order to get a better estimate – leading to *overdetermined* linear equations
- an exact solution to  $y = X\beta$  does not usually exist; however, it can be solved by **linear least-squares** formulation

# Problem statement

**overdetermined linear equations:**

$$X\beta = y, \quad X \text{ is } m \times n \text{ with } m > n$$

for most  $y$  cannot solve for  $\beta$

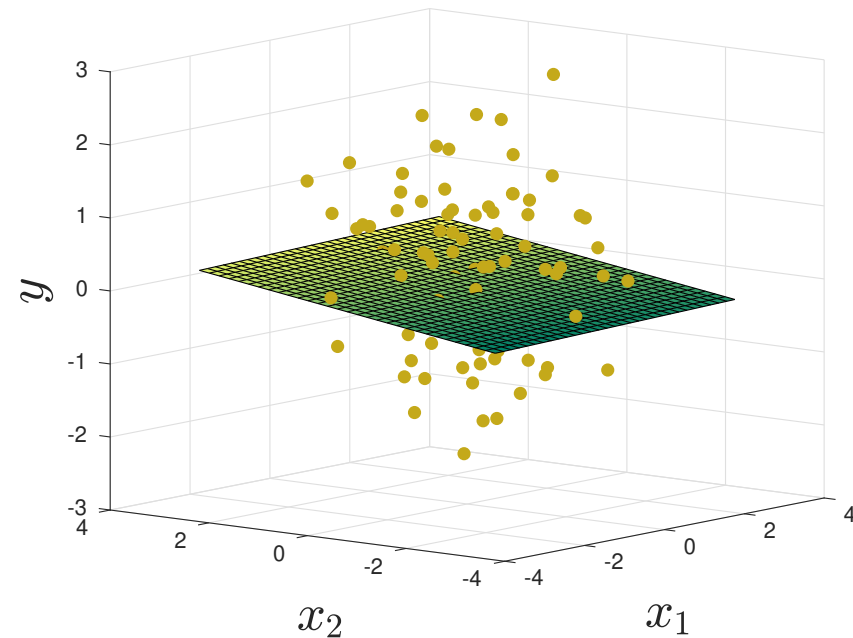
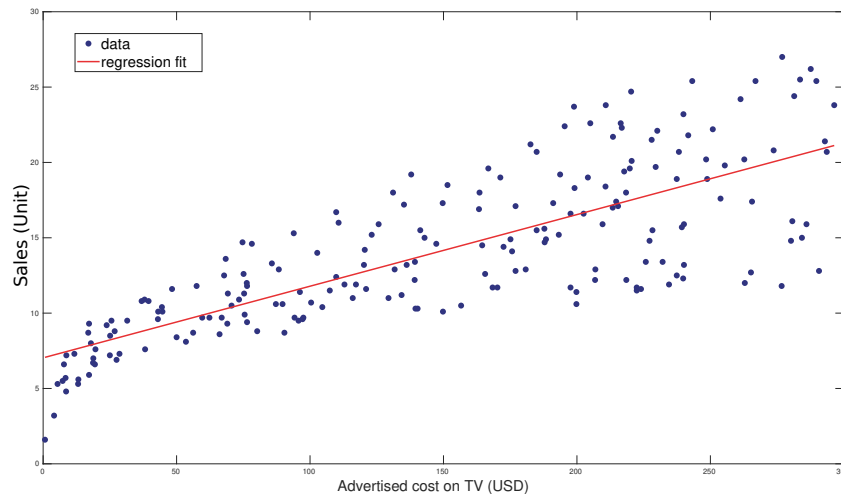
**linear least-squares formulation:**

$$\underset{\beta}{\text{minimize}} \quad \|y - X\beta\|_2 = \left( \sum_{i=1}^m \left( \sum_{j=1}^n X_{ij}\beta_j - y_i \right)^2 \right)^{1/2}$$

- $r = y - X\beta$  is called *the residual error*
- $\beta$  with smallest residual norm  $\|r\|$  is called *the least-squares solution*
- equivalent to minimizing  $\|y - X\beta\|^2$

# Fitting linear least-squares

left: explain the sale amount by advertising on TV



- left: sum squared distance of data points to the line is minimum (this line fits best)
- right: for two predictors, LS solution is the normal vector of hyperplane that lies closest to all data points of  $y$

## Example 1: data fitting

given data points  $\{(t_i, y_i)\}_{i=1}^m$ , we aim to approximate  $y$  using a function  $g(t)$

