

- Names for  $\{f_j(x_i)\}$ : ( $j$ -th) **feature, predictor, covariate, independent variable**
- Names for  $\{y_i\}$ : **response, response variable, dependent variable, target, label**

- Def. Observed response variables:**  $y_1, y_2, \dots, y_n$
- Def. Features:**  $z_{ij}$  for  $i = 1, \dots, n$  and  $j = 1, \dots, p$
- Def. Regression coefficients:**  $\beta := (\beta_1, \dots, \beta_p)$
- Def. Squared error:**

$$S(\beta) := \sum_{i=1}^n (y_i - \beta^\top z_i)^2$$

- Def. Least squares estimate:**

$$\hat{S} := \min_{\beta \in \mathbb{R}^p} S(\beta)$$

- Def. Least squares regression coefficients:**

$$\hat{\beta} := (\hat{\beta}_1, \dots, \hat{\beta}_p) := \arg \min_{\beta \in \mathbb{R}^p} S(\beta)$$

- Def. These  $p$  equations are known as the Normal Equation** (bc. normal is a synonym to perpendicular)
- We have

$$(\hat{\epsilon}_1, \dots, \hat{\epsilon}_n)^\top (z_{1j}, \dots, z_{nj}) = 0, \quad j = 1, \dots, p$$

where

$$\hat{\epsilon}_i := y_i - \hat{\beta}^\top z_i, \quad i = 1, \dots, n$$

are the **residuals**

Suppose  $Y \sim \mathcal{N}(\mu, \Sigma)$  and that  $\Sigma^{-1} \in \mathbb{R}^{n \times n}$  exists. Then

$$(Y - \mu)^\top \Sigma^{-1} (Y - \mu) \sim \chi_n^2$$

$$\frac{\partial S}{\partial \beta_j} = 0 \Rightarrow 2 \sum_{i=1}^n (y_i - \beta^\top z_i) (-z_{ij}) = 0, \quad j = 1, \dots, p$$

$$\hat{y} = Hy, \quad H := Z(Z^\top Z)^{-1} Z^\top$$

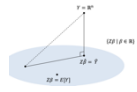
(Tukey called  $H$  the "hat" matrix)

- Properties of  $H$ :

- Symmetric:  $H = H^\top$
- Idempotent:  $H^2 = H$  (a symmetric idempotent matrix such as  $H$  is called a perpendicular projection matrix (PPM))
- The eigenvalues of a real PPM are all either 0 or 1
- If  $Z$  is invertible,  $H$  has  $p$  non-zero eigenvalues
- $I - H$  is PPM

- Def. Coefficient of determination:**

$$R^2 := \frac{SS_{Fit}}{SS_{Tot}} = 1 - \frac{SS_{Res}}{SS_{Tot}}$$



- Proportion of variation accounted for by all variables compared to the sum of squares error under the model  $y_i = \beta_0 + \epsilon_i$
- Measures how well  $Y$  is predicted or determined by  $Z\hat{\beta}$ :
- $R := \sqrt{R^2}$  is called the **coefficient of multiple correlation** - it measures how well the response  $y$  correlates with the  $p$  predictors in  $Z$  taken collectively
- When  $z_i = (1, x_i) \in \mathbb{R}^2$ ,  $R$  is the Pearson correlation of  $\{x_i\}$  and  $\{y_i\}$

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

- $SS_{Tot} := \sum_{i=1}^n (y_i - \bar{y})^2$  is the **Total (or centered) sum of square**
- $SS_{Fit} := \sum_{i=1}^n (\hat{y}_i - \bar{y})^2$  is the **Centered sum of squares of fitted values**
- $SS_{Res} := \sum_{i=1}^n (y_i - \hat{y}_i)^2$  is the **Residual sum of squares**

$$E[Y|X=x] = \beta_0 + \beta_1 x + \beta_2 [x-x]_+ + \dots$$

$z_+ := \max\{0, z\} = z \cdot \mathbb{1}_{z>0}$

$$E[Y|X=x] = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_{n-1} x_{n-1}$$

(group 0 has mean  $\beta_0$ , mean of group  $j>0$  is  $\beta_0 + \beta_j$ )

- $\hat{y}_i = H_i y$  ( $H_i$  is the  $i$ -th row of  $H$ )
- $H_{ij} = z_i^\top (Z^\top Z)^{-1} z_j = H_{ji}$  (the contribution of  $y_j$  to  $\hat{y}_i$  equals that of  $y_j$  to  $\hat{y}_i$ )
- $H_{ii} = z_i^\top (Z^\top Z)^{-1} z_i \geq 0$  (Exc.)
- $H$  projects vectors onto the **columns space** of  $Z$   
 $\text{Col}(Z) := \mathcal{M} = \{Z\beta \mid \beta \in \mathbb{R}^p\}$
- $I - H$  projects vectors onto the **null space** of  $Z$   
 $\text{Null}(Z) := \mathcal{M}^\perp := \{v \in \mathbb{R}^n \mid Zv = 0\}$  (the set of vectors orthogonal to vectors in  $\mathcal{M}$ )

$$SS_{Tot} = SS_{Fit} + SS_{Res}$$

## Chi-squared distribution $\chi^2$

- Let  $Z_1, \dots, Z_k \stackrel{iid}{\sim} \mathcal{N}(0, 1)$ . The distribution  $\chi_k^2$  is defined as

$$\sum_{i=1}^k Z_i^2 \sim \chi_k^2$$

- PDF:

$$f(x; k) = \frac{x^{\frac{k}{2}-1} e^{-\frac{x}{2}}}{2^{\frac{k}{2}} \Gamma(\frac{k}{2})} \mathbf{1}_{x \geq 0}$$

