Basics of Linear Models

Motivation for models of the mean function

Previously we assumed that rvs Y_1, Y_2, \ldots, Y_n are iid. $\Rightarrow E(Y_i) = E(Y_j)$ for every i, j. A more interesting model is

$$E(Y_i) = f_i(\underbrace{\text{observed variables}}_{\text{covariates, predictors, explanatory variables}})$$

E.g. Y_i : score of *i*-th student on the final exam. f_i : function of study time, difficulty of exam, past performance on quizzes, etc.

The mean function f_i relates the expectation of Y_i —response variable—to the corresponding explanatory variables. Mathematically,

$$E(Y_i) = f_i(\underbrace{x_{i1}, x_{i2}, \dots, x_{im}}_{\boldsymbol{x}_i^T}, \boldsymbol{\beta}) \Rightarrow \begin{cases} Y_i = \underbrace{Y_i - E(Y_i)}_{\text{error}_i} + E(Y_i) \\ = E(Y_i) + \text{error}_i \\ = f_i(\boldsymbol{x}_i^T, \boldsymbol{\beta}) + \text{error}_i \end{cases}$$

Most generally, this is a nonlinear model, i.e., $f_i(\boldsymbol{x}_i^T, \boldsymbol{\beta})$ is a nonlinear function of the coefficients $\boldsymbol{\beta}$.

Linear Models

If $f_i(\boldsymbol{x}_i^T, \boldsymbol{\beta}) = \boldsymbol{x}_i^T \boldsymbol{\beta} = \sum_{j=1}^m x_{ij} \beta_j$ where \boldsymbol{x}_i^T is a vector of explanatory variables and $\boldsymbol{\beta}$ is the vector of coefficients. Then we have a <u>statistical linear model (LM)</u>, meaning that the mean function is <u>linear in the coefficients</u> β_j ; the mean function need not be linear in covariates. Examples:

- $\mathrm{E}(Y_i) = \beta_0$
- $\bullet \ \mathrm{E}(Y_i) = \beta_0 + \beta_1 x_{i1}$
- $E(Y_i) = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i1}^2$
- \rightarrow these are LMs since expectation is linear in β_i 's.
 - $E(Y_i) = \exp(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2})$
- \rightarrow not an LM.

Our focus: statistical linear models; hence, no more f_i 's to denote the mean functions.

The (linear) least squares problem: given a vector of observations Y and a matrix of covariates X, find a vector of model coefficients b that minimizes

$$\sum_{i=1}^{n} (Y_i - \boldsymbol{x}_i^T \boldsymbol{b})^2 = (\boldsymbol{Y} - \boldsymbol{X} \boldsymbol{b})^T (\boldsymbol{Y} - \boldsymbol{X} \boldsymbol{b}) = \text{SSE}(\boldsymbol{b}), \text{ the sum of squared errors.}$$

 $Y_i = \boldsymbol{x}_i^T \boldsymbol{\beta} + \operatorname{error}_i \Rightarrow \operatorname{estimate} \boldsymbol{\beta} \text{ as the value of } \boldsymbol{b} \text{ that minimizes SSE}(\boldsymbol{b}).$

Example: Let $Y_i = \beta_0 + \beta_1 x_i + \text{error}_i$.

 \Rightarrow we find a line $\widehat{\beta}_0 + \widehat{\beta}_1 x$ that minimizes SSE (\boldsymbol{b}) , the sum of squared vertical distances to the points (x_i, y_i) from line $\widehat{\beta}_0 + \widehat{\beta}_1 x$. In matrix form

$$Y_{i} = \begin{bmatrix} 1 & x_{i}^{T} \end{bmatrix} \cdot \begin{bmatrix} \beta_{0} \\ \beta_{1} \end{bmatrix} + \text{error}_{i}$$

$$Y = \begin{bmatrix} 1 & x_{1}^{T} \\ 1 & x_{2}^{T} \\ \vdots & \vdots \\ 1 & x_{n}^{T} \end{bmatrix} \cdot \begin{bmatrix} \beta_{0} \\ \beta_{1} \end{bmatrix} + \text{error}_{i},$$

In statistics, if x_i is a scalar, this is known as simple linear regression. If x_i^T is a vector, we have multiple linear regression.

