Topic VII:
Regression Models

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Introduction

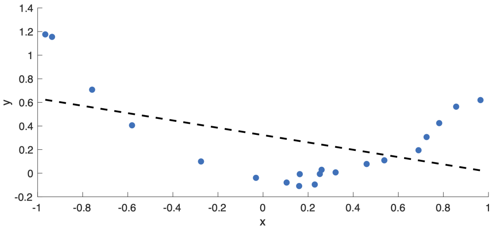
In simple linear regression, we analyze the linear relationship between the response Y and an predictor x.

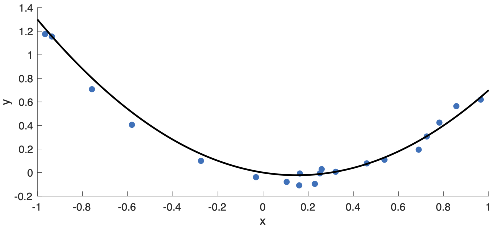
$$Y = \alpha + \beta x + \varepsilon.$$

- Estimation
- Inference

What if the relationship is not linear?

- $Y = \alpha + \beta x + \varepsilon$? No!
- $Y = \beta_0 + \beta_1 x + \beta_2 x^2 + \varepsilon$.
- Conventional explanation: Fit a parabola to data.





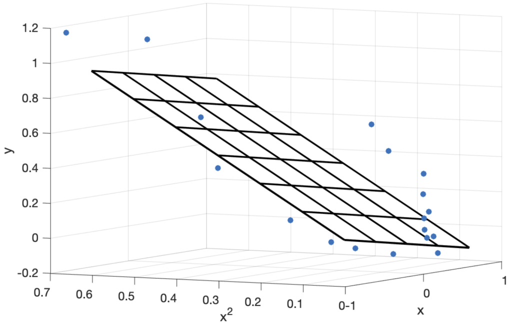
Enlarge the Feature Space

- Alternatively: Let

$$x_1 = x, \quad x_2 = x^2$$

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \varepsilon.$$

- Bottomline: Although Y is quadratic in x, it is linear in the unknown parameters.



More generally, we use non-linear function of the inputs $\boldsymbol{\phi}(\boldsymbol{x})$ and assume

$$Y = \boldsymbol{\beta}^\top \boldsymbol{\phi}(\boldsymbol{x}) + \varepsilon.$$

If $\boldsymbol{\phi}(\boldsymbol{x}) = (1, x, x^2, x^3, \ldots, x^d)$ is the vector of polynomial basis functions, it is called a **polynomial regression**.

Multiple Regression

Multiple linear regression model

For $i = 1, \ldots, n$

$$Y_i = \beta_1 x_{i1} + \cdots + \beta_p x_{ip} + \varepsilon_i.$$

Or in vector form

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon},$$

where $\boldsymbol{Y} \in \mathbb{R}^{n \times 1}$, $\boldsymbol{X} \in \mathbb{R}^{n \times p}$, $\boldsymbol{\beta} \in \mathbb{R}^{p \times 1}$.

- $\boldsymbol{X}$ is called the design matrix, $\boldsymbol{Y}$ is the response;
- the j-th column of $\boldsymbol{X}$, $\mathrm{x}_j = x_{\cdot j} \in \mathbb{R}^n$ is the vector of the j-th predictor;
- $\boldsymbol{\beta}$ is the unknown parameter; ε_i is the error of observation i.
- We usually set $x_{i1} = 1$ to have a non-zero intercept.

Goal: find the parameter values that fits the data the best.

Examples

$\boldsymbol{X}$ is usually called the design matrix.

$$\mathcal{N}(\mu_1,\sigma^2)\begin{cases} Y_1 \\ \vdots \\ Y_n \end{cases} \qquad \mathcal{N}(\mu_2,\sigma^2)\begin{cases} Y_{n+1} \\ \vdots \\ Y_{n+m} \end{cases} \qquad X = \begin{pmatrix} 1 & 0 \\ \vdots & \vdots \\ 1 & 0 \\ 0 & 1 \\ \vdots & \vdots \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}$$

- The location model: $p = 1$, $\boldsymbol{X} = (1, \cdots, 1)^\top$, $\beta_1 = \mu$.

$$Y = \mu + \varepsilon.$$

- The 2-sample model: $p = 2$, $\boldsymbol{X} = \begin{pmatrix} 1 & \cdots & 1 & 0 & \dots & 0 \\ 0 & \cdots & 0 & 1 & \dots & 1 \end{pmatrix}^\top$, $\beta = (\mu_1, \mu_2)^\top$.
- One-way (simple) analysis of variance (ANOVA), compare the mean of k groups: $p = k$, $\boldsymbol{X} =?$
- Simple linear regression: $Y = \alpha + \beta x + \varepsilon$.

$$\boldsymbol{X} = \begin{pmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix}, \quad \beta = (\alpha, \beta)^\top.$$

Examples

- Higher order regression: $Y = \alpha + \beta_1 x + \beta_2 x^2 + \varepsilon$.

$$\boldsymbol{X} = \begin{pmatrix} 1 & x_1 & x_1^2 \\ \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 \end{pmatrix}, \quad \beta = (\alpha, \beta_1, \beta_2)^\top.$$

  This seems very powerful combined with the following fact: any continuous function can be approximated arbitrarily well by polynomials. (Weierstrass Theorem)

- Multiplicative model: $Y = \alpha x^\beta \exp(\varepsilon)$. If we take logarithm of both sides, we have $\log(Y) = \log(\alpha) + \beta \log(x) + \varepsilon$.

$$\boldsymbol{X} = \begin{pmatrix} 1 & \log(x_1) \\ \vdots & \vdots \\ 1 & \log(x_n) \end{pmatrix}, \quad \beta = (\log(\alpha), \beta)^\top.$$

Method of Least Squares

Consider the following linear regression model

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

- How to find a good estimator $\boldsymbol{\beta}$?
- For a given $\widehat{\boldsymbol{\beta}}$, the fitted values are $\widehat{\boldsymbol{Y}} = \boldsymbol{X}\widehat{\boldsymbol{\beta}}$.
- $\widehat{\boldsymbol{\varepsilon}}(\widehat{\boldsymbol{\beta}}) \triangleq \boldsymbol{Y} - \widehat{\boldsymbol{Y}} = \boldsymbol{Y} - \boldsymbol{X}\widehat{\boldsymbol{\beta}}$ is called the vector of the residuals.
- To estimate $\boldsymbol{\beta}$, minimize the **residual sum of squares (RSS)**:

$$\widehat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} \|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}\|_2^2.$$

RSS is also called sum of squared error (SSE) or sum of squared residuals (SSR).

Least Squares Estimator

$$\widehat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} \|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}\|_2^2.$$

- Take partial derivative of $\|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}\|_2^2 = (\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta})^\top(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta})$ with respect to $\boldsymbol{\beta}$, and set them to zero:

$$-2\boldsymbol{X}^\top(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}) = \boldsymbol{0} \quad \Rightarrow \quad \boldsymbol{X}^\top\boldsymbol{X}\widehat{\boldsymbol{\beta}} = \boldsymbol{X}^\top\boldsymbol{Y}$$

Let $f(x) = (f_1(x), \ldots, f_m(x))^\top \in \mathbb{R}^m$ for $x \in \mathbb{R}^n$, define $\frac{\partial f}{\partial x} \triangleq [\frac{\partial f_i}{\partial x_j}] \in \mathbb{R}^{m\times n}$.