- If  $X \sim \chi_k^2$ , then

$$\mathbb{E}[X] = k, \quad \text{Var}[X] = 2k$$

- For non-random matrices  $A \in \mathbb{R}^{n \times p}$  and  $B \in \mathbb{R}^{m \times m}$   
 $\text{Cov}(AX, BY) = A \text{Cov}(X, Y) B^\top$
- For a constant vector  $b$ ,  
 $\text{Var}[AX + b] = A \text{Var}[X] A^\top$

$$\sqrt{n}(\bar{X}_n - \mu) \xrightarrow{D} \mathcal{N}(0, \sigma^2).$$

- $\mu(\bar{X}) = \mu$
- $\sigma^2(\bar{X}) = \sigma^2/n$
- $\gamma(\bar{X}) = \gamma/\sqrt{n}$
- $\kappa(\bar{X}) = \kappa/n$

- Taking  $h(x) = x^k$  gives the  $k$ -th moment of  $X$
- Some special moments of interest have given names:

- The **mean**  $\mu = \mathbb{E}[X]$  corresponds to  $h(x) = x$
- The **variance** of  $X$  is  $\sigma^2 := \mathbb{E}[(X - \mu)^2]$
- The **skewness** of  $X$  is  $\gamma := \mathbb{E}[(X - \mu)^3] / \sigma^3$
- The (excess) **kurtosis** of  $X$  is  $\kappa := \mathbb{E}[(X - \mu)^4] / \sigma^4 - 3$

- $\gamma$  is useful as a measure of symmetry; it is zero for symmetric distributions
- $\kappa = 0$  when  $X \sim \mathcal{N}(0, 1)$ .  $\kappa$  is useful in measuring whether the tails of the distribution are heavier ( $\kappa > 0$ ) or lighter ( $\kappa < 0$ ) than the tails of the normal distribution

## F-distribution

$$F = \frac{\frac{1}{p-q} (SS_{Total} - SS_{Full})}{\frac{1}{n-p} SS_{Full}} \sim F_{p-q, n-p}$$

- The normalized ratio of two Chisquared distribution:

$$F_{d_1, d_2} := \frac{\frac{1}{d_1} \chi_{d_1}^2}{\frac{1}{d_2} \chi_{d_2}^2}$$

- PDF:

$$f(x; d_1, d_2) = \frac{1}{B(\frac{d_1}{2}, \frac{d_2}{2})} \left(\frac{d_1}{d_2}\right)^{d_1/2} x^{d_1/2-1} \left(1 + \frac{d_1}{d_2} x\right)^{-(d_1+d_2)/2}$$

- If  $X \sim F_{n_1, n_2}$ , then

$$\mathbb{E}[X] = \frac{d_2}{d_2 - 2}, \quad d_2 > 2$$

- In particular, if

$$\begin{bmatrix} X \\ Y \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mu_x \\ \mu_y \end{bmatrix}, \begin{bmatrix} \sigma_x^2 & \rho \sigma_x \sigma_y \\ \rho \sigma_x \sigma_y & \sigma_y^2 \end{bmatrix}\right)$$

then the conditional distribution of  $Y$  given  $X$  is

$$\mathcal{L}(Y|X) = \mathcal{N}\left(\mu_y + \rho \sigma_y \frac{X - \mu_x}{\sigma_x}, \sigma_y^2 (1 - \rho^2)\right)$$

- If  $\Sigma$  is invertible, then the density of  $Y$  is

$$f_Y(y) = \frac{1}{(2\pi)^{m/2} \sqrt{|\Sigma|}} \exp\left(-\frac{1}{2} (y - \mu)^\top \Sigma^{-1} (y - \mu)\right)$$

(here  $y = (y_1, \dots, y_m)$ )

variance

- we can test  $H_0$  using the extra SS principle:

$$F = \frac{\frac{1}{k-1} (SS_{Tot} - SS_{within})}{\frac{1}{n-k} SS_{within}}$$

reject  $H_0$  at level  $\alpha$  if

$$F > F_{k-1, n-k}^{1-\alpha}$$

$$\mathbb{E}[Y_2|Y_1] = \mu_2 + \Sigma_{21} \Sigma_{11}^{-1} (Y_1 - \mu_1)$$

$$\text{Var}[Y_2|Y_1] = \Sigma_{22} - \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12}$$

## t-distribution

- Suppose that  $Z \sim \mathcal{N}(0, 1)$  and  $X \sim \chi_k^2$ ,  $X$  and  $Z$  independent. Then

$$\frac{Z}{\sqrt{\frac{X}{k}}} \sim t_k$$

- PDF:

$$f(t) = \frac{\Gamma(\frac{\nu+1}{2})}{\sqrt{\nu\pi} \Gamma(\frac{\nu}{2})} \left(1 + \frac{t^2}{\nu}\right)^{-\frac{\nu+1}{2}}$$