Aside: β_0 is known as an "intercept", estimated by $\widehat{\beta}_0$. In the model, the column of ones can be absorbed into the x_i^T 's.

How to solve the least squares problem? \Rightarrow find $\frac{\partial \text{SSE}(b)}{\partial b}$, set to 0, solve, get $\hat{\beta} = (X^T X)^{-1} X^T Y$, assuming X is of full rank $(X \text{ is } n \times m, n > m)$.

How to solve the least squares problem "statistically"? Assume:

$$Y_i = \underbrace{\boldsymbol{x}_i^T \boldsymbol{\beta}}_{\sum_{j=1}^m x_{ij}\beta_j} + \varepsilon_i$$

where ε_i 's are iid Normal $(0, \sigma^2)$. In vector-matrix form,

$$oldsymbol{Y}_{n imes 1} = oldsymbol{X} oldsymbol{eta}^{m imes 1} + oldsymbol{arepsilon}_{n imes 1} + oldsymbol{arepsilon}_{n imes 1}$$

 $Y_i \sim \text{Normal}(\boldsymbol{x}_i^T \boldsymbol{\beta}, \sigma^2)$, the Y_i 's are independent but not identically distributed. Since we know the joint pdf of the Y_i 's let's use ML estimation to estimate $\boldsymbol{\beta}$ and σ^2 . • Step 1: write down the likelihood; here, $f_i(\cdot|\boldsymbol{\beta}, \sigma^2)$ is the pdf of Y_i :

 $\ell\left(\boldsymbol{\beta},\sigma^2\right) = \ln\left(\mathrm{L}\left(y_1,\ldots,y_n\mid\boldsymbol{\beta},\sigma^2\right)\right)$

$$L(y_1, \dots, y_n \mid \boldsymbol{\beta}, \sigma^2) = \prod_{i=1}^n f_i(y_i \mid \boldsymbol{\beta}, \sigma^2) = \prod_{i=1}^n (2\pi\sigma^2)^{-1/2} \exp\left(-\frac{(y_i - \boldsymbol{x}_i^T \boldsymbol{\beta})^2}{2\sigma^2}\right)$$
$$= (2\pi\sigma^2)^{-n/2} \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \boldsymbol{x}_i^T \boldsymbol{\beta})^2\right)$$

 $(u-X\beta)^T(u-X\beta)$

• Step 2: log-likelihood:

$$=-rac{n}{2}\ln(2\pi)-rac{n}{2}\ln(\sigma^2)-rac{1}{2\sigma^2}(oldsymbol{y}-oldsymbol{X}oldsymbol{eta})^T(oldsymbol{y}-oldsymbol{X}oldsymbol{eta}).$$

 $\frac{\partial \ell(\boldsymbol{\beta}, \sigma^2)}{\partial \boldsymbol{\beta}} = -\frac{1}{2\sigma^2} 2\boldsymbol{X}^T (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})$

• Step 3. Find the gradient of $\ell(\boldsymbol{\beta}, \sigma^2)$ with respect to $\boldsymbol{\beta}$ and σ^2 , set the gradient to 0, solve for $\boldsymbol{\beta}$ and σ^2 .

$$\frac{\partial \ell\left(\boldsymbol{\beta}, \sigma^{2}\right)}{\partial \sigma^{2}} = -\frac{n}{2} \frac{1}{\sigma^{2}} - \frac{1}{2} \frac{(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})^{T}(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})}{(\sigma^{2})^{2}}$$

$$\Rightarrow \text{ solve, get } \widehat{\boldsymbol{\beta}} = \left(\boldsymbol{X}^{T}\boldsymbol{X}\right)^{-1} \boldsymbol{X}^{T}\boldsymbol{y} \text{ and } \widehat{\sigma}^{2} = \frac{1}{n}(\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{\beta}})^{T}(\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{\beta}}).$$