Matrix differentiation

Let $A \in \mathbb{R}^{m\times n}, B \in \mathbb{R}^{n\times n}$, $x \in \mathbb{R}^{n\times 1}$. Let $f(x) = Ax \in \mathbb{R}^m, g(x) = x^\top Bx \in \mathbb{R}$, then

$$\frac{\partial f}{\partial x} = A \in \mathbb{R}^{m\times n}, \quad \frac{\partial g}{\partial x} = x^\top(B + B^\top) \in \mathbb{R}^{1\times n}.$$

Normal equation

$$\boldsymbol{X}^\top \boldsymbol{X}\widehat{\boldsymbol{\beta}} = \boldsymbol{X}^\top \boldsymbol{Y}.$$

- We assumed that $n \geq p$ and $\boldsymbol{X}$ has full (column) rank, so that $\boldsymbol{X}^\top \boldsymbol{X}$ is invertible.
- Given $n \geq p$ and $\boldsymbol{X}$ is full-rank, we have the **least square estimator (LSE)**

$$\widehat{\boldsymbol{\beta}} = (\boldsymbol{X}^\top \boldsymbol{X})^{-1}\boldsymbol{X}^\top \boldsymbol{Y},$$

- The **fitted value** of $\boldsymbol{Y}$ is

$$\widehat{\boldsymbol{Y}} = \boldsymbol{X}\widehat{\boldsymbol{\beta}} = \boldsymbol{X}(\boldsymbol{X}^\top \boldsymbol{X})^{-1}\boldsymbol{X}^\top \boldsymbol{Y}.$$

Collinearity

Collinearity is a phenomenon in which one predictor variable in a multiple regression model can be linearly predicted from the others with a substantial degree of accuracy. In this case, $\boldsymbol{X}^\top \boldsymbol{X}$ has extremely small eigenvalues, i.e., it is nearly non-invertible, and the estimation of parameter is sensitive to small changes in the model and data.

Least Squares Estimator – Computation Considerations

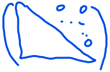
$$\boldsymbol{X}^\top \boldsymbol{X}\widehat{\boldsymbol{\beta}} = \boldsymbol{X}^\top \boldsymbol{Y}.$$

The normal equation is usually solved via the Cholesky decomposition of the matrix $\boldsymbol{X}^\top \boldsymbol{X}$ or a QR decomposition of X.

- Cholesky decomposition

  $$\boldsymbol{X}^\top \boldsymbol{X} = LL^\top \Rightarrow LL^\top \widehat{\boldsymbol{\beta}} = \boldsymbol{X}^\top \boldsymbol{Y},$$

  where L is a lower triangular matrix.

- To solve the least square, first let $\boldsymbol{z} = L^\top \widehat{\boldsymbol{\beta}}$ and solve $L\boldsymbol{z} = \boldsymbol{X}^\top \boldsymbol{Y}$ for $\boldsymbol{z}$ using forward substitution, and then solve $L^\top \widehat{\boldsymbol{\beta}} = \boldsymbol{z}$ for $\boldsymbol{\beta}$ using backward substitution.

Least Squares Estimator – Computation Considerations

$$\boldsymbol{X}^\top \boldsymbol{X} \widehat{\boldsymbol{\beta}} = \boldsymbol{X}^\top \boldsymbol{Y}.$$

- QR decomposition
$$\boldsymbol{X} = QR,$$
where Q is an orthogonal matrix ($QQ^\top = Q^\top Q = I$) and R is an upper triangular matrix.
- $X = QR \Rightarrow \boldsymbol{X}^\top \boldsymbol{X} = R^\top R$, QR for X is equivalent to Cholesky for $\boldsymbol{X}^\top \boldsymbol{X}$.
- But with n observations and p features, the Cholesky decomposition requires $p^3 + np^2/2$ operations, while the QR decomposition requires np^2 operations.

Depending on the relative size of n and p, the Cholesky can sometimes be faster; on the other hand, it can be less numerically stable (Lawson and Hansen, 1974).

Simple Linear Regression

Example: Simple linear regression. $Y = \alpha + \beta x + \varepsilon$.

$$S_{xx} = \sum_{i=1}^{n}(x_i - \bar{x})^2 = \sum_{i=1}^{n} x_i^2 - n\bar{x}^2, \qquad S_{YY} = \sum_{i=1}^{n}(Y_i - \bar{Y})^2 = \sum_{i=1}^{n} Y_i^2 - n\bar{Y}^2$$

$$S_{xY} = \sum_{i=1}^{n}(x_i - \bar{x})(Y_i - \bar{Y}) = \sum_{i=1}^{n} x_i Y_i - n\bar{x}\bar{Y}$$

Least Square Estimators

$$\widehat{\beta} = \frac{S_{xY}}{S_{xx}}, \quad \widehat{\alpha} = \bar{Y} - \widehat{\beta}\bar{x}, \quad RSS = \sum_{i=1}^{n}(Y_i - \widehat{\alpha} - \widehat{\beta}x_i)^2 = \frac{S_{xx}S_{YY} - S_{xY}^2}{S_{xx}}$$

Geometric Interpretation

Column space of $\boldsymbol{X} \in \mathbb{R}^{n \times p}$

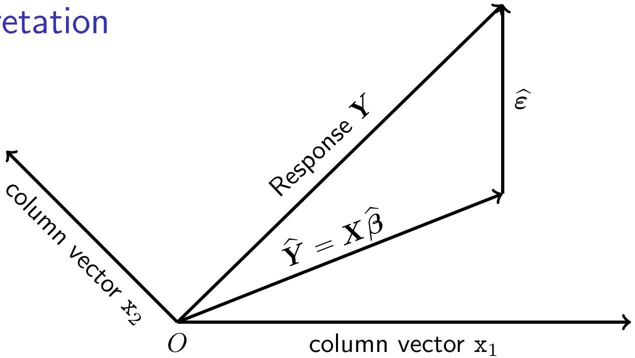
A dimension p subspace of $\mathbb{R}^n$, spanned by the column vectors of $\boldsymbol{X}$.

$$\boldsymbol{X}\boldsymbol{\beta} = \beta_1 \mathrm{x}_1 + \beta_2 \mathrm{x}_2 + \cdots + \beta_p \mathrm{x}_p, \quad \boldsymbol{\beta} \in \mathbb{R}^p.$$

Here $\mathrm{x}_j \in \mathbb{R}^n$ is the j-th column of $\boldsymbol{X}$.

- The fitted value
$$\widehat{\boldsymbol{Y}} = \boldsymbol{X}\widehat{\boldsymbol{\beta}} = \boldsymbol{X}(\boldsymbol{X}^\top \boldsymbol{X})^{-1}\boldsymbol{X}^\top \boldsymbol{Y}$$
belongs to the column space.
- For the LSE $\widehat{\boldsymbol{\beta}}$, we know by normal equation that
$$\widehat{\boldsymbol{\varepsilon}}^\top \boldsymbol{X} = (\boldsymbol{Y} - \boldsymbol{X}\widehat{\boldsymbol{\beta}})^\top \boldsymbol{X} = 0.$$
It implies that $\widehat{\boldsymbol{\varepsilon}}$ is orthogonal to the $\boldsymbol{X}$-column space.

Geometric Interpretation



- $\widehat{\boldsymbol{Y}} = P\boldsymbol{Y}$ is the projection of $\boldsymbol{Y}$ on the X-column space, where
$$P \triangleq \boldsymbol{X}(\boldsymbol{X}^\top\boldsymbol{X})^{-1}\boldsymbol{X}^\top$$
is the projection matrix.
- $\widehat{\boldsymbol{\varepsilon}} = Q\boldsymbol{Y}$ where $Q = I - P$, which is orthogonal to $\widehat{\boldsymbol{Y}} = P\boldsymbol{Y}$, i.e., $\widehat{\boldsymbol{Y}}^\top\widehat{\boldsymbol{\varepsilon}} = 0$.
Note that $PQ = QP = 0$.