- If  $Y \sim t_k$ , then

$$\mathbb{E}[Y] = 0, \quad \text{Var}[Y] = \frac{k}{k-2}, \quad k \geq 3$$

- The  $t$ -distribution converges to the normal distribution as  $k \rightarrow \infty$ . It has heavier tails than that of the normal distribution

$$\begin{aligned} &= P\left(-\frac{t_{n-1}^{1-\alpha/2}}{\sqrt{n}} < T < \frac{t_{n-1}^{1-\alpha/2}}{\sqrt{n}}\right) \\ &= P\left(-\frac{t_{n-1}^{1-\alpha/2}}{\sqrt{n}} < \frac{\bar{Y} - \mu}{\frac{s}{\sqrt{n}}} < \frac{t_{n-1}^{1-\alpha/2}}{\sqrt{n}}\right) \\ &= P\left(\bar{Y} - \frac{s}{\sqrt{n}} t_{n-1}^{1-\alpha/2} < \bar{Y} < \bar{Y} + \frac{s}{\sqrt{n}} t_{n-1}^{1-\alpha/2}\right) \end{aligned}$$

Thm.

$$\frac{1}{\sigma^2} \sum_{i=1}^n \hat{\epsilon}_i^2 = \frac{\|\hat{\epsilon}\|^2}{\sigma^2} \sim \chi_{n-p}^2$$

One Sample t-test

Data:  $y_1, y_2, \dots, y_n$

$$t = \frac{\bar{y} - \mu_0}{s/\sqrt{n}} \quad s^2 = \frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2$$

Two-Sample t-test:

$$t = \frac{\bar{y}_1 - \bar{y}_2}{s \sqrt{1/n_1 + 1/n_2}} = \frac{\bar{y}_1 - \bar{y}_2}{s \sqrt{\frac{1}{n_1} + \frac{1}{n_2}}}$$

(the unbiased estimator of  $\sigma^2$ )

$$s^2 = \frac{1}{n-2} \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2$$
$$= \frac{\sum_{i=1}^{n_0} (y_{0i} - \bar{y}_0)^2 + \sum_{i=1}^{n_1} (y_{1i} - \bar{y}_1)^2}{n_0 + n_1 - 2}$$

$$t = \frac{\bar{y}_A - \frac{2}{3}\bar{y}_B - \frac{1}{3}\bar{y}_C}{s \sqrt{\frac{1}{n_A} + \frac{4}{9n_B} + \frac{1}{9n_C}}}$$

$$s^2 = \frac{1}{n-3} \sum_{c \in \{A, B, C\}} \sum_{j=1}^{n_c} (y_{c,j} - \bar{y}_c)^2$$

Statistical power:

$$s^2 = \frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2 \sim \frac{\sigma^2}{s^2/\sigma^2} \sim F_{1, n-1}$$
$$= P_r \left( \frac{(Z + \sqrt{n}(\frac{\mu_0 - \mu}{\sigma}))^2}{V/(n-1)} > F_{1, n-1}^{1-\alpha} \right)$$

Where  $Z \sim N(0,1)$   $Z = \frac{\sqrt{n}(\bar{y} - \mu)}{\sigma}$   
 $V \sim \chi^2_{n-1}$   $V = \frac{s^2}{\sigma^2} (n-1)$   
 $\lambda = n(\frac{\mu_0 - \mu}{\sigma})^2$

$\frac{N^2(\bar{y}, 1)}{\frac{1}{k} \chi^2_k}$  is known as the non-central F dist.  
with 1 DoF over k DoF  
(denoted  $F_{1,k}(\lambda)$ )  $\chi^2 = \left( \sqrt{n}(\frac{\mu_0 - \mu}{\sigma}) \right)^2$

The SVD

$$Z \in \mathbb{R}^{n \times p}$$
$$Z = U \Sigma V^T$$

where  $U \in \mathbb{R}^{n \times n}$   $\Sigma \in \mathbb{R}^{n \times p}$   $V \in \mathbb{R}^{p \times p}$

$$U^T U = U U^T = I_n \quad V^T V = V V^T = I_p$$
$$\Sigma = \text{diag}(\sigma_1, \dots, \sigma_r) \quad \sigma_i \geq 0 \quad k = \min\{n, p\}$$

overall:

(I)  $Z = U \Sigma V^T$

(II)  $y^* = \sigma^2 y$

(III)  $\hat{\beta}_j^* = \begin{cases} y_j^* / \sigma_j & \sigma_j \neq 0 \\ 0 & \sigma_j = 0 \end{cases}$

(IV)  $\hat{\beta} = V \hat{\beta}^*$

Computing SVD is done in  $\mathcal{O}(np^2)$

Theorem (BH '95)

If all p-values are independent, then  $FDR \leq \frac{m_0}{m} \alpha \leq \alpha$

K-Groups (ANOVA):

Cell mean model:

$$Y_{ij} = \mu_i + \epsilon_{ij} \quad \epsilon_{ij} \stackrel{iid}{\sim} N(0, \sigma^2)$$