- Step 4. Make sure we found the maximizers of L (β, σ^2) by showing that all eigenvalues of the matrix of second derivatives of L (β, σ^2) —known as the Hessian—are negative. (Equivalently, (-1) · Hessian is positive definite.)
- Some jargon: estimating $\boldsymbol{\beta}$ and $\sigma^2 \equiv$ "fitting the model"
- $\widehat{\boldsymbol{\beta}} \equiv \mathrm{ML}$ and LS estimator of $\boldsymbol{\beta}$.
 - $\hat{Y} = X\hat{\beta}$ is the vector of fitted values (it estimates $X\beta$).
 - $m{arepsilon} = m{Y} m{X}m{eta} \; : \; ext{vector of true errors.} \ \widehat{m{arepsilon}} = m{Y} m{X}\widehat{m{eta}} \; : \; ext{vector of residuals.}$ (do not confuse residuals with true errors)
 - $ullet \ \widehat{oldsymbol{Y}} = oldsymbol{X} \widehat{oldsymbol{eta}} = oldsymbol{X} \left(oldsymbol{X}^T oldsymbol{X}
 ight)^{-1} oldsymbol{X}^T oldsymbol{Y} = oldsymbol{H} oldsymbol{Y}$

Let P be a matrix such that

$$oldsymbol{P} = egin{bmatrix} oldsymbol{P}_1 & oldsymbol{P}_2 \ n imes m & n imes(n-m) \end{bmatrix}$$

1. Columns of P form an orthonormal basis for \mathbb{R}^N , (columns are "perpendicular" and have length 1), i.e., $P^TP = I$.

- 2. Columns of P_1 form an orthonormal basis for the column space of X. Column space of $X: \{z \in \mathbb{R}^n : z = Xd, d \in \mathbb{R}^M\}$
- 3. Columns of P_2 form a basis for the orthogonal complement of column space for X (null space of X^T : $\{z \in \mathbb{R}^n : X^T z = 0\}$.

Observation: one can write

$$\bullet \ \boldsymbol{H} = \boldsymbol{X} \left(\boldsymbol{X}^T \boldsymbol{X} \right)^{-1} \boldsymbol{X}^T = \boldsymbol{P}_1 \boldsymbol{P}_1^T$$

- $\bullet \ (\boldsymbol{I} \boldsymbol{H}) = \boldsymbol{P}_{2} \boldsymbol{P}_{2}^{T}.$
- $\bullet \ \ \boldsymbol{X}\widehat{\boldsymbol{\beta}} = \boldsymbol{H}\boldsymbol{Y} = \boldsymbol{H}\boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{H}\boldsymbol{\varepsilon} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{P}_{1}\boldsymbol{P}_{1}^{T}\boldsymbol{\varepsilon}$
- $\bullet \ \ \widehat{\boldsymbol{\varepsilon}} = (\boldsymbol{I} \boldsymbol{H})(\boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}) = (\boldsymbol{X} \boldsymbol{X}\underbrace{\left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{X}}_{\boldsymbol{I}})\boldsymbol{\beta} + \boldsymbol{P}_2\boldsymbol{P}_2^t\boldsymbol{\varepsilon} = \boldsymbol{P}_2\boldsymbol{P}_2^T\boldsymbol{\varepsilon}$

Let
$$U = P_1^T \varepsilon$$
, $W = P_2^T \varepsilon$, $V = P^T \varepsilon$ so that $V = \begin{bmatrix} P_1^T \\ P_2^T \end{bmatrix} \varepsilon = \begin{bmatrix} U \\ W \end{bmatrix}$
Program: show that U and W are independent. Hence $h(V)$ and $g(W)$ are independent for any choice of h and g .