Probabilistic Model

Now suppose we have the following assumptions

- Exogeneity: $\mathbb{E}[\varepsilon_i] = 0$.
- Homoscedasticity: $\mathbb{E}\left[\varepsilon_i^2\right] = \sigma^2$.
- ε_i's are independent normal random variables.

The likelihood function of y under parameter $\boldsymbol{\beta}, \sigma^2$:

$$L(\boldsymbol{\beta}, \sigma^2) \propto \frac{1}{\sigma^n} \exp\left(-\frac{\sum_{i=1}^n (Y_i - \boldsymbol{x}_i \boldsymbol{\beta})^2}{2\sigma^2}\right) = \frac{1}{\sigma^n} \exp\left(-\frac{\|\boldsymbol{Y} - X\boldsymbol{\beta}\|_2^2}{2\sigma^2}\right).$$

The MLE of $\boldsymbol{\beta}$ coincides with LSE (does not depend on σ^2).

Best Unbiased Linear Estimator (BLUE)

Assuming exogeneity and Homoscedasticity (but not normality) and under the model $\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$, we have the following:

Theorem (Gauss-Markov)

1. *(Unbiasedness)* $\mathbb{E}[\widehat{\boldsymbol{\beta}}] = \mathbb{E}\left[(\boldsymbol{X}^\top\boldsymbol{X})^{-1}\boldsymbol{X}^\top\boldsymbol{Y}\right] = \mathbb{E}\left[(\boldsymbol{X}^\top\boldsymbol{X})^{-1}\boldsymbol{X}^\top(\boldsymbol{X}\boldsymbol{\beta}+\boldsymbol{\varepsilon})\right] = \boldsymbol{\beta}$.
2. *(Conditional standard error)* $\mathrm{Cov}[\widehat{\boldsymbol{\beta}}] = \sigma^2(\boldsymbol{X}^\top\boldsymbol{X})^{-1}$.
3. *The least-squares estimator $\widehat{\boldsymbol{\beta}}$ is the best linear unbiased estimator (BLUE).*

BLUE

For any given vector $\boldsymbol{a}$, $\boldsymbol{a}^\top\widehat{\boldsymbol{\beta}}$ is a linear[a] unbiased estimator of the parameter $\theta = \boldsymbol{a}^\top\boldsymbol{\beta}$. Further, for any linear unbiased estimator $\boldsymbol{b}^\top\boldsymbol{Y}$ of θ, its variance is at least as large as that of $\boldsymbol{a}^\top\widehat{\boldsymbol{\beta}}$.

[a] An estimator in the form of $\hat{\beta} = AY + \mu$ for some matrix A and vector μ.

Proof of BLUE. Obviously, $\boldsymbol{a}^\top \widehat{\boldsymbol{\beta}}$ is unbiased and linear. The variance is

$$\mathrm{Var}(\boldsymbol{a}^\top \widehat{\boldsymbol{\beta}}) = \sigma^2 \boldsymbol{a}^\top (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{a}.$$

Consider any linear unbiased estimator $\boldsymbol{b}^\top \boldsymbol{Y}$ of $\theta = \boldsymbol{a}^\top \boldsymbol{\beta}$. Unbiasedness requires that

$$\boldsymbol{b}^\top \boldsymbol{X} \boldsymbol{\beta} = \mathbb{E}[\boldsymbol{b}^\top \boldsymbol{Y}] = \boldsymbol{a}^\top \boldsymbol{\beta}, \quad \forall \boldsymbol{\beta}.$$

Hence $\boldsymbol{b}^\top \boldsymbol{X} = \boldsymbol{a}^\top$. Furthermore, the variance is

$$\mathrm{Var}(\boldsymbol{b}^\top \boldsymbol{Y}) = \sigma^2 \boldsymbol{b}^\top \boldsymbol{b}.$$

Plugging in $\boldsymbol{a} = \boldsymbol{X}^\top \boldsymbol{b}$, we have

$$\mathrm{Var}(\boldsymbol{b}^\top \boldsymbol{Y}) - \mathrm{Var}(\boldsymbol{a}^\top \widehat{\boldsymbol{\beta}}) = \sigma^2 \boldsymbol{b}^\top Q \boldsymbol{b} \geq 0.$$

Properties of LSE

1. $E[\widehat{\boldsymbol{Y}}] = \mathbb{E}[\boldsymbol{Y}] = \boldsymbol{X}\boldsymbol{\beta}$.
2. $\mathrm{Cov}[\widehat{\boldsymbol{Y}}] = \mathrm{Cov}[\boldsymbol{X}\boldsymbol{\beta} + P\boldsymbol{\varepsilon}] = \sigma^2 P$.
3. $\mathrm{Cov}[\widehat{\boldsymbol{\varepsilon}}] = \mathrm{Cov}[Q\boldsymbol{Y}] = \mathrm{Cov}[Q\boldsymbol{\varepsilon}] = \sigma^2 Q$.
4. $\mathrm{Cov}[\widehat{\boldsymbol{Y}}, \widehat{\boldsymbol{\varepsilon}}] = 0$ as $QP = 0$.

The following is an unbiased estimator of σ^2

$$\widehat{\sigma}^2 = \frac{\sum_{i=1}^n (Y_i - \widehat{Y}_i)^2}{n-p} = \frac{\|\widehat{\boldsymbol{\varepsilon}}\|_2^2}{n-p}.$$

Proof. Note that

$$\sum_{i=1}^{n}(Y_i - \widehat{Y}_i)^2 = \widehat{\boldsymbol{\varepsilon}}^\top \widehat{\boldsymbol{\varepsilon}} = \boldsymbol{Y}^\top Q^\top Q \boldsymbol{Y} = \boldsymbol{\varepsilon}^\top Q^\top Q \boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^\top Q \boldsymbol{\varepsilon}.$$

Use the fact that $\mathrm{tr}(AB) = \mathrm{tr}(BA)$, we have

$$\sum_{i=1}^{n}(Y_i - \widehat{Y}_i)^2 = \mathrm{tr}(\varepsilon^\top Q \boldsymbol{\varepsilon}) = \mathrm{tr}(Q \boldsymbol{\varepsilon} \boldsymbol{\varepsilon}^\top)$$

Finally,

$$\mathbb{E}\left[\sum_{i=1}^{n}(Y_i - \widehat{Y}_i)^2\right] = \mathbb{E}\left[\mathrm{tr}(Q \boldsymbol{\varepsilon} \boldsymbol{\varepsilon}^\top)\right] = \mathrm{tr}\left(Q \mathbb{E}[\boldsymbol{\varepsilon} \boldsymbol{\varepsilon}^\top]\right) = \sigma^2 \mathrm{tr}(Q).$$

To calculate $\mathrm{tr}(Q)$, recall that trace is equal to the summation of the eigenvalues, and note that eigenvalues of Q is either 0 or 1 and the rank of Q is $n - p$ (if we assume $\boldsymbol{X}^\top \boldsymbol{X}$ is invertible).

Generalized Least Square

What if ε is not i.i.d., but $\sim N(\mathbf{0}, \sigma^2\Sigma)$

- Σ is always positive semi-definite.
- We assume that Σ is **positive definite**, so that $\Sigma = AA^\top$, where A is invertible. (e.g. Cholesky decomposition)
- We assume that Σ is known.
- We can reduce to the standard model

$$\tilde{\boldsymbol{Y}} \triangleq A^{-1}Y = A^{-1}(X\boldsymbol{\beta} + \boldsymbol{\varepsilon}) = A^{-1}X\boldsymbol{\beta} + A^{-1}\boldsymbol{\varepsilon}$$

- New independent variables $\tilde{X} = A^{-1}X$, new i.i.d. error $\tilde{\boldsymbol{\varepsilon}} = A^{-1}\boldsymbol{\varepsilon}$.
- Check:

$$\mathbb{E}[\tilde{\boldsymbol{\varepsilon}}] = \mathbb{E}[A^{-1}\boldsymbol{\varepsilon}] = A^{-1}\mathbb{E}[\boldsymbol{\varepsilon}] = \mathbf{0}$$
$$\mathrm{Cov}[\tilde{\boldsymbol{\varepsilon}}] = A^{-1}\mathrm{Cov}[\boldsymbol{\varepsilon}](A^{-1})^\top = A^{-1}\sigma^2(AA^\top)(A^{-1})^\top = \sigma^2 I$$

GLS Cont.