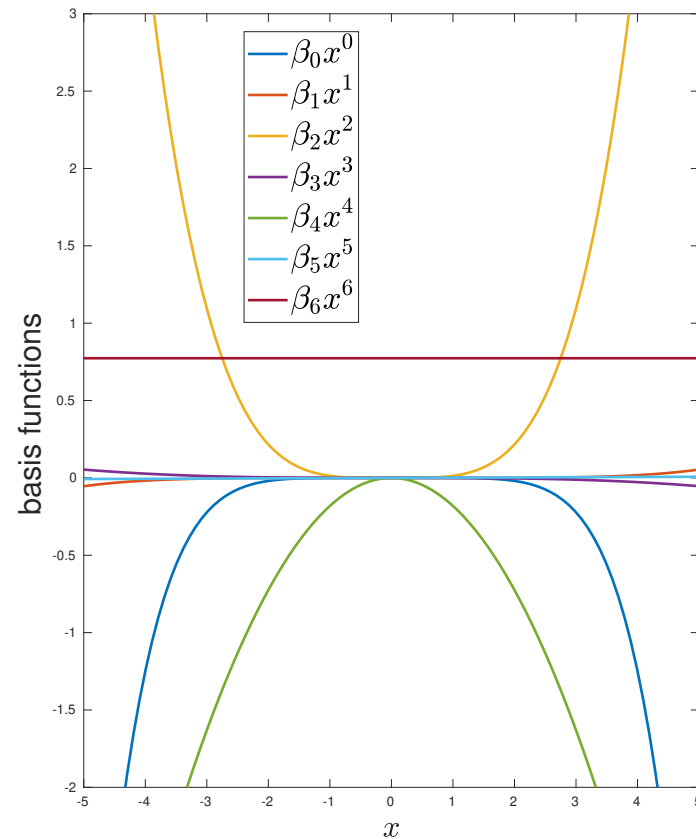
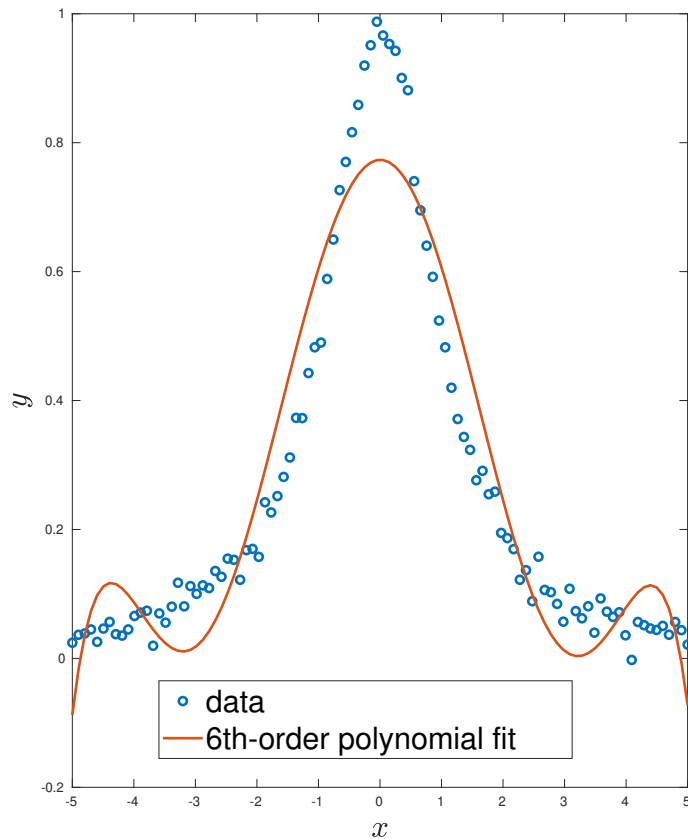
$$y = g(t) := \beta_1 g_1(t) + \beta_2 g_2(t) + \cdots + \beta_n g_n(t)$$

- $g_k(t) : \mathbf{R} \rightarrow \mathbf{R}$  is a basis function
  - polynomial functions:  $1, t, t^2, \dots, t^n$
  - sinusoidal functions:  $\cos(\omega_k t), \sin(\omega_k t)$  for  $k = 1, 2, \dots, n$
- the linear regression model can be formulated as

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} = \begin{bmatrix} g_1(t_1) & g_2(t_1) & \cdots & g_n(t_1) \\ g_1(t_2) & g_2(t_2) & \cdots & g_n(t_2) \\ \vdots & \vdots & & \vdots \\ g_1(t_m) & g_2(t_m) & \cdots & g_n(t_m) \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_n \end{bmatrix} \triangleq y = X\beta$$

- often have  $m \gg n$ , *i.e.*, explaining  $y$  using a few parameters in the model

fitting a 6th-order polynomial to data points generated from  $f(t) = 1/(1 + t^2)$



- (right) the weighted sum of basis functions ( $x^k$ ) is the fitted polynomial
- the ground-truth function  $f$  is nonlinear, but can be decomposed as a sum of polynomials

## Example 2: scalar first-order model

given data set:  $\{(u(t), y(t))\}_{t=1}^N$ , we aim to estimate a scalar ARX model

$$y(t) = ay(t-1) + bu(t-1) + e(t)$$

$y(t)$  is linear in model parameters:  $a, b$

$$\begin{bmatrix} y(2) \\ y(3) \\ \vdots \\ y(N) \end{bmatrix} = \begin{bmatrix} y(1) & u(1) \\ y(2) & u(2) \\ \vdots & \vdots \\ y(N-1) & u(N-1) \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix}$$

- the model is first-order, the equation is initialized with  $y(1), u(1)$
- the model can be generalized to