Goal: find the distribution of $V = h(\varepsilon) = P^T \varepsilon$. Recall: in one dimension, if Z = h(T) then

$$\underbrace{f_Z(z)}_{\text{pdf of }Z} = \underbrace{f_T\left(h^{-1}(z)\right)}_{\text{pdf of }T} \cdot \underbrace{\left|\frac{\partial h^{-1}(z)}{\partial z}\right|}_{\substack{\text{Jacobian of the inverse transformation}}$$

$$V = P^T \varepsilon \Rightarrow \varepsilon = h^{-1}(V) = (P^T)^{-1} V$$
. Since $P^T P = I \Rightarrow P = (P^T)^{-1}$

$$f_{oldsymbol{V}}(oldsymbol{v}) = f_{oldsymbol{arepsilon}}ig(h^{-1}(oldsymbol{v})ig) \cdot |\mathrm{det}(oldsymbol{P})|$$

$$f_{m{arepsilon}}(m{arepsilon}) = \prod_{i=1}^{n} (2\pi\sigma^2)^{-1/2} \exp\left(-rac{arepsilon_i^2}{2\sigma^2}
ight) = (2\pi\sigma^2)^{-n/2} \cdot \exp\left(-rac{m{arepsilon}^T m{arepsilon}}{2\sigma^2}
ight)$$
 $f_{m{V}}(m{v}) = (2\pi\sigma^2)^{-n/2} \cdot \exp\left(-rac{m{v}^T m{P}^T m{P} m{v}}{2\sigma^2}
ight) \cdot |\det(m{P})|$

$$= (2\pi\sigma^2)^{-n/2} \cdot \exp\left(-\frac{\boldsymbol{v}^T\boldsymbol{v}}{2\sigma^2}\right) \cdot |\det(\boldsymbol{P})|$$

$$=(2\pi\sigma^2)^{-n/2}\cdot\exp\left(-rac{oldsymbol{u}^Toldsymbol{u}+oldsymbol{w}^Toldsymbol{w}}{2\sigma^2}
ight)\cdot|\det(oldsymbol{P})|$$

since $\boldsymbol{v} = \begin{pmatrix} \boldsymbol{u} \\ \boldsymbol{w} \end{pmatrix}, \boldsymbol{v}^T \boldsymbol{v} = \boldsymbol{u}^T \boldsymbol{u} + \boldsymbol{w}^T \boldsymbol{w} = \sum_{i=1}^m u_i^2 + \sum_{j=1}^{m-n} w_j^2$

$$= (2\pi\sigma^2)^{-m/2} \exp\left(-\frac{\boldsymbol{u}^T \boldsymbol{u}}{2\sigma^2}\right) \cdot \underbrace{|\det(\boldsymbol{P})|}_{=1} \cdot (2\pi\sigma^2)^{-(n-m)/2} \cdot \exp\left(-\frac{\boldsymbol{w}^T \boldsymbol{w}}{2\sigma^2}\right)$$

 \Rightarrow using factorization criterion, \boldsymbol{U} and \boldsymbol{W} are independent, actually, U_i 's and W_j 's are iid Normal $(0, \sigma^2)$.

Implications:

$$\widehat{\boldsymbol{\varepsilon}}^T \widehat{\boldsymbol{\varepsilon}} = \boldsymbol{\varepsilon}^T \underbrace{(\boldsymbol{I} - \boldsymbol{H})^T (\boldsymbol{I} - \boldsymbol{H})}_{(\boldsymbol{I} - \boldsymbol{H}) = \boldsymbol{P}_2 \boldsymbol{P}_2^T} \boldsymbol{\varepsilon} = \boldsymbol{W}^T \boldsymbol{W}$$

$$W_i \overset{\text{iid}}{\sim} \text{Normal}(0, \sigma^2), \quad \boldsymbol{W}^T \boldsymbol{W} = \sum_{i=1}^{n-m} W_i^2 = \sigma^2 \sum_{i=1}^{n-m} \left(\frac{W_i}{\sigma}\right)^2 \sim \chi_{n-m}^2$$

$$\Rightarrow \widetilde{\sigma}^2 = \frac{\widehat{\boldsymbol{\varepsilon}}^T \widehat{\boldsymbol{\varepsilon}}}{n-m} : \text{ unbiased estimator of } \sigma^2$$