- Apply LSE,

$$
\begin{aligned}
&\min \|\tilde{\boldsymbol{Y}} - \tilde{X}\boldsymbol{\beta}\|_2^2 = (\boldsymbol{Y} - X\boldsymbol{\beta})^\top \Sigma^{-1} (\boldsymbol{Y} - X\boldsymbol{\beta}) \\
\Rightarrow &\widehat{\boldsymbol{\beta}} = (X^\top \Sigma^{-1} X)^{-1} X^\top \Sigma^{-1} \boldsymbol{Y}.
\end{aligned}
$$

- This is called the generalized least squares estimate.

$$
\widehat{\boldsymbol{\beta}} \sim N(\boldsymbol{\beta}, \sigma^2 (X^\top \Sigma^{-1} X)^{-1}).
$$

- One can derive test statistics based on the distribution.

GLS Remarks

- A special case is when Σ is a diagonal matrix $diag(v_1, \ldots, v_n)$. In this case, we are minimizing the weighted squared error $\sum_i \varepsilon_i^2 / v_i$. This is called the **weighted least square**.
- In practice we usually don't know Σ. So we can run a standard LSE, estimate $\widehat{\Sigma}$ (need to impose some structures), and then applied GLS. This is referred to as the Cochrane-Orcutt procedure.
- If Σ is not positive definite (only semi-definite), one can use the Gram-Schmidt process (Schmidt orthonormalization) to find a set of standard normal random variables and the matrix that transform them to the original error terms.
  - Think about the geometric interpretation of covariance and use the fact that uncorrelated means independence for normal random variables.
  - Read the wikipedia page for Gram-Schmidt process.

Properties of LSE – Distributions

Now we impose the additional normal assumption, $\boldsymbol{\varepsilon} \sim N(\mathbf{0}, \sigma^2 I_{n\times n})$.

- $\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon} \sim N(\boldsymbol{X}\boldsymbol{\beta}, \sigma^2 I_{n\times n})$
- $\widehat{\boldsymbol{\beta}} = (\boldsymbol{X}^\top \boldsymbol{X})^{-1}\boldsymbol{X}^\top(\boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}) \sim N(\boldsymbol{\beta}, \sigma^2(\boldsymbol{X}^\top \boldsymbol{X})^{-1})$.
- $\widehat{\boldsymbol{Y}} = P\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + P\boldsymbol{\varepsilon} \sim N(\boldsymbol{X}\boldsymbol{\beta}, \sigma^2 P), P = \boldsymbol{X}(\boldsymbol{X}^\top \boldsymbol{X})^{-1}\boldsymbol{X}^T$.
- $\widehat{\boldsymbol{\varepsilon}} = Q\boldsymbol{Y} = Q\boldsymbol{\varepsilon} \sim N(0, \sigma^2 Q), Q = I - P$. Note that $PQ = QP = 0$.
- $\widehat{\boldsymbol{Y}}$ and $\widehat{\boldsymbol{\varepsilon}}$ are independent: $\mathrm{Cov}(P\boldsymbol{Y}, Q\boldsymbol{Y}) = P\sigma^2 I_{n\times n} Q = 0$.
- $\widehat{\boldsymbol{\beta}} = (\boldsymbol{X}^\top \boldsymbol{X})^{-1}\boldsymbol{X}^\top \boldsymbol{X}\widehat{\boldsymbol{\beta}} = (\boldsymbol{X}^\top \boldsymbol{X})^{-1}\boldsymbol{X}^\top \widehat{\boldsymbol{Y}} \Rightarrow \widehat{\boldsymbol{\beta}}$ and $\widehat{\sigma}^2 = \frac{\|\widehat{\boldsymbol{\varepsilon}}\|_2^2}{n-p}$ are independent.
- Use the lemma for chi-squared distribution from Lecture 2,

$$(n-p)\widehat{\sigma}^2/\sigma^2 = \frac{\|\widehat{\boldsymbol{\varepsilon}}\|_2^2}{\sigma^2} = \frac{\sum_{i=1}^n (Y_i - \widehat{Y}_i)^2}{\sigma^2} \sim \chi^2_{n-p}.$$

Statistical Inference for β_i

To test whether a particular variable x_i has no effect on $\boldsymbol{Y}$:

- Recall that $\widehat{\boldsymbol{\beta}}$ and $\widehat{\sigma}^2 = \frac{\|\widehat{\varepsilon}\|_2^2}{n-p} = RSS/(n-p)$ are independent.
- For each β_i,

$$\frac{\widehat{\beta}_i - \beta_i}{\widehat{\sigma}\sqrt{(\boldsymbol{X}^\top\boldsymbol{X})^{-1}_{ii}}} = \frac{(\widehat{\beta}_i - \beta_i)/\sqrt{\sigma^2(\boldsymbol{X}^\top\boldsymbol{X})^{-1}_{ii}}}{\sqrt{[(n-p)\widehat{\sigma}^2/\sigma^2]/(n-p)}} \sim t_{n-p}.$$

Hypothesis Test – β_i

H_0	H_1	TS	Significance level α	p-value
$\beta_i = 0$	$\beta_i \neq 0$	$\frac{\widehat{\beta}_i}{\widehat{\sigma}\sqrt{(\boldsymbol{X}^\top\boldsymbol{X})^{-1}_{ii}}}$	Reject if $\lvert TS\rvert > t_{n-p}(1-\alpha/2)$	$2\mathbb{P}\{T_{n-p} > TS\}$

- The $1-\alpha$ confidence interval for β_i is

$$\left[\widehat{\beta}_i - t_{n-p}(1-\alpha/2)\widehat{\sigma}\sqrt{(\boldsymbol{X}^\top\boldsymbol{X})^{-1}_{ii}}, \widehat{\beta}_i + t_{n-p}(1-\alpha/2)\widehat{\sigma}\sqrt{(\boldsymbol{X}^\top\boldsymbol{X})^{-1}_{ii}}\right]$$

Simple Linear Regression

Example: Simple linear regression. $y = \alpha + \beta x + \varepsilon$.