Effect means model

$$Y_{ij} = \mu + \alpha_i + \epsilon_{ij} \quad \epsilon_{ij} \stackrel{iid}{\sim} N(0, \sigma^2)$$

The SS for the cell means:

$$SS_{within} := SS_{res} = \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_{i.})^2$$

The total SS:

$$SS_{tot} = \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_{..})^2$$

We can test  $H_0$  using the extra SS principle:

$$F = \frac{\frac{1}{k-1} (SS_{tot} - SS_{within})}{\frac{1}{n-k} SS_{within}}$$

reject  $H_0$  at level  $\alpha$  if  $F > F_{k-1, n-k}^{1-\alpha}$

$\sigma^2 = \frac{SS_{within}}{n-k}$   
 $Var(\hat{\beta}_1) = \frac{\sigma^2}{S_{xx}}$

We also define

$$SS_{between} := SS_{fit} = SS_{tot} - SS_{within}$$
$$= \sum_{i=1}^k n_i (\bar{y}_{i.} - \bar{y}_{..})^2$$

Source	DoF	SS	MS
Groups	k-1	SS <sub>between</sub>	SS <sub>between</sub> / (k-1)
Error	n-k	SS <sub>within</sub>	SS <sub>within</sub> / (n-k)
Total	n-1	SS <sub>tot</sub>	

$MS_{within} = s^2$

In general:

$$\sum_{i=1}^k \lambda_i = 0 \quad \sum_{i=1}^k \lambda_i^2 > 0 \quad t = \frac{\sum_{i=1}^k \lambda_i \bar{y}_{i.}}{s \sqrt{\sum_{i=1}^k \frac{\lambda_i^2}{n_i}}} \sim t_{n-k}$$

Contrasts:

$$t = \frac{\bar{y}_1 + \bar{y}_2 + \bar{y}_3}{3} - \frac{\bar{y}_4 + \bar{y}_5 + \bar{y}_6}{3}$$
$$s^2 = MSE_{within} = \frac{1}{9} \left( \frac{1}{n_1} + \frac{1}{n_2} + \frac{1}{n_3} \right) + \frac{1}{16} \left( \frac{1}{n_4} + \dots + \frac{1}{n_7} \right)$$
$$t \sim t_{n-7}$$

Bonferroni's Union Bound

- we have m tests (e.g.  $m = \binom{k}{2}$ )
- we conduct each test at level  $\alpha/m$  (e.g. for z-tests, we reject based on  $z_{1-\alpha/(2m)}^2$ )

(BH)

FDR controlling using Benjamini & Hochberg

- Perform each test; sort the p-values from lowest to highest  $p_{(1)} \leq p_{(2)} \leq \dots \leq p_{(m)}$
- Define  $\ell_i = \alpha \cdot \frac{i}{m}$  (line with slope  $\frac{\alpha}{m}$ )
- Define  $i^* = \max \{i: p_{(i)} \leq \ell_i\}$
- Reject all  $H_{0,i} \quad p_{(i)} \leq p_{(i^*)}$

If the tests are independent

Suppose that  $y \sim N(Z\beta, \sigma^2 I)$  and that  $(Z^T Z)^{-1}$  is invertible.

- $\hat{\beta} \sim N(\beta, \sigma^2 (Z^T Z)^{-1})$
- $\hat{y} = Z \hat{\beta} \sim N(Z\beta, H \sigma^2)$
- $\hat{\epsilon} = y - \hat{y} \sim N(0, (I-H) \sigma^2)$

Regression line:  $E(y | x) = \mu_y + \rho \frac{\sigma_y}{\sigma_x} (x - \mu_x)$

The linear model:

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$
$$Z = \begin{pmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix} \quad p = \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} \quad \hat{\beta} = (Z^T Z)^{-1} Z^T y$$

We have:

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (x_i - \bar{x}) y_i}{\sum_{i=1}^n (x_i - \bar{x})^2} = \frac{\frac{1}{n} \sum_{i=1}^n (x_i - \bar{x}) y_i}{\frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2}$$

and  $\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$

$$Var(\hat{\beta}_0) = \dots = \frac{\sigma^2}{n} \frac{1}{S_{xx}}$$

$$Var(\hat{\beta}_0 + \hat{\beta}_1 x) = \dots = \frac{\sigma^2}{n} \left( 1 + \left[ \frac{x - \bar{x}}{S_{xx}} \right]^2 \right)$$

$$\hat{\beta}_0 + \hat{\beta}_1 x \in \left( \hat{\beta}_0 + \hat{\beta}_1 x \pm t_{n-2}^{1-\alpha/2} s \sqrt{\frac{1}{n} + \frac{(x - \bar{x})^2}{S_{xx}}} \right)$$

w.p. 1- $\alpha$

$$y_{n+1} \in \left( \hat{\beta}_0 + \hat{\beta}_1 x_{n+1} \pm t_{n-2}^{1-\alpha/2} s \sqrt{1 + \frac{1}{n} + \frac{(x_{n+1} - \bar{x})^2}{S_{xx}}} \right)$$

w.p. 1- $\alpha$

we set a bound if we evaluate this for every  $x_{n+1} \in \mathbb{R}$

In general:

$$Z_0^T \hat{\beta} \in \left( Z_0^T \hat{\beta} \pm t_{n-p}^{1-\alpha/2} s \sqrt{Z_0^T (Z^T Z)^{-1} Z_0} \right)$$

w.p. 1- $\alpha$   $Z_0 \in \mathbb{R}^p$

False-Discovery Rate (FDR)

Suppose we make m hypotheses tests  $\{H_{0,i}\}_{i=1}^m$ . Each has either rejected or not.