Shortcut notation: let \bot denote "independence", i.e. $U \bot W$ if U is independent of W. Recall:

$$oldsymbol{U} = oldsymbol{P}_1^T oldsymbol{arepsilon}, \quad oldsymbol{X} \widehat{oldsymbol{eta}} = oldsymbol{X} oldsymbol{eta} + oldsymbol{P}_1 \cdot oldsymbol{\underline{P}}_1^T oldsymbol{arepsilon}, \quad \widetilde{\sigma}^2 = rac{oldsymbol{W}^T oldsymbol{W}}{n-m} = rac{\sum_{j=1}^n \widehat{arepsilon}_j^2}{n-m}$$

Hence $X\widehat{\beta} \perp \widetilde{\sigma}^2$ since these are made from disjoint subsets of independent random variables (the $V_i's$).

$$\widehat{\boldsymbol{\beta}} = \left(\boldsymbol{X}^T \boldsymbol{X}\right)^{-1} \boldsymbol{X}^T \cdot \boldsymbol{X} \widehat{\boldsymbol{\beta}} \perp \widetilde{\sigma}^2$$

$$\boldsymbol{a}^T \widehat{\boldsymbol{\beta}} = \sum_{i=1}^m a_i \widehat{\beta}_i \perp \widetilde{\sigma}^2 \quad \boldsymbol{a} \colon m \times 1 \text{ constant vector}$$

Goal: find the distribution of $a^T \hat{\beta}$.

$$oldsymbol{a}^T \widehat{eta} = oldsymbol{a}^T \left(oldsymbol{X}^T oldsymbol{X}
ight)^{-1} oldsymbol{X}^T oldsymbol{Y} = oldsymbol{a}^T \left(oldsymbol{X}^T oldsymbol{X}
ight)^{-1} oldsymbol{X}^T oldsymbol{X} eta + oldsymbol{a}^T \left(oldsymbol{X}^T oldsymbol{X}
ight)^{-1} oldsymbol{X}^T oldsymbol{\varepsilon} = oldsymbol{a}^T oldsymbol{eta} + oldsymbol{c}^T oldsymbol{arepsilon} oldsymbol{v} \cdot oldsymbol{v$$

Recall: $\varepsilon_i \stackrel{\text{iid}}{\sim} \text{Normal}(0, \sigma^2)$. Mgf of ε_i is $m(t) = \exp(t^2 \sigma^2/2)$. What is the distribution of $Z = \sum_{i=1}^n c_i \varepsilon_i$? Mgf of Z is

$$M_Z(t) = \operatorname{E}\left(e^{tZ}\right) = \operatorname{E}\left(\exp\left(t \cdot \sum_{i=1}^n c_i \varepsilon_i\right)\right) = \prod_{i=1}^n \operatorname{E}\left(\exp\left(t c_i \varepsilon_i\right)\right) \text{ by independence of } \varepsilon_i\text{'s}$$

$$= \prod_{i=1}^n \exp\left(\frac{t^2 c_i^2 \sigma^2}{2}\right) = \exp\left(\frac{t^2}{2} \cdot \sum_{i=1}^n c_i^2 \cdot \sigma^2\right)$$

which is the mgf of Normal $(0, \sigma^2 \sum_{i=1}^n c_i^2)$.