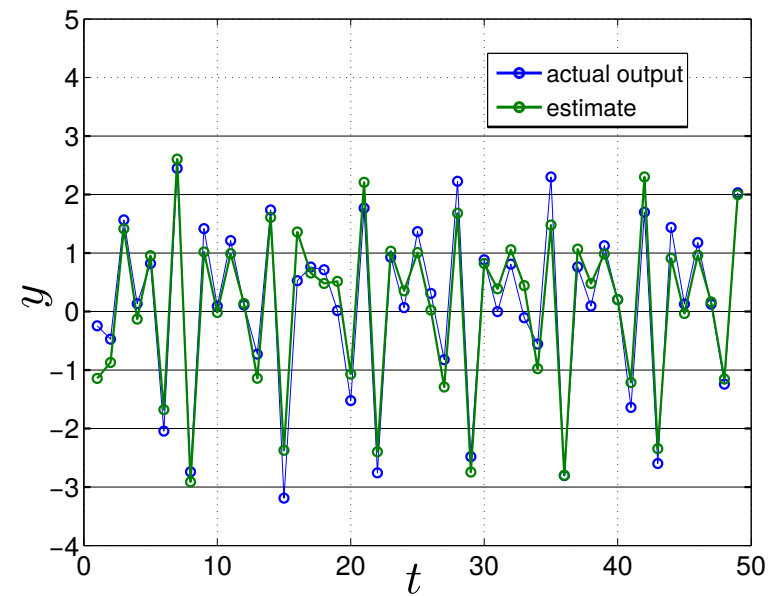
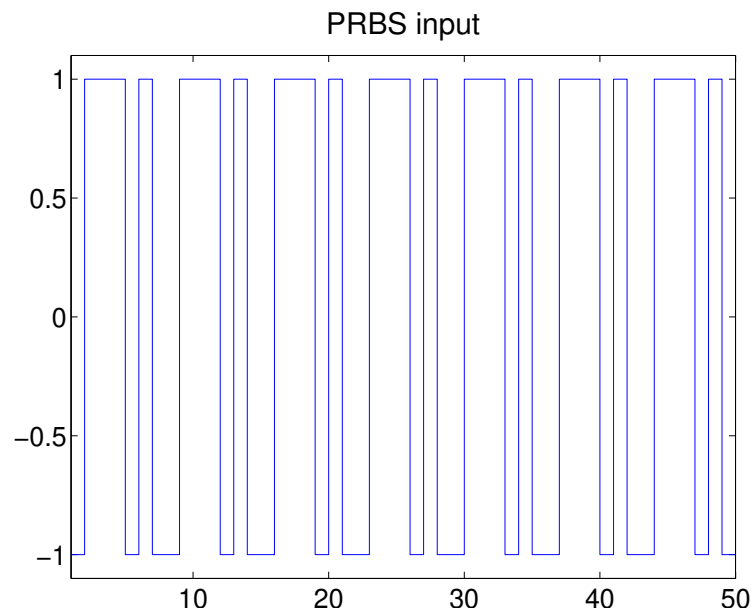
$$y(t) = a_1y(t-1) + \dots + a_p y(t-p) + b_1u(t-1) + \dots + b_m u(t-m) + e(t)$$

where  $\theta = (a_1, a_2, \dots, a_p, b_1, b_2, \dots, b_m)$  is the parameter vector



data generation:

- $a = 0.8, b = 1$  are true parameters
- $e$  is white noise with variance 0.1
- PRBS input



estimated parameters:  $\hat{a} = 0.75, \hat{b} = 1.08$

## Closed-form of least-squares estimate

the zero gradient condition of LS objective is

$$\frac{d}{d\beta} \|y - X\beta\|_2^2 = -X^T(y - X\beta) = 0$$

which is equivalent to the **normal equation**

$$X^T X \beta = X^T y$$

if  $X$  is **full rank**:

- least-squares solution can be found by solving the normal equations
- $n$  equations in  $n$  variables with a positive definite coefficient matrix
- the closed-form solution is  $\beta = (X^T X)^{-1} X^T y$
- $(X^T X)^{-1} X^T$  is a *left inverse* of  $X$

# Properties of full rank matrices

suppose  $X$  is an  $m \times n$  matrix; we always have

$$\text{rank}(X) \leq \min(m, n)$$

if  $X$  is full rank with  $m \geq n$  (tall matrix)

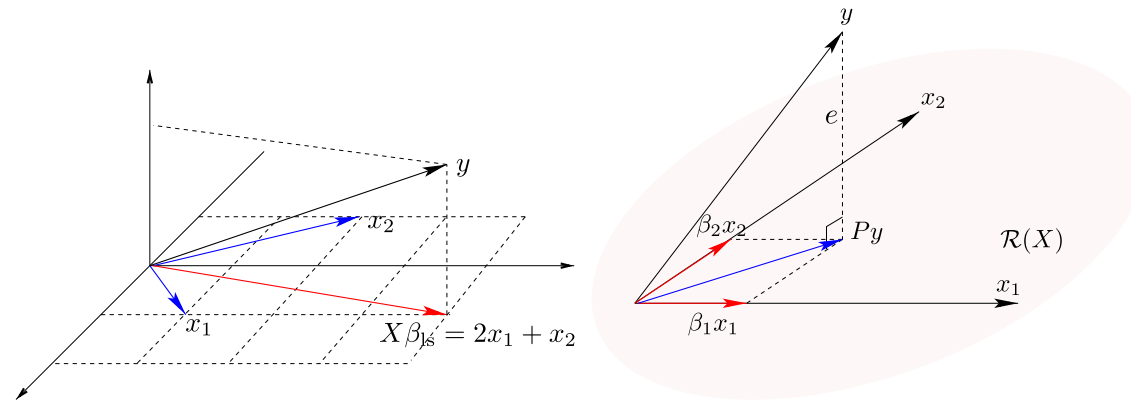
- $\text{rank}(X) = n$  and  $\mathcal{N}(X) = \{0\}$  ( $Xz = 0 \Leftrightarrow z = 0$ )
- $X^T X$  is positive definite: for any  $z \neq 0$  then