We summarize the situation in a table:

	# not rej.	# rej.	Total
$H_{0,i}$ true	U	V	$m_0$
$H_{0,i}$ false	T	S	$m_1$
Total	$m-R$	R	m

Def. false discovery proportion is  $FDP = \frac{SV}{R}$   $R > 0$   
 $\begin{cases} 0 & R = 0 \end{cases}$

Def. false discovery rate is  $E[FDP]$

Under general dependency structure:

- we should be more conservative
- we use  $\ell_i = \alpha \cdot \frac{i}{m} \cdot \frac{1}{c_m}$

$$c_m = \sum_{i=1}^m \frac{1}{b_i} \approx \ln(m) + \gamma - \frac{1}{2m} \approx \ln(m)$$

Euler's constant

can false disc. of m measurements in this case:

$$y_{n+1} \in \left( \hat{\beta}_0 + \hat{\beta}_1 x_{n+1} \pm t_{n-2}^{1-\alpha/2} s \sqrt{1 + \frac{1}{n} + \frac{(x_{n+1} - \bar{x})^2}{S_{xx}}} \right)$$

w.p. 1- $\alpha$

## Simultaneous Bands

- Contain  $(\beta + \beta_1 \cdot x)_{x \in R}$  with prob.  $1 - \alpha$
- In  $p$  dim. contain  $(z^T \beta)_{z \in R^p}$
- From the distribution of  $\hat{\beta}$ :  

$$Pr((\hat{\beta} - \beta)^T (Z^T Z)^{-1} (\hat{\beta} - \beta) \leq s^2 p \cdot F_{p, n-p}^{-1}) = 1 - \alpha$$
 This define an ellipsoid in  $R^p$

## Working Hotelling Bands:

- Confidence:  $\hat{\beta} \pm \sqrt{2 F_{2, n-2}^{-1-\alpha}} \cdot s \sqrt{\frac{1}{n} + \frac{(x - \bar{x})^2}{S_{xx}}}$
- Prediction:  $\hat{\beta} \pm \sqrt{2 F_{2, n-2}^{-1-\alpha}} \cdot s \sqrt{1 + \frac{1}{n} + \frac{(x - \bar{x})^2}{S_{xx}}}$
- Avg. of  $m$  predictions:  $\hat{\beta} \pm \sqrt{2 F_{2, n-2}^{-1-\alpha}} \cdot s \sqrt{\frac{1}{m} + \frac{1}{n} + \frac{(x - \bar{x})^2}{S_{xx}}}$
- (these are wider than earlier-mentioned bands)

## Competing Variables:

- $\hat{\beta}_1$  is significant if  $x_2$  is not in the model
- $\hat{\beta}_2$  is significant if  $x_1$  is not in the model.

## collaborating Variables:

- $\hat{\beta}_1$  is sig. if  $x_2$  is in the model
- $\hat{\beta}_2$  is sig. if  $x_1$  is in the model

## Def. Partial Correlation $P_{ijk}$

Partial correlation of  $x_i, x_j$ , adjusting for  $x_k$  is the correlation of resid. for  $x_i$  on  $x_k$  and resid. for  $x_j$  on  $x_k$

For Gaussian data:

$$P_{ijk} = \frac{P_{ij} - P_{ik}P_{jk}}{\sqrt{(1 - P_{ik}^2)(1 - P_{jk}^2)}}$$

(with or without hats)

$$\hat{P}_{ij} = \frac{x_i^T x_j}{\|x_i\| \|x_j\|} \quad P_{ij} = \frac{\text{Cov}(x_i, x_j)}{\sqrt{\text{Var}(x_i) \text{Var}(x_j)}}$$

**Forward approach:** we start at  $\emptyset$  and add the best predictor if the new model is statistically significant; we stop otherwise (using F-test for extra sum of squares)

**Backward approach:** we start with all predictors, and drop the least significant / the one that leaves you with maximal SSres if the old model is not statistically significant better than the new one; otherwise, stop

## Cross Validation in linear models

- The residuals:

$$\frac{y_i - \hat{y}_i^{(i)}}{1 - H_{ii}} = \frac{\hat{\epsilon}_i}{1 - H_{ii}}$$

- Overall:

$$CV = \sum_i^n (y_i - \hat{y}_i^{(i)})^2 = \sum_{i=1}^n \frac{\hat{\epsilon}_i^2}{(1 - H_{ii})^2}$$

$$\hat{y}_i^{(i)} = \frac{\hat{y}_i - H_{ii} y_i}{1 - H_{ii}}$$

Least trimmed regression (80% smallest residuals example):

$$\hat{\beta} = \arg \min_{\beta} \sum_{i=1}^{\lfloor 0.8n \rfloor} |\hat{\epsilon}_{(i)}(\beta)|^2$$

bias: the prediction error resulting from miss-specifying the model  
 Variance: the prediction error resulting from variations in the data used for fitting