- TS for β, $H_0 : \beta = \beta_0$, implies that $\sqrt{\frac{S_{xx}}{\widehat{\sigma}^2}}(\widehat{\beta} - \beta_0) \sim t_{n-2}$ under H_0.
- $(1-\gamma)$ CI for β:

$$\left(\widehat{\beta} - t_{n-2}(1-\gamma/2)\frac{\widehat{\sigma}}{\sqrt{S_{xx}}}, \widehat{\beta} + t_{n-2}(1-\gamma/2)\frac{\widehat{\sigma}}{\sqrt{S_{xx}}}\right)$$

- TS for α, $H_0 : \alpha = \alpha_0$, implies that $\sqrt{\frac{S_{xx} n}{\widehat{\sigma}^2 \sum_i x_i^2}}(\widehat{\alpha} - \alpha_0) \sim t_{n-2}$ under H_0.
- $(1-\gamma)$ CI for α:

$$\left(\widehat{\alpha} - \sqrt{\frac{\widehat{\sigma}^2 \sum_i x_i^2}{S_{xx} n}} t_{n-2}(1-\gamma/2), \widehat{\alpha} + \sqrt{\frac{\widehat{\sigma}^2 \sum_i x_i^2}{S_{xx} n}} t_{n-2}(1-\gamma/2)\right)$$

Statistical Inference for $\boldsymbol{\beta}$

To test whether the parameter is $\boldsymbol{\beta}_0$, i.e., $H_0 : \boldsymbol{\beta} = \boldsymbol{\beta}_0$ versus $H_1 : \boldsymbol{\beta} \neq \boldsymbol{\beta}_0$.

$$\frac{(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0)^\top (\boldsymbol{X}^\top \boldsymbol{X})(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0)}{p\widehat{\sigma}^2} = \frac{\frac{\boldsymbol{\varepsilon}^\top P \boldsymbol{\varepsilon}}{\sigma^2}/p}{\frac{\boldsymbol{\varepsilon}^\top Q \boldsymbol{\varepsilon}}{\sigma^2}/(n-p)} \sim F_{p,n-p}, \text{ under } H_0.$$

(Check independence!) This is because the numerator equals $\boldsymbol{\varepsilon}^\top P \boldsymbol{\varepsilon}$ and $tr(P) = p$ and $\widehat{\sigma}^2 = \frac{\|\widehat{\boldsymbol{\varepsilon}}\|_2^2}{n-p} = \boldsymbol{Y}^\top Q \boldsymbol{Y}/(n-p) = \boldsymbol{\varepsilon}^\top Q \boldsymbol{\varepsilon}/(n-p)$ and $tr(Q) = n - p$.

- Reject if test statistic $\geq F_{p,n-p}(1-\alpha)$.

$(1-\alpha)$ confidence set

$$\left\{\boldsymbol{\beta} : (\boldsymbol{\beta} - \widehat{\boldsymbol{\beta}})^\top (\boldsymbol{X}^\top \boldsymbol{X})(\boldsymbol{\beta} - \widehat{\boldsymbol{\beta}}) \leq p\widehat{\sigma}^2 F_{p,n-p}(1-\alpha)\right\}$$

An ellipsoid.

Statistical Inference for the True Location of the Hyperplane

- For each experimental condition $\boldsymbol{x}_0$: Let $Y_0 = \boldsymbol{x}_0^\top \boldsymbol{\beta}$ and $\widehat{Y}_0 = \boldsymbol{x}_0^\top \widehat{\boldsymbol{\beta}}$

$$\frac{\widehat{Y}_0 - \mathbb{E}[Y_0]}{\widehat{\sigma}\sqrt{\boldsymbol{x}_0^\top (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{x}_0}} \sim t_{n-p}.$$

$\Rightarrow$ Confidence interval such that the true hyperplane cross at this $\boldsymbol{x}_0$.
Pointwise confidence band (CB)

$$\mathbb{P}(\boldsymbol{x}_0^\top \widehat{\boldsymbol{\beta}} - w(\boldsymbol{x}_0) \leq \boldsymbol{x}_0^\top \boldsymbol{\beta} \leq \boldsymbol{x}_0^\top \widehat{\boldsymbol{\beta}} + w(\boldsymbol{x}_0)) = 1 - \alpha.$$

- Can we construct a confidence band for the entire true hyperplane ($Y = \boldsymbol{x}^\top \boldsymbol{\beta}$)?
Simultaneous CB

$$\mathbb{P}(\boldsymbol{x}^\top \widehat{\boldsymbol{\beta}} - w(\boldsymbol{x}) \leq \boldsymbol{x}^\top \boldsymbol{\beta} \leq \boldsymbol{x}^\top \widehat{\boldsymbol{\beta}} + w(\boldsymbol{x}), \text{ for all } \boldsymbol{x}) = 1 - \alpha.$$

Statistical Inference for the True Location of the Hyperplane

For simultaneous band, by Cauchy-Schwartz for $\langle \alpha, \beta \rangle = \alpha^\top (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \beta$

$$
\begin{aligned}
|\boldsymbol{x}_0^\top \widehat{\boldsymbol{\beta}} - \boldsymbol{x}_0^\top \boldsymbol{\beta}|^2 &= |\boldsymbol{x}_0^\top (\boldsymbol{X}^\top \boldsymbol{X})^{-1} (\boldsymbol{X}^\top \boldsymbol{X})(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta})|^2 = \langle \boldsymbol{x}_0, (\boldsymbol{X}^\top \boldsymbol{X})(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}) \rangle^2 \\
&\leq (\boldsymbol{x}_0^\top (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{x}_0) \left((\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta})^\top (\boldsymbol{X}^\top \boldsymbol{X})(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}) \right)
\end{aligned}
$$

From previous slides, we know that

$$
\frac{(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0)^\top (\boldsymbol{X}^\top \boldsymbol{X})(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0)}{p \widehat{\sigma}^2} \sim F_{p, n-p}
$$

Confidence band

$$
|\boldsymbol{x}_0^\top \widehat{\boldsymbol{\beta}} - \boldsymbol{x}_0^\top \boldsymbol{\beta}|^2 \leq (\boldsymbol{x}_0^\top (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{x}_0) p \widehat{\sigma}^2 F_{p, n-p}(1 - \alpha).
$$

Simple Linear Regression

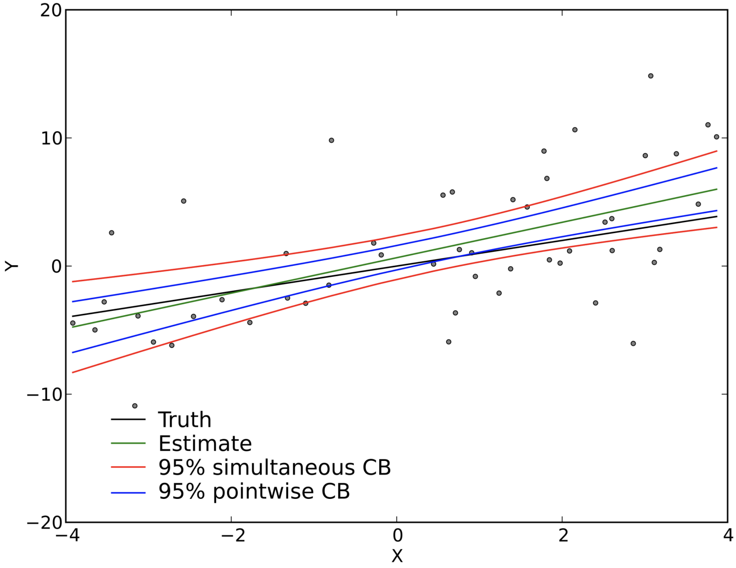
Example: Simple linear regression

Confidence interval for the new observation at x_0

$$\widehat{\alpha} + \widehat{\beta}x_0 \pm t_{n-2}(1-\gamma/2) \cdot \sqrt{\frac{RSS}{(n-2)}\left[\frac{1}{n} + \frac{(x_0-\bar{x})^2}{S_{xx}}\right]}$$

Simultaneous confidence band for the regression line x_0

$$\widehat{\alpha} + \widehat{\beta}x_0 \pm \sqrt{2F_{n-2}(1-\gamma/2)} \cdot \sqrt{\frac{RSS}{(n-2)}\left[\frac{1}{n} + \frac{(x_0-\bar{x})^2}{S_{xx}}\right]}$$


20
10
0
−10
−20
Y
−4
−2
0
2
4
X
Truth
Estimate
95% simultaneous CB
95% pointwise CB

Prediction Interval

In the previous slides, we see confidence band for mean response $\mathbb{E}[Y] = \boldsymbol{x}^\top \boldsymbol{\beta}$.

What about the response $Y = \boldsymbol{x}^\top \boldsymbol{\beta} + \varepsilon$?