$$z^T X^T X z = \|Xz\|^2 > 0$$

similarly, if  $X$  is full rank with  $m \leq n$  (fat matrix)

- $\text{rank}(X) = m$  and  $\mathcal{N}(X^T) = \{0\}$
- $XX^T$  is positive definite

# Geometric interpretation of a LS problem



- $\|y - X\beta\|_2$  is the distance from  $y$  to

$$X\beta = \beta_1x_1 + \beta_2x_2 + \cdots + \beta_nx_n$$

- solution  $\beta_{ls}$  gives the linear combination of the columns of  $X$  closest to  $y$
- $X\beta_{ls}$  is the **orthogonal projection** of  $y$  to the range of  $X$
- $Py$  gives the best approximation; for any  $\hat{y} \in \mathcal{R}(X)$  and  $\hat{y} \neq Py$

$$\|y - Py\| < \|y - \hat{y}\|$$

# Numerical computation

we can solve a least-squares problem via

- Cholesky factorization: factor  $X^T X \succ 0$  into  $LL^T$  where  $L$  is lower triangular
- QR factorization

most programming languages provide built-in commands

returned output	MATLAB	Python
$\hat{\beta}$	<code>X\y</code>	<code>scipy.linalg.lstsq</code>
estimated model	<code>fitlm</code>	<code>sklearn.linear_model.LinearRegression</code>

the closed-form  $\hat{\beta} = (X^T X)^{-1} X^T y$  is for analysis purpose

we do not actually compute  $\hat{\beta}$  from this expression

# Analysis of LS estimate

- linear regression model in estimation
- analysis of LS estimate
  - LS model with deterministic/fixed regressor
  - LS model with stochastic regressor
- identification
- consistency
- asymptotic distribution

# General regression model

the general regression model with additive errors is given by

$$y = \mathbf{E}[y|X] + u$$

- the data are  $(y, X)$  where  $y$  is observation and  $X$  is a matrix of explanatory variables
- $\mathbf{E}[y|X]$  is considered as a conditional function that gives the average value of  $y$  given  $X$
- $u$  is a vector of unknown random errors/noise/disturbances

a linear regression model is obtained when  $\mathbf{E}[y|X]$  is linear in  $X$

# Linear regression model

a linear regression model is

$$y_i = x_i^T \beta + u, \quad i = 1, 2, \dots, N$$

in matrix notation

$$y = X\beta + u$$

- $X \in \mathbf{R}^{N \times n}$  is regression or sensor matrix
- $y \in \mathbf{R}^N$  is the measurement, also called dependent variable or endogenous variable
- $\beta \in \mathbf{R}^n$  is the parameter vector (to be estimated)
- $u \in \mathbf{R}^N$  is the error vector
- each row vector of  $X$ ,  $x_i^T$  is referred to as regressors/predictors or covariates



# Least-squares estimation

from the linear regression model

$$y = X\beta + u$$

the method is to choose an estimate  $\hat{\beta}$  that minimizes

$$\|X\hat{\beta} - y\|$$

*i.e.*, minimize the deviation between what we actually observed ( $y$ ), and what we would observe if  $\beta = \hat{\beta}$ , and there were no noise ( $u = 0$ )

the LS estimate is given by

$$\hat{\beta}_{\text{ls}} = (X^T X)^{-1} X^T y$$

provided that  $X$  is full rank

# Analysis of the LS estimate (static case)

## assumptions:

- $u$  is *white noise* with zero mean and covariance matrix  $\Sigma$
- the least-square estimate is given by

$$\hat{\beta} = \operatorname{argmin} \|X\beta - y\|$$

- the regressor  $X$  is *deterministic*

then the following properties hold:

- $\hat{\beta}$  is an unbiased estimate of  $\beta$  ( $\mathbf{E}\hat{\beta} = \beta$ , or  $\hat{\beta} = \beta$  when  $u = 0$ )
- the covariance matrix of  $\hat{\beta}$  is given by

$$\mathbf{cov}(\hat{\beta}) = (X^T X)^{-1} X^T \Sigma X (X^T X)^{-1}$$

**short proof:** we can write the LS estimate as

$$\hat{\beta} = (X^T X)^{-1} X^T y = (X^T X)^{-1} X^T (X\beta + u) = \beta + (X^T X)^{-1} X^T u$$