## Penalty on number of variables:

$$AIC := n \cdot \log\left(\frac{SS_{res}}{n}\right) + 2p$$

$$BIC = n \log \frac{SS_{res}}{n} + p \log n$$

Regularization: Ridge regression (L2) was created originally to handle the case when  $Z^T Z$  is (nearly)

$$\tilde{\beta}_\lambda = (Z^T Z + \lambda I)^{-1} Z^T y \quad \lambda > 0$$

Variation: if we don't want to shrink the intercept:

$$\tilde{\beta}_\lambda = \left( Z^T Z + \lambda \begin{pmatrix} 0 & \\ & I_{p-1} \end{pmatrix} \right)^{-1} Z^T y, \quad \lambda > 0$$

$$\ell(\beta; y, Z, \lambda) = \|y - Z\beta\|^2 + \lambda \|\beta\|^2$$

## Advantages:

- More accurate with predictions
- More stable when predictors are correlated

Disadvantages: gives non zero values to all predictors

## L1 Lasso:

$$\ell(\beta; y, Z, \lambda) = \|y - Z\beta\|^2 + \lambda \|\beta\|_1$$

$$\|\beta\|_1 = \sum_{j=1}^p |\beta_j|$$

- If we regress  $y$  on  $Z$

$$\beta_{OLS} = (Z^T Z)^{-1} Z^T (Z\beta + \tilde{\epsilon} \cdot \tilde{\beta})$$

$$= \hat{\beta} + (Z^T Z)^{-1} Z^T \tilde{\epsilon} \cdot \tilde{\beta}$$

- Suppose  $E[y] = Z\beta + \tilde{\epsilon} \cdot \tilde{\beta}$   
 $\tilde{\epsilon} \in R^n, \tilde{\beta} \in R$

- Conditions for CLT:
- 1)  $\lambda_{\min}(Z^T Z) \rightarrow \infty$   
 $Z^T Z$  is a matrix version of  $n$
  - 2) No  $Z_{ij}$  is "too large"
  - 3)  $\epsilon_i$  is not heavy tailed

## Detection QQ plot:

- 1) Sort  $\hat{\epsilon}_i$  so that  $\hat{\epsilon}_{(1)} \leq \hat{\epsilon}_{(2)} \leq \dots \leq \hat{\epsilon}_{(n)}$
- 2) Plot  $\hat{\epsilon}_{(i)}$  vs.  $\Phi\left(\frac{i - \frac{n+1}{2}}{n}\right)$

The model is robust if less than 20% are outliers

## Detecting Heteroscedasticity:

- If we know  $V$ , we can use generalized LS:

$$V = P^T \Delta P \quad P^T P = P P^T = I$$

$$\Delta = \text{diag}(\lambda_1, \dots, \lambda_n)$$

$$\text{let: } D := \Delta^{-\frac{1}{2}} P$$

- we have:  $\tilde{D}y = D(Z\beta + \epsilon) = \tilde{D}Z\beta + \tilde{D}\epsilon$

$$\tilde{y} = \tilde{Z}\beta + \tilde{\epsilon}$$

$$\text{Where: } \text{Var}(\tilde{\epsilon}) = D \text{Var}(\epsilon) D^T$$

$$= D P^T \Delta P D^T$$

$$= \Delta^{-\frac{1}{2}} P P^T \Delta P P^T \Delta^{-\frac{1}{2}} = I$$

- he took:

$$\hat{\beta}_{GLS} = (\tilde{Z}^T \tilde{Z})^{-1} \tilde{Z}^T \tilde{y}$$

so that  $\hat{\beta}_{GLS}$  minimizes  $\|Dy - DZ\beta\|^2$

- If  $V = \text{diag}(\sigma_1^2, \dots, \sigma_n^2)$

then we can use

$$\tilde{\sigma}_i^2 = \tilde{u}_i^T, \quad \tilde{u}_i = y_i - z_i^T \hat{\beta}_{OLS}$$

we can also compute the correlation between the residuals:

$$\hat{\rho}_{ik} = \frac{\frac{1}{n} \sum_{i=1}^n \tilde{\epsilon}_i \tilde{\epsilon}_{i-k}}{\sqrt{\frac{1}{n} \sum_{i=1}^n \tilde{\epsilon}_i^2} \sqrt{\frac{1}{n} \sum_{i=1}^n \tilde{\epsilon}_{i-k}^2}}$$

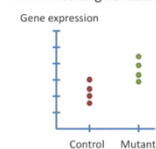
- The p-value:

$$p = \frac{\# \text{ of permutations with } \bar{y}_i - \bar{y}_0 \geq \bar{y}_i - \bar{y}_0}{\binom{n_0 + n_1}{n_0}}$$

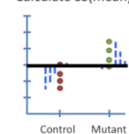
- if the number of permutations is too large, consider a random sample of  $N$  permutations.

$$p = \frac{1 + (\# \text{ of sampled perm with } \bar{y}_i - \bar{y}_0 \geq \text{observed } |\bar{y}_i - \bar{y}_0|)}{N + 1}$$

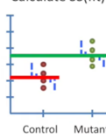
The original data.