For each experimental condition $\boldsymbol{x}_0$:

$$\frac{\widehat{Y}_0 - Y_0}{\widehat{\sigma}\sqrt{1 + \boldsymbol{x}_0^\top (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{x}_0}} \sim t_{n-p}.$$

Example: Simple linear regression

(For the mean) $$\left(\widehat{\alpha} + \widehat{\beta} x_0 \pm t_{n-2}(1-\alpha/2) \sqrt{\frac{RSS}{(n-2)} \left[\frac{1}{n} + \frac{(x_0 - \bar{x})^2}{S_{xx}}\right]}\right)$$

(For the response) $$\left(\widehat{\alpha} + \widehat{\beta} x_0 \pm t_{n-2}(1-\alpha/2) \sqrt{\frac{RSS}{(n-2)} \left[1 + \frac{1}{n} + \frac{(x_0 - \bar{x})^2}{S_{xx}}\right]}\right)$$

Nested Model Test – F-statistic

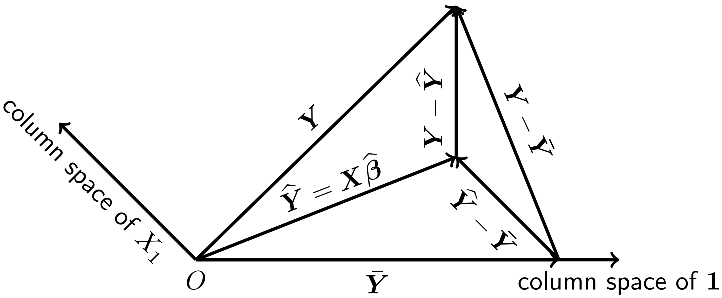
The F statistic checks whether a non-trivial linear model is not rejected.

- $X = \begin{pmatrix} 1 & x_{12} & \cdots & x_{1p} \\ 1 & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n2} & \cdots & x_{np} \end{pmatrix} = (\mathbf{1}, X_1)$, $\beta = (\beta_1, \beta_2, \ldots, \beta_p)^\top$.
- Consider null hypothesis $H_0 : \beta_2 = \beta_3 = \cdots = \beta_p = 0$, the MLE under the null hypothesis is $\bar{\boldsymbol{Y}}$.

Nested Model Test – F-statistic

The F-statistic

$$F = \frac{\|\bar{\boldsymbol{Y}} - \widehat{\boldsymbol{Y}}\|_2^2/(p-1)}{\|\boldsymbol{Y} - \widehat{\boldsymbol{Y}}\|_2^2/(n-p)} \sim F_{p-1,n-p}$$



This can be considered as testing two nested models. $H_0 : \beta_2 = \beta_3 = \cdots = \beta_p = 0$ is the simpler model, and if we allow any $\boldsymbol{\beta}$, this is the full model.

Nested Model

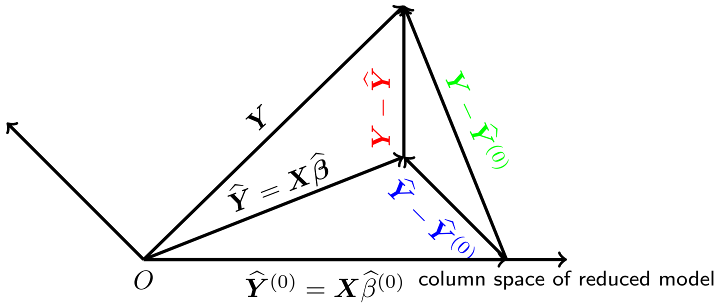
- H_1: all features play a role $\boldsymbol{Y} = X\boldsymbol{\beta} + \boldsymbol{\varepsilon}$.
- Null hypothesis H_0: a reduced model where some parameters are redundant $B\boldsymbol{\beta} = \boldsymbol{b}$.
- For example, $\beta_2 = \beta_3 = \cdots = \beta_p = 0$. Or $\beta_1 + \beta_2 = 3$, which means we can reduce $\beta_2 = 3 - \beta_1$ and need only $p - 1$ features.
- For example, B is $(p-q) \times p$, $\boldsymbol{b} = \boldsymbol{0}$. Test if $p - q$ of the coefficients are zero.

$$B = \begin{pmatrix} 1 & 0 & \ldots & 0 & 0 & \ldots & 0 \\ 0 & 1 & \ldots & 0 & 0 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & 1 & 0 & \ldots & 0 \end{pmatrix}$$

- Can we represent the relationship by a simpler model?

Nested Model Test

- If the null hypothesis H_0 is true, say $\beta_2 = 0$. Then the column space of $X^{(0)}$ is a subspace of X.
- Geometric interpretation and Pythagoras theorem.



- Define $RSS = \|\mathbf{Y} - \widehat{\mathbf{Y}}\|_2^2$ under H_1 and $RSS_0 = \|\mathbf{Y} - \widehat{\mathbf{Y}}^{(0)}\|_2^2$ under H_0.

Nested Model Test

- Recall the properties of LSE: $RSS/(n-p)$ is an unbiased estimator of σ^2, under both hypotheses. $(RSS_0 - RSS)/(p-q)$ is an unbiased estimator of σ^2 under H_0. More importantly, they are orthogonal!
- Pythagoras theorem: $\|\boldsymbol{Y} - \widehat{\mathbf{Y}}^{(0)}\|_2^2 = \|\boldsymbol{Y} - \widehat{\boldsymbol{Y}}\|_2^2 + \|\widehat{\mathbf{Y}} - \widehat{\mathbf{Y}}^{(0)}\|_2^2$.
- This implies a statistic under H_0:

$$\frac{(RSS_0 - RSS)/(p-q)}{RSS/(n-p)} = \frac{\|\widehat{\mathbf{Y}} - \widehat{\mathbf{Y}}^{(0)}\|_2^2/(p-q)}{\|\boldsymbol{Y} - \widehat{\boldsymbol{Y}}\|_2^2/(n-p)} \sim F_{p-q,n-p}.$$

- Reject the simpler model if the test statitic is large.

Nested Model Test – ANOVA

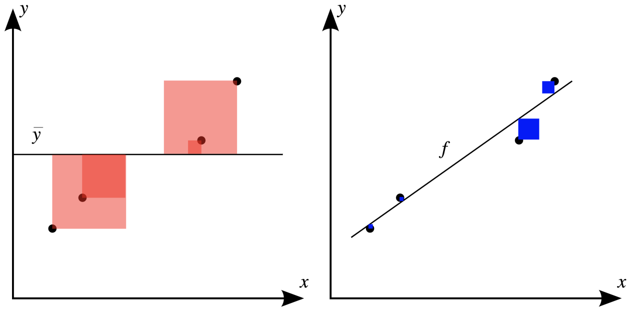
Analysis of variance (ANOVA) is a special case of the nested model test.