- since  $X$  is deterministic and  $u$  is zero mean, we have  $\mathbf{E}\hat{\beta} = \beta$
- the covariance of  $\hat{\beta}$  is derived by

$$\mathbf{cov}(\hat{\beta}) = \mathbf{E}[(\hat{\beta} - \mathbf{E}\hat{\beta})(\hat{\beta} - \mathbf{E}\hat{\beta})^T]$$

but  $\mathbf{E}\hat{\beta} = \beta$  and that  $\hat{\beta} - \mathbf{E}\hat{\beta} = (X^T X)^{-1} X^T u$ , hence,

$$\begin{aligned}\mathbf{cov}(\hat{\beta}) &= \mathbf{cov}[(X^T X)^{-1} X^T u] \\ &= (X^T X)^{-1} X^T \mathbf{cov}(u) X (X^T X)^{-1} \\ &= (X^T X)^{-1} X^T \Sigma X (X^T X)^{-1}\end{aligned}$$

if  $\Sigma = \sigma^2 I$ , then it reduces to  $\mathbf{cov}(\hat{\beta}) = \sigma^2 (X^T X)^{-1}$

## BLUE property

assumptions:  $u$  is white noise with zero mean and **unit** covariance ( $\text{cov}(u) = I$ )

the estimator defined by

$$\hat{\beta}_{\text{ls}} = (X^T X)^{-1} X^T y$$

is the **optimum unbiased linear least-mean-squares** estimator of  $\beta$

assume  $\hat{\beta} = By$  is any other linear estimator of  $\beta$

- require  $BX = I$  in order for  $\hat{\beta}$  to be unbiased
- $\text{cov}(\hat{\beta}) = BB^T$
- $\text{cov}(\hat{\beta}_{\text{ls}}) = BX(X^T X)^{-1} X^T B^T$  (apply  $BX = I$ )

Using  $I - X(X^T X)^{-1} X^T \succeq 0$ , we conclude that

$$\text{cov}(\hat{\beta}) - \text{cov}(\hat{\beta}_{\text{ls}}) = B(I - X(X^T X)^{-1} X^T)B^T \succeq 0$$

- BLUE property is also known as **Gauss-Markov theorem**
- the assumption that  $\text{cov}(u) = I$  (or could be  $\sigma^2 I$ ) is equivalent to
  - $\text{var}(u_i) = \sigma^2$  for all  $i$ , *i.e.*, the error terms have the same variance (**homoskedasticity**)
  - $\text{cov}(u_i, u_j) = 0$  for  $i \neq j$ , *i.e.*, the error terms are uncorrelated
- the proof on the optimality use the fact that  $P = X(X^T X)^{-1} X^T$  is an **orthogonal projection** matrix with
  - $P^T = P$
  - $P^2 = P$
  - $\|Px\| \leq \|x\|$  for all  $x \in \mathbf{R}^n$

these properties imply that  $I - P \succeq 0$

## Properties of estimation errors

under the homoskedastic assumption  $u_i \sim \mathcal{N}(0, \sigma^2)$  and define

$$\hat{u} = y - X\hat{\beta}_{\text{ls}}, \quad \text{RSS} = \sum_{i=1}^N \hat{u}_i^2, \quad s^2 = \text{RSS}/(N - n) = (N - n)^{-1} \sum_{i=1}^N \hat{u}_i^2$$

### Facts:

- $s^2$  is an unbiased estimate for  $\sigma^2$
- $(N - n)s^2/\sigma^2 \sim \chi^2(N - n)$  (require Gaussian assumption of  $u_i$ )

## proof sketch:

- unbiased property of  $s^2$ 
  - $\hat{u} = (I - P)y \triangleq My$  where  $M$  is also an orthogonal projection matrix
  - $\hat{u} = Mu$  from the dgp:  $y = X\beta + u$  and that  $MX = 0$
  - since  $M = I - X(X^T X)^{-1}X^T$  we have and  $\text{tr}(M) = \text{tr}(I_N) - \text{tr}(I_n)$
  - use  $\mathbf{E}\|\hat{u}\|_2^2 = \mathbf{E}[u^T M u] = \mathbf{E}[\text{tr}(u^T M u)]$
- chi-square distribution of  $s^2$ 
  - $(N - n)s^2/\sigma^2 = \hat{u}^T \hat{u}/\sigma^2 = u^T M u/\sigma^2$
  - use that  $u_i/\sigma$  is standard Gaussian and that  $M$  is idempotent

# Analysis of the LS estimate (stochastic case)

$X$  is not a deterministic matrix (e.g. LS estimate of time series model)

we will explore the following properties of LS estimate

- identification
- consistency
- asymptotic distribution



# Identification of LS estimate

the ability of LS estimate to permit identification of  $\mathbf{E}[y|X]$  is follows

for the linear model,  $\beta$  is identified if

1.  $\mathbf{E}[y|X] = X\beta$

2.  $X\alpha = X\beta$  if and only if  $\alpha = \beta$

- 1st assumption: the conditional mean is correctly specified ensures that  $\beta$  is of intrinsic interest
- 2nd assumption: equivalent to  $\mathcal{N}(X) = \{0\}$  or  $X$  is full rank

# Consistency of LS estimate

assumptions:

1. the data generating process (dgp) is actually the linear model on page 6-16
2.  $\mathbf{plim}(N^{-1}X^T X)^{-1}$  converges in probability to a finite nonzero matrix
3.  $\mathbf{plim} N^{-1}X^T u = 0$

the LS estimate can be expressed as

$$\hat{\beta}_{\text{ls}} = \beta + (X^T X)^{-1} X^T u = \beta + (N^{-1} X^T X)^{-1} N^{-1} X^T u$$

apply rules of limit in probability and use the assumptions

$$\mathbf{plim} \hat{\beta}_{\text{ls}} = \beta + \mathbf{plim}(N^{-1}X^T X)^{-1} \cdot \mathbf{plim} N^{-1}X^T u = \beta$$

## Distribution of LS estimator

assumptions:

1. the dgp model is  $y = X\beta + u$  or  $y_i = x_i^T \beta_i + u_i$  for  $i = 1, \dots, N$
2. data are **independent** over  $i$  (but not identically distributed) with

$$\mathbf{E}[u|X] = 0, \quad \mathbf{E}[uu^T|X] = D = \mathbf{diag}(\sigma_i^2)$$

3.  $X$  is full rank
4.  $\Sigma_x = \mathbf{plim} N^{-1} X^T X$  exists and finite nonsingular
5. by CLT,  $\frac{1}{\sqrt{N}} X^T u \xrightarrow{d} \mathcal{N}(0, \Sigma_{ux})$  where  $\Sigma_{ux} = \mathbf{plim} N^{-1} X^T uu^T X$

then the LS estimate  $\hat{\beta}_{\text{ls}}$  is **consistent** for  $\beta$  and

$$\sqrt{N}(\hat{\beta}_{\text{ls}} - \beta) \xrightarrow{d} \mathcal{N}(0, \Sigma_x^{-1} \Sigma_{ux} \Sigma_x^{-1})$$

*Proof.* with rescaling from page 6-26, the LS estimate can be expressed as

$$\sqrt{N}(\hat{\beta}_{\text{ls}} - \beta) = \left( \frac{1}{N} X^T X \right)^{-1} \frac{1}{\sqrt{N}} X^T u$$

- assumption 2:  $x_i u_i$  are independent, so by CLT (on page 5-43) and weak LLN

$$(1/\sqrt{N}) X^T u = (1/\sqrt{N}) \sum_{i=1}^N x_i u_i \xrightarrow{d} \mathcal{N}(0, \Sigma_{ux}), \quad \text{where}$$

$$\Sigma_{ux} = \lim \frac{1}{N} \sum_{i=1}^N \mathbf{E}[x_i x_i^T u_i^2] \quad (\text{note: } \mathbf{E}[u_i x_i] = 0)$$

$$= \lim \frac{1}{N} \sum_i \mathbf{E}[\mathbf{E}[u_i^2 x_i x_i^T | x_i]] = \lim \frac{1}{N} \sum_i \mathbf{E}[\mathbf{E}[u_i^2 | x_i] x_i x_i^T]$$

$$= \lim \frac{1}{N} \sum_i \mathbf{E}[\sigma_i^2 x_i x_i^T] = \lim \frac{1}{N} \mathbf{E}[X^T D X]$$

- assumption 3,4 and by weak LLN (on page 5-12)

$$\frac{1}{N}X^T X = \frac{1}{N} \sum_{i=1}^N x_i x_i^T \xrightarrow{p} \Sigma_x = \lim \frac{1}{N} \sum_{i=1}^N \mathbf{E}[x_i x_i^T]$$

- by continuous mapping theorem and that the inverse operator is continuous on the space of invertible matrices

$$\left( \frac{1}{N}X^T X \right)^{-1} \xrightarrow{p} \Sigma_x^{-1}$$

- by product limit normal rule (on page 5-17), we obtained the desired result where

$$\sqrt{N}(\hat{\beta}_{ls} - \beta) \xrightarrow{d} \mathcal{N}(0, \Sigma_x^{-1} \Sigma_{ux} \Sigma_x^{-1})$$

## Error assumptions

we explore the variance of LS estimate under two conditions on the error,  $u$

- (conditional) homoskedasticity:  $u_i$  has the same variance for all  $i$ ,  $\sigma^2$

$$\mathbf{E}[uu^T|X] = D = \sigma^2 I$$

- (conditional) heteroskedasticity:  $u_i$  may have different variance,  $\sigma_i^2$

$$\mathbf{E}[uu^T|X] = D = \mathbf{diag}(\sigma_i^2)$$

for both cases, it means  $u_i$ 's are uncorrelated, *i.e.*,  $D$  is diagonal

if  $u_i$ 's are correlated, then  $D$  is only symmetric

## Asymptotic Variance Matrix of LS estimate

the asymptotic variance matrix of the distribution and the estimate are

$$P = \Sigma_x^{-1} \Sigma_{ux} \Sigma_x^{-1}, \quad \mathbf{Avar}(\hat{\beta}) = N^{-1} P$$

where

$$\Sigma_{ux} = \lim \frac{1}{N} \mathbf{E}[X^T D X], \quad \Sigma_x = \lim \frac{1}{N} \mathbf{E}[X^T X], \quad D = \mathbf{diag}(\sigma_i^2)$$

define the LS residual

$$\hat{u} = y - X \hat{\beta}$$

the asymptotic covariance matrices can be substituted by their estimates

$$\hat{\Sigma}_{ux} = \frac{1}{N} X^T \hat{D} X, \quad \hat{\Sigma}_x = \frac{1}{N} X^T X, \quad \hat{D} = \mathbf{diag}(\hat{u}^2)$$