Calculate SS(mean)



Calculate SS(fit)



$$F = \frac{SS(\text{mean}) - SS(\text{fit}) / (p_{fit} - p_{mean})}{SS(\text{fit}) / (n - p_{fit})}$$

$y = \text{overall mean}$   
 $y = \text{mean}_{\text{control}} + \text{mean}_{\text{mutant}}$

$p_{\text{mean}} = 1$   
 $p_{\text{fit}} = 2$

	F	MS between	MS within
MS		$\frac{SS \text{ between}}{R - 1}$	$\frac{SS \text{ within}}{n - R}$
SS		$\sum_{i=1}^R n_i (\bar{y}_i - \bar{y})^2$	$\sum_{i=1}^R \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2$
DoF		$R - 1 = 1$	$n - R = n_0 + n_1 - 2$
Source	Group	Error	Total

2. ANOVA table for  $k=2$ :



Increasing the number of measurements improves the accuracy in estimating the LS coefficients  $\beta_j$  using  $\hat{\beta}_j$  in the sense that the confidence interval for  $\beta_j$  (centered at  $\hat{\beta}_j$ ) gets smaller with  $n$  (this is the formal way of saying that the accuracy is increased). Connecting this back to test of significance against  $\beta_j = 0$ : if 0 is not in the  $1 - \alpha$  confidence interval of  $\beta_j$ , then the t-test P-value must be smaller than  $\alpha$ . The ability to handle singular design matrices is one of the motivations of using ridge regression. We assume that the variations of all samples around their group mean are normally distributed, independent, and of equal variance. Under the null distribution  $H_0$  we have  $t \sim t_{n-3}$ . We reject  $H_0$  at significance level  $\alpha = 0.05$  if  $|t|$  exceeds  $t_{0.975, n-3}$ .

**Answer: (i):** We set  $H_0$  as the hypothesis that  $y_{new} \sim \mathcal{N}(\mu, \sigma^2)$ . Under  $H_0$ ,

$$y_{new} - \bar{y} \sim \mathcal{N}(0, \sigma^2(1 + 1/n)),$$

so

$$t = \frac{y_{new} - \bar{y}}{s\sqrt{1 + 1/n}} \sim t_{n-1}, \quad s^2 = \frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2.$$

Our test rejects  $H_0$  at significance level  $\alpha = 0.05$  if  $|t| > t_{n-1}^{0.975}$  (another acceptable answer is to incorporate  $y_{new}$  into  $s^2$ . However, this may inflate  $s^2$  under the alternative hence result in a test of lesser power)

(ii)  $y_{new} \in \bar{y} \pm s\sqrt{1 + 1/n} \cdot t_{n-1}^{0.975}$

(iii) The best option is to use the two-sample t-test with  $n_1 = n$  and  $n_2 = 2$ . In this case,

$$t = \frac{\bar{y}_{new} - \bar{y}}{s\sqrt{\frac{1}{2} + \frac{1}{n}}}, \quad s^2 = \frac{1}{n+2-2} \left( \sum_{i=1}^n (y_i - \bar{y})^2 + (y_{new1} - \bar{y}_{new})^2 + (y_{new2} - \bar{y}_{new})^2 \right)$$

We reject the null if  $|t|$  exceeds  $t_n^{0.975}$ .

Another option is to use  $\bar{y}_{new} = (y_{new1} + y_{new2})/2$  in a procedure similar to (i). With this option, under the null we have

$$\bar{y}_{new} - \bar{y} \sim \mathcal{N}\left(0, \sigma^2\left(\frac{1}{2} + \frac{1}{n}\right)\right),$$

so

$$t = \frac{\bar{y}_{new} - \bar{y}}{s\sqrt{\frac{1}{2} + \frac{1}{n}}}, \quad s^2 = \frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2.$$

We reject the null if  $|t|$  exceeds  $t_{n-1}^{0.975}$ .

A type I error (false-positive) occurs if an investigator rejects a null hypothesis that is actually true in the population; a type II error (false-negative) occurs if the investigator fails to reject a null hypothesis that is actually false in the population. Although type I and type II errors can never be avoided entirely, the investigator can reduce their likelihood by increasing the sample size  
If R2 is closed to 1, the predictor explains the response well. Increasing the number of predictors never decreases R2.

```
n = len(y_t)
p = 3
q = 1
SSful = np.sum(np.square(y_t - np.dot(beta_hat1, Z1.T)))
SSsub = np.sum(np.square(y_t - np.dot(beta_hat2, Z2.T)))
F = (1/(p-q) * (SSsub - SSful))/(1/(n-p) * SSful)

pvalue = stats.f.sf(F, 2, n-p)
print(pvalue)

9.631240818725029e-11
```

Since the pvalue is really small, we can say that we reject the null hypothesis that says that the two models are similar. Therefore, we conclude that the fitted model significantly improves the trivial model.

The two sample t test quantifies the difference between the arithmetic means of the two months over the years. The p-value quantifies the probability of observing as or more extreme values assuming that the rainfall doesn't change over the years. The paired t test measures whether the average score differs significantly across samples (years). If we observe a large p-value then we cannot reject the null hypothesis of identical average scores. If the p-value is smaller than the threshold, then we reject the null hypothesis of equal averages. Therefore, from previous questions, the two sample ttest would be better since we don't want to generalize that if we reject the null hypothesis for one year, then the rainfall do change over the years.