- $X = \begin{pmatrix} 1 & \cdots & 1 & 0 & \cdots & 0 & \cdots & 0 & \cdots & 0 \\ 0 & \cdots & 0 & 1 & \cdots & 1 & \cdots & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & 0 & \cdots & 0 & \cdots & 1 & \cdots & 1 \end{pmatrix}^{\top}, \beta = (\mu_1, \mu_2, \ldots, \mu_k)^{\top}.$
- MLE is $(\bar{Y}_{1\cdot}, \ldots, \bar{Y}_{k\cdot})$.
- Consider null hypothesis $H_0 : \mu_1 = \mu_2 = \cdots = \mu_k$, the MLE under the null hypothesis is $\widehat{\boldsymbol{Y}}^{(0)} = \bar{\boldsymbol{Y}}$.
- $\|\boldsymbol{Y} - \widehat{\boldsymbol{Y}}^{(0)}\|_2^2 = \|\boldsymbol{Y} - \widehat{\boldsymbol{Y}}\|_2^2 + \|\widehat{\boldsymbol{Y}}^{(0)} - \widehat{\boldsymbol{Y}}\|_2^2 \Rightarrow SST = SSB + SSW.$

Coefficient of Determination

$$R^2 \triangleq \frac{TSS - RSS}{TSS} = 1 - \frac{RSS}{TSS}, \quad TSS = \|\boldsymbol{Y} - \bar{\boldsymbol{Y}}\|_2^2.$$

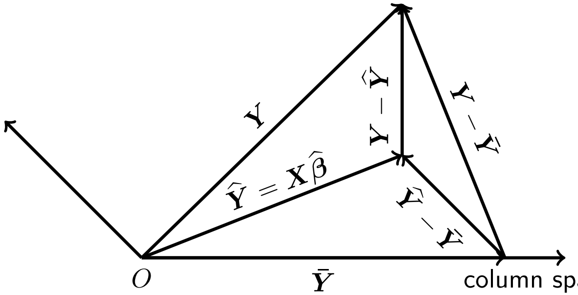
- Total Sum of Squares is the error *not captured by the sample mean*.
- $RSS = \sum(Y_i - \widehat{Y}_i)^2$ reflects the variance *not captured by the regression model*.



When $R^2 \approx 1$, it means $RSS \approx 0$, the fit is perfect!

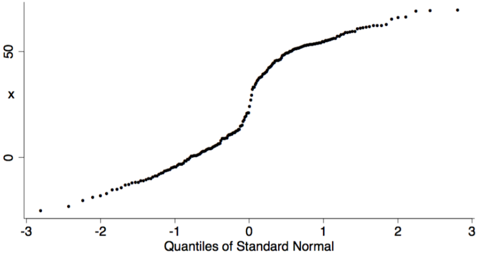
When $R^2 \approx 0$, it means the regression model is not much better than $\bar{y}$.

- One can check that
$$R^2 = \frac{\|\widehat{\mathbf{Y}} - \bar{\mathbf{Y}}\|_2^2/(p-1)}{\|\mathbf{Y} - \bar{\mathbf{Y}}\|_2^2/(n-p)}.$$
- Also a F distribution? NO!



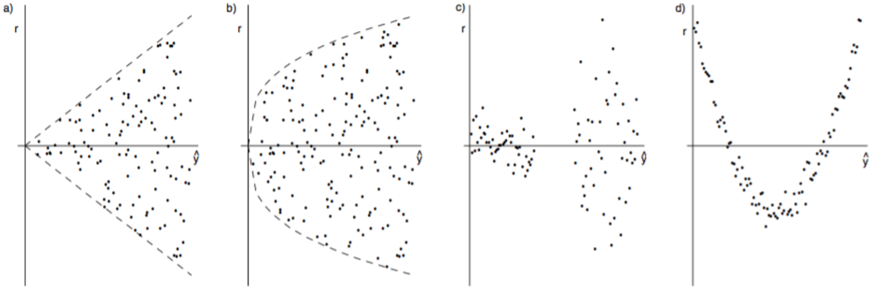
Normality

- Model assumption: ϵ_i has normal distribution.
- Normal probability plot: check whether a random sample $x_1, \ldots, x_n$ have normal distribution. Plot $\Phi^{-1}((i-0.5)/n)$ against $(x_{(i)} - \mu)/\sigma$ on the plane.
- If X is indeed normal, the plot should be roughly a straight line.
- Check the residuals: $\widehat{\epsilon_i} = Y_i - \widehat{Y}_i$ should be approximately normal when n is large.



Homoscedasticity

- Model assumption: ϵ_i are i.i.d. random variables.
- Plot $\widehat{Y}_i$ against $\widehat{\epsilon}_i$. What are the problems of the following figures?



Transformation

In practice we usually take a transformation of the response variable before fitting a regression model.

Example: $Y \propto x_1^{\beta_1} x_2^{\beta_2} \cdots x_p^{\beta_p}$, in which case we take the logarithm

$$\log(Y) = \sum_{i=1}^{p} \beta_i \log(x_i) + \varepsilon.$$

Box and Cox (1964) proposed a systematic way to find a transformation from the data.

To some extend, Box-Cox transformation can be used to address cases where normality or homoscedasticity assumptions are violated.

Box-Cox Transformation

Consider a parametric family of transformation functions. Let $Y^{(\lambda)}$ denote the transformed response, where λ is a parameter.

$$Y^{(\lambda)} = \begin{cases} \frac{Y^{\lambda}-1}{\lambda}, & \text{if } \lambda \neq 0, \\ \log(Y), & \text{if } \lambda = 0. \end{cases}$$

Box-Cox model

$$Y^{(\lambda)} = \boldsymbol{X}^{\top}\boldsymbol{\beta} + \varepsilon, \quad \text{where } \varepsilon \overset{i.i.d.}{\sim} N(0, \sigma^2)$$

The likelihood function of the Box-Cox model is

$$L(\lambda, \boldsymbol{\beta}, \sigma^2 | \boldsymbol{X}, \boldsymbol{Y}) = \frac{1}{(2\pi)^{n/2}\sigma^n} e^{-\frac{1}{2\sigma^2}\|\boldsymbol{Y}^{(\lambda)} - \boldsymbol{X}\boldsymbol{\beta}\|^2} \cdot J(\lambda, \boldsymbol{Y})$$

where the Jacobian is $J(\lambda, \boldsymbol{Y}) = \prod_{i=1}^n |d\boldsymbol{Y}^{(\lambda)}/d\boldsymbol{Y}| = \prod_{i=1}^n |Y_i|^{\lambda-1}$.

MLE for Box-Cox model

- Given a λ, the MLE for $\boldsymbol{\beta}, \sigma^2$ are the usual

$$\widehat{\boldsymbol{\beta}}(\lambda) = (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{X}^\top \boldsymbol{Y}^{(\lambda)}, \quad \widehat{\sigma}^2(\lambda) = \frac{1}{n}\|\boldsymbol{Y}^{(\lambda)} - \widehat{\boldsymbol{Y}}^{(\lambda)}\|^2.$$

- Plugging $\widehat{\boldsymbol{\beta}}(\lambda)$ and $\widehat{\sigma}^2(\lambda)$ into the likelihood, we have

$$\log L(\lambda) = (\lambda - 1)\sum_{i=1}^n \log(|Y_i|) - \frac{n}{2}\log \widehat{\sigma}^2(\lambda) - \frac{n}{2} \Rightarrow \widehat{\lambda}_{\text{MLE}} = \arg\max_\lambda \log L(\lambda).$$

- The MLE is $(\widehat{\lambda}_{\text{MLE}}, \widehat{\boldsymbol{\beta}}(\widehat{\lambda}_{\text{MLE}}), \widehat{\sigma}^2(\widehat{\lambda}_{\text{MLE}}))$.

Nonlinear regression

Recall our motivating example – polynomial regression

$$Y = \boldsymbol{\beta}^\top \boldsymbol{\phi}(\boldsymbol{x}) + \varepsilon,$$

where $\boldsymbol{\phi}(\boldsymbol{x}) = (1, x, x^2, x^3, \ldots, x^d)$.

Weierstrass Theorem

Any continuous $f(X)$ on $[0, 1]$ can be uniformly approximated by a polynomial function.

Spline regression

- One problem of polynomial regression: not suitable for functions with varying degrees of smoothness.
- Solution: use piece-wise polynomial.

Spline

A degree-d spline is a piecewise polynomials with degree d, which is continuous differentiable up to order $d-1$. The points where discontinuity (in the derivatives) occurs are called the <u>knots</u>.