**homoskedasticity assumption:** the estimated variance matrix can be simplified

if we assume homoskedasticity,  $\mathbf{E}[u_i^2|x_i]$  is the same across  $i$ , *i.e.*,  $D = \sigma^2 I$

hence,  $\Sigma_{ux} = \sigma^2 \Sigma_x$  and the asymptotic variance matrix reduces to

$$\mathbf{Avar}(\hat{\beta}_{ls}) = N^{-1} P = N^{-1} \sigma^2 \Sigma_x^{-1}$$

its estimate is given by

$$\hat{\sigma}^2 = \|\hat{u}\|_2^2 / (N - n), \quad \widehat{\mathbf{Avar}}(\hat{\beta}_{ls}) = N^{-1} \hat{\sigma}^2 \hat{\Sigma}_x^{-1} = \hat{\sigma}^2 (X^T X)^{-1}$$

- compare with the result on page 6-18
- $\hat{\sigma}^2$  is a consistent estimate of  $\sigma^2$ , regardless of the normalization  $N - n$
- many computer packages use this as the *default* OLS variance estimate



consistency proof of  $\hat{\sigma}^2$

- apply the definition and dgp:  $y = X\beta + u$  where  $u$  is homoskedastic

$$\hat{\sigma}^2 = \frac{1}{N-n} u^T M u = \frac{N}{N-n} \left[ \frac{u^T u}{N} - \left( \frac{u^T X}{N} \right) \left( \frac{X^T X}{N} \right)^{-1} \left( \frac{X^T u}{N} \right) \right]$$

- apply the limit in probability and the product limit rule

- $\lim_{N \rightarrow \infty} N/(N-n) = 1$
- $\text{plim}(1/N)u^T u = \sigma^2$  (weak LLN)
- $\text{plim}(1/N)X^T X = \Sigma_x$  (assume to obtain positive matrix in large samples)
- $\text{plim}(1/N)X^T u = 0$  (assume  $\mathbf{E}[u|X] = 0$ )

$$(1/N)X^T u = (1/N) \sum_{i=1}^N u_i x_i \xrightarrow{p} \mathbf{E}[u_i x_i] = \mathbf{E}_x[\mathbf{E}[u_i x_i | x_i]] = \mathbf{E}_x[x_i \mathbf{E}[u_i | x_i]] = 0$$

- note that the proof follows even when the division is not  $N-n$  (e.g.,  $N$ )

**heteroskedascity assumption:** the asymptotic variance matrix is

$$\mathbf{Avar}(\hat{\beta}_{ls}) = N^{-1} \Sigma_x^{-1} \Sigma_{ux} \Sigma_x^{-1}$$

and its estimate is

$$\widehat{\mathbf{Avar}}(\hat{\beta}_{ls}) = N^{-1} \hat{\Sigma}_x^{-1} \hat{\Sigma}_{ux} \hat{\Sigma}_x^{-1} = (X^T X)^{-1} X^T \hat{D} X (X^T X)^{-1}$$

where  $\hat{D} = \mathbf{diag}(\hat{u}^2)$  and  $\hat{u} = y - X\hat{\beta}$

- $\widehat{\mathbf{Avar}}(\hat{\beta}_{ls})$  is called **heteroskedastic-consistent** estimate of  $\mathbf{Avar}(\hat{\beta}_{ls})$
- many names for the standard errors, the square roots of the diagonals of  $\widehat{\mathbf{Avar}}(\hat{\beta}_{ls})$ 
  - white standard errors
  - heteroskedasticity-robust standard errors
  - huber standard errors

# Weighted least-squares

given  $W$  a positive definite matrix that can be factorized as  $W = L^T L$

a weighted least-squares (WLS) problem is

$$\underset{x}{\text{minimize}} (X\beta - y)^T W (X\beta - y)$$

- equivalent formulation:  $\underset{x}{\text{minimize}} \|L(X\beta - y)\|^2$
- can be solved from the modified normal equation

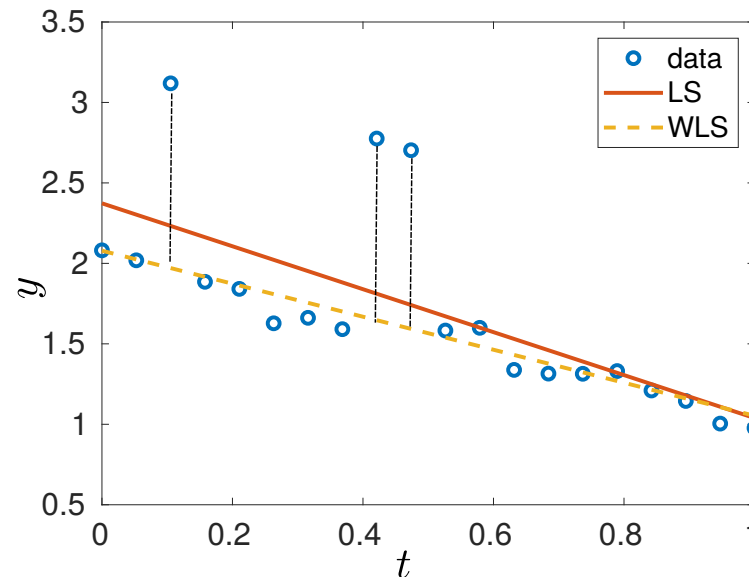
$$X^T W X \beta = X^T W y$$

- the solution is  $\hat{\beta}_{\text{wls}} = (X^T W X)^{-1} X^T W y$  (if  $X$  is full rank)
- $X\hat{\beta}_{\text{wls}}$  is the *orthogonal projection* on  $\mathcal{R}(X)$  w.r.t the new inner product