In this example we want to ask whether the number of fireplaces affects positively on the price of a house, so that we know to build some in order to increase the value of ours. However, what if the number of fireplaces is merely a function of the number of rooms which responsible to the increase. In this case, adding additional fireplaces would not affect the price (because we did not changed the number of rooms). To account for the effect of fireplaces, we can adjust for the number of rooms.

```
import statsmodels.api as sm

varX = 'Fireplaces'
varY = 'SalePrice'
varZ = 'TotRmsAbvGrd' # total rooms above ground level

model_LotFrontageYearBuilt = smf.ols(formula=f"{varX} ~ {varZ}", data=data2).fit()
model_SalePriceYearBuilt = smf.ols(formula=f"{varY} ~ {varZ}", data=data2).fit()

X = sm.add_constant(model_LotFrontageYearBuilt.resid)
y = model_SalePriceYearBuilt.resid
model_res = sm.OLS(y, X).fit()
plt.scatter(model_LotFrontageYearBuilt.resid, model_SalePriceYearBuilt.resid)
plt.title(f"Regressing residuls. Partial Correlation ({varX},{varY}), adjusting for {varZ} is $R^2 = {m
```

$$\begin{aligned} n &= n_o + n_i \\ SS_{between} &= \sum_{i=1}^k n_i (\bar{y}_{i\cdot} - \bar{y}_{\cdot\cdot})^2 \\ &= n_o (\bar{y}_{o\cdot} - \bar{y}_{\cdot\cdot})^2 + n_i (\bar{y}_{i\cdot} - \bar{y}_{\cdot\cdot})^2 \\ SS_{within} &= \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_{i\cdot})^2 \\ &= \sum_{j=1}^{n_o} (y_{oj} - \bar{y}_{o\cdot})^2 + \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_{i\cdot})^2 \\ SS_{tot} &= \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_{\cdot\cdot})^2 \\ &= \sum_{j=1}^{n_o} (y_{oj} - \bar{y}_{\cdot\cdot})^2 + \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_{\cdot\cdot})^2 \end{aligned}$$

$$\begin{aligned} SS_{tot} &= \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_{\cdot\cdot})^2 \\ &= \sum_{i=1}^k \sum_{j=1}^{n_i} ((y_{ij} - \bar{y}_{i\cdot}) + (\bar{y}_{i\cdot} - \bar{y}_{\cdot\cdot}))^2 \\ &= \sum_{i=1}^k \sum_{j=1}^{n_i} ((y_{ij} - \bar{y}_{i\cdot})^2 + 2(y_{ij} - \bar{y}_{i\cdot})(\bar{y}_{i\cdot} - \bar{y}_{\cdot\cdot}) + (\bar{y}_{i\cdot} - \bar{y}_{\cdot\cdot})^2) \\ &= \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_{i\cdot})^2 + 2 \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_{i\cdot})(\bar{y}_{i\cdot} - \bar{y}_{\cdot\cdot}) + \sum_{i=1}^k \sum_{j=1}^{n_i} (\bar{y}_{i\cdot} - \bar{y}_{\cdot\cdot})^2 \\ &= 2 \cdot \sum_{i=1}^k (\bar{y}_{i\cdot} - \bar{y}_{\cdot\cdot}) \left( \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_{i\cdot}) \right) \\ &= 2 \cdot \sum_{i=1}^k (\bar{y}_{i\cdot} - \bar{y}_{\cdot\cdot}) \left( \sum_{j=1}^{n_i} y_{ij} - \sum_{j=1}^{n_i} \bar{y}_{i\cdot} \right) \\ &= 2 \sum_{i=1}^k (\bar{y}_{i\cdot} - \bar{y}_{\cdot\cdot}) \left( \sum_{j=1}^{n_i} y_{ij} - \sum_{j=1}^{n_i} \frac{1}{n_i} \sum_{j=1}^{n_i} y_{ij} \right) \\ &= 2 \sum_{i=1}^k (\bar{y}_{i\cdot} - \bar{y}_{\cdot\cdot}) \left( \sum_{j=1}^{n_i} y_{ij} - \frac{n_i}{n_i} \sum_{j=1}^{n_i} y_{ij} \right) \\ &= 2 \sum_{i=1}^k (\bar{y}_{i\cdot} - \bar{y}_{\cdot\cdot}) (0) \end{aligned}$$
$$\begin{aligned} p_r(\min p_i \leq \alpha/n \mid H_0 = \text{true}) &= 1 - p_r(\min p_i > \frac{\alpha}{n} \mid H_0 = \text{true}) \\ &= 1 - p_r(p_1 > \frac{\alpha}{n}, p_2 > \frac{\alpha}{n}, \dots, p_n > \frac{\alpha}{n} \mid H_0 = \text{true}) \\ &= 1 - \prod_{i=1}^n p_r(p_i > \frac{\alpha}{n} \mid H_0 = \text{true}) \\ &= 1 - (1 - \frac{\alpha}{n})^n \end{aligned}$$