Example: Linear spline with knots $\tau_1 < \tau_2$.

$$f(x) = \begin{cases} \beta_0 + \beta_1 x, & x \in (-\infty, \tau_1] \\ \beta_0 + \beta_1 x + \beta_2 (x - \tau_1)^+, & x \in (\tau_1, \tau_2] \\ \beta_0 + \beta_1 x + \beta_2 (x - \tau_1)^+ + \beta_3 (x - \tau_2)^+, & x \in (\tau_2, \infty). \end{cases}$$

The basis functions

$$B_0(x) = 1, B_1(x) = x, B_2(x) = (x - \tau_1), B_3(x) = (x - \tau_2)^+.$$

Example: Cubic spline with knots $\tau_1 < \tau_2$.

$$f(x) = \begin{cases} \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3, & x \in (-\infty, \tau_1] \\ \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4((x-\tau_1)^+)^3, & x \in (\tau_1, \tau_2] \\ \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4((x-\tau_1)^+)^3 + \beta_5((x-\tau_2)^+)^3, & x \in (\tau_2, \infty). \end{cases}$$

The basis functions

$$B_0(x) = 1, B_1(x) = x, B_2(x) = x^2, B_3(x) = x^3, B_4(x) = ((x-\tau_1)^+)^3, B_5(x) = ((x-\tau_2)^+)^3.$$

- Try to write down cubic splines with k knots.

Spline regression

$$\boldsymbol{Y} = \boldsymbol{\beta}^\top \boldsymbol{B}(\boldsymbol{x}) + \varepsilon.$$

- A multiple linear regression model.
- Versatile and tractable: Cubic splines are widely used.
- Later on, we will look at a fully nonparametric multiple regression called <u>kernel ridge regression</u>.

Influence of Individual Observations on the LSE

Cook's distance for the ith observation

$$D_i = \frac{(\widehat{\boldsymbol{\beta}}^{(-i)} - \widehat{\boldsymbol{\beta}})^\top (\boldsymbol{X}^\top \boldsymbol{X})(\widehat{\boldsymbol{\beta}}^{(-i)} - \widehat{\boldsymbol{\beta}})}{p\widehat{\sigma}^2} \sim F_{p,n-p}.$$

- Observations with large Cook's distance alters the LSE by a lot, and thus can be considered an outlier.
- It may not be appropriate to simply discard outlier.
- For data that deviates from normal distribution (check by Q-Q plot), especially for those distributions with heavy tails, outliers appear more often.
- So we need robust methods for regression.

Robust Regression

Recall that the multiple linear regression model can be obtained by minimizing the least square error, i.e.,

$$\widehat{\boldsymbol{\beta}}_{\mathrm{OLS}} = \arg\min_{\boldsymbol{\beta}} l(\boldsymbol{\beta}) = \arg\min_{\boldsymbol{\beta}} \sum_{i=1}^{n} (Y_i - \widehat{Y}_i)^2 = \arg\min_{\boldsymbol{\beta}} \|\boldsymbol{Y} - \widehat{\boldsymbol{Y}}\|_2^2.$$

- The loss function is quadratic $\Rightarrow$ loss for outliers have much more impact on the estimation.

Consider the alternative loss function

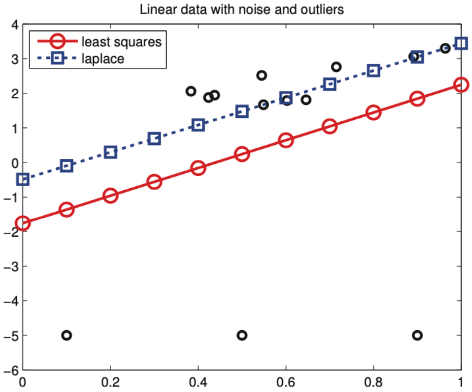
$$\widehat{\boldsymbol{\beta}}_{\mathrm{Robust}} = \arg\min_{\boldsymbol{\beta}} \sum_{i=1}^{n} |Y_i - \widehat{Y}_i| = \arg\min_{\boldsymbol{\beta}} \|\boldsymbol{Y} - \widehat{\boldsymbol{Y}}\|_1.$$

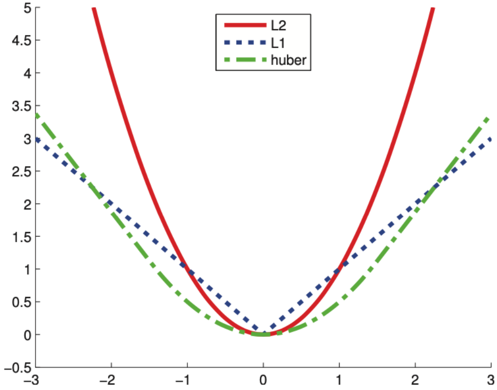
- This is called **robust regression**.

Robust Regression

Robust regression is equivalent to assuming that the response y follows a Laplace distribution.

$$p(Y|\boldsymbol{X}, \boldsymbol{\beta}, b) = \text{Laplace}(Y|\boldsymbol{X}, \boldsymbol{\beta}, b) \propto \exp(-|Y - \boldsymbol{x}^\top \boldsymbol{\beta}|/b).$$





Robust Regression

The loss function in robust regression is not differentiable at 0 and is nonlinear. Fortunately, it can be solved using linear program.

- Consider writing $\varepsilon = \varepsilon^+ - \varepsilon^-$, where $\varepsilon^+ = \max\{0, \varepsilon\}$ and $\varepsilon^- = \max\{0, -\varepsilon\}$.
- One can show that the robust regression estimation is equivalent to

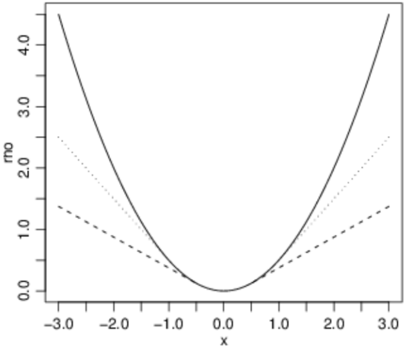
$$\begin{aligned} \widehat{\boldsymbol{\beta}}_{\text{Robust}} = \mathop{\arg\min}_{\boldsymbol{\beta}, \boldsymbol{\varepsilon}^+, \boldsymbol{\varepsilon}^-} \quad & \sum_{i=1}^{n} (\varepsilon_i^+ - \varepsilon_i^-) \\ \text{suchthat} \quad & \varepsilon_i^+ \geq 0, \varepsilon_i^- \geq 0, \boldsymbol{X}_i^\top \boldsymbol{\beta} + \varepsilon_i^+ + \varepsilon_i^- = Y_i. \end{aligned}$$

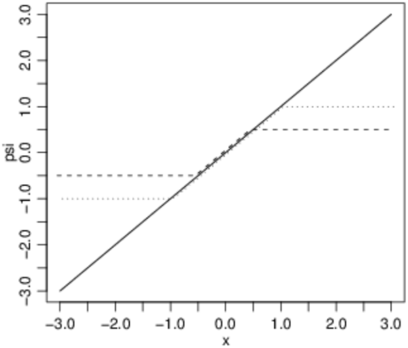
- The resulting linear program can be slow because the dimension is $p + 2n$.

Huber Regression

The loss function in robust regression is not differentiable at 0.

- A trade-off between ordinary least square and robust regression is the **Huber regression**.
- In Huber regression, the error ε is ε^2 for $\varepsilon \leq \delta$ and is $\delta|\varepsilon| - \delta^2/2$.





Robustness of the sample mean

Example: Let $X_1, \cdots, X_n$ be i.i.d. $N(\mu, \sigma^2)$. Sample mean can be obtained as the LSE for the location model $p = 1$, $X = (1, \cdots, 1)^\top$, $\beta_1 = \mu$.

$$Y = \mu + \varepsilon.$$

- We know $\bar{