$$\langle x, y \rangle_W = \langle Wx, y \rangle$$

# Interpretation of WLS

when  $m$ -measurements contain some outliers (samples 3,9,10)



using  $W = \mathbf{diag}(w_1, w_2, \dots, w_m)$  gives WLS objective:  $\sum_{i=1}^m w_i (y_i - x_i^T \beta)^2$

- use relatively **low**  $w_3, w_9, w_{10}$  to penalize **less** on those samples
- the linear model tends not to adapt to outliers – making WLS a more robust method than LS

# Generalized Least-Squares Estimator

revisit BLUE property of LS: suppose  $\text{cov}(u)$  is *not*  $I$ , says  $\mathbf{E}[uu^T] = \Sigma \succ 0$

scale the equation  $y = X\beta + u$  by  $\Sigma^{-1/2}$

$$\Sigma^{-1/2}y = \Sigma^{-1/2}X\beta + \Sigma^{-1/2}u$$

the optimal unbiased linear least-mean-squares estimator of  $\beta$  is

$$\hat{\beta}_{\text{glS}} = (X^T \Sigma^{-1} X)^{-1} X^T \Sigma^{-1} y$$

this is a special case of weighted least-squares solution when  $W = \Sigma^{-1}$

- if  $\Sigma$  is known the weighted LS estimate is BLUE if  $W = \Sigma^{-1}$
- large  $\Sigma_{ii}$  means  $u_i$  is more uncertain, so we should put less penalty on this residual
- this solution is known as **generalized least-squares estimator**

# Feasible Generalized Least-Squares Estimator

the GLS estimator cannot be implemented because  $\text{cov}(u) = \Sigma$  is not known

if we replace  $\Sigma$  by a  $\hat{\Sigma}$  in GLS estimator then it yields

$$\hat{\beta}_{\text{fgls}} = (X^T \hat{\Sigma}^{-1} X)^{-1} X^T \hat{\Sigma}^{-1} y$$

known as the **feasible generalized least-squares (FGLS) estimator**

let us specify that  $\Sigma = \Sigma(\gamma)$  where  $\gamma$  is a parameter vector

$$\sqrt{N}(\hat{\beta}_{\text{fgls}} - \beta) \xrightarrow{d} \mathcal{N} \left[ 0, (\text{plim } N^{-1} X^T \Sigma^{-1} X)^{-1} \right]$$

if we use  $\hat{\Sigma} = \Sigma(\hat{\gamma})$  and  $\hat{\gamma}$  is consistent for  $\gamma$

conclusion: FGLS estimator is a special case of weighted LS estimator

# Analysis of the WLS estimate (static case)

## assumptions:

- the dgp is  $y = X\beta + u$
- $u$  is *white noise* with zero mean and covariance matrix  $\Sigma$
- the weighted least-square estimate is given by  $\hat{\beta} = (X^T W X)^{-1} X^T W y$
- the regressor  $X$  is *deterministic*

then the following properties hold:

- $\hat{\beta}$  is an unbiased estimate of  $\beta$  ( $\mathbf{E}\hat{\beta} = \beta$ , or  $\hat{\beta} = \beta$  when  $u = 0$ )
- the covariance matrix of  $\hat{\beta}$  is given by

$$\text{cov}(\hat{\beta}) = (X^T W X)^{-1} X^T W \Sigma W X (X^T W X)^{-1}$$

# Asymptotic asymptotic covariance matrix of WLS

assumptions: (dynamic case)

- the dgp is  $y = X\beta + u$
- $u$  is *white noise* with zero mean and covariance matrix  $\Sigma$
- the weighted least-square estimate is given by  $\hat{\beta} = (X^T W X)^{-1} X^T W y$
- the regressor  $X$  is *stochastic*

then the **estimated asymptotic covariance matrix** of WLS estimator is

$$\widehat{\mathbf{Avar}}(\hat{\beta}_{\text{wls}}) = (X^T W X)^{-1} X^T W \hat{\Sigma} W X (X^T W X)^{-1}$$

where  $\hat{\Sigma}$  (estimated covariance matrix of error) is such that

$$\mathbf{plim} N^{-1} X^T W \hat{\Sigma} W X = \mathbf{plim} N^{-1} X^T W \Sigma W X$$

conclusion:  $W$  must be chosen to be a good estimate of  $\Sigma^{-1}$



# MATLAB functions

- `fitlm` fits a linear regression
- `glmfit` fit a generalized linear model (linear regression is a special case and the default option)
- `fgls` solve feasible generalized least squares
- `robustfit` fit robust regressions

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