$$\sum_{i=1}^{n} c_i^2 = \boldsymbol{c}^T \boldsymbol{c} = \boldsymbol{a}^T \left(\boldsymbol{X}^T \boldsymbol{X} \right)^{-1} \underbrace{\boldsymbol{X}^T \boldsymbol{X} \left(\boldsymbol{X}^T \boldsymbol{X} \right)^{-1}}_{\boldsymbol{I}} \boldsymbol{a} = \boldsymbol{a}^T \left(\boldsymbol{X}^T \boldsymbol{X} \right)^{-1} \boldsymbol{a}.$$

$$\Rightarrow \boldsymbol{a}^T \widehat{\boldsymbol{\beta}} \sim \operatorname{Normal} \left(\boldsymbol{a}^T \boldsymbol{\beta}, \sigma^2 \boldsymbol{a}^T \left(\boldsymbol{X}^T \boldsymbol{X} \right)^{-1} \boldsymbol{a} \right)$$

Special Cases

• Let I be an $m \times n$ identity matrix. Let $I_{i\bullet}$ be the i-th row of I and $I_{\bullet j}$ be the j-th column of I. $\Rightarrow I_{\bullet i} = (I_{i\bullet})^T \Rightarrow \widehat{\beta}_i = I_{i\bullet}\widehat{\beta}$

$$\Rightarrow \widehat{\beta}_i \sim \operatorname{Normal}(\beta_i, \sigma^2 \underbrace{I_{i\bullet} (X^T X)^{-1} I_{\bullet i}}_{\text{the } i\text{-th entry on main diagonal}}).$$

• let $\boldsymbol{a}^T = \boldsymbol{x}_{\text{New}}^T$ be a vector of covariates for a new random variable $\boldsymbol{Y}_{\text{New}}$. $\boldsymbol{Y}_{\text{New}} \sim \text{Normal}(\boldsymbol{x}_{\text{New}}^T \boldsymbol{\beta}, \sigma^2)$. An estimator of $\boldsymbol{x}_{\text{New}}^T \boldsymbol{\beta}$ is $\boldsymbol{x}_{\text{New}}^T \widehat{\boldsymbol{\beta}}$.

$$oldsymbol{x}_{ ext{New}}^T \widehat{oldsymbol{eta}} \sim ext{Normal} ig(oldsymbol{x}_{ ext{New}}^T oldsymbol{eta}, \sigma^2 oldsymbol{x}_{ ext{New}}^T ig(oldsymbol{X}^T oldsymbol{X} ig)^{-1} oldsymbol{x}_{ ext{New}} ig).$$

$\underline{ ext{CIs}}$ and tests for $oldsymbol{a}^Toldsymbol{eta}$

Let $\theta = \boldsymbol{a}^T \boldsymbol{\beta}$.

$$P(\theta) = \frac{\boldsymbol{a}^{T} \widehat{\boldsymbol{\beta}} - \theta}{\sqrt{\sigma^{2}} \sqrt{\boldsymbol{a}^{T} \left(\boldsymbol{X}^{T} \boldsymbol{X}\right)^{-1} \boldsymbol{a}}} \sim \text{Normal}(0, 1)$$

If σ^2 were known, can use as a pivot for θ . If σ^2 is unknown: replace σ^2 by $\tilde{\sigma}^2$.

$$P(\theta) = \frac{\boldsymbol{a}^T \widehat{\boldsymbol{\beta}} - \theta}{\sqrt{\widehat{\sigma}^2} \sqrt{\boldsymbol{a}^T (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{a}}} \cdot \frac{\sqrt{\sigma^2}}{\sqrt{\sigma^2}} = \frac{N(0, 1)}{\sqrt{\frac{\chi_{n-m}^2}{n-m}}} \quad \text{and numerator } \perp \text{ denominator.}$$
$$\Rightarrow P(\theta) \sim t(\text{df} = n - m).$$

E.g., if H_0 : $\theta = \theta_0$, then $P(\theta_0) \sim t(df = n - m)$ under H_0 when σ^2 is unknown and is estimated by $\tilde{\sigma}^2$. \Rightarrow Can do tests and CIs about θ as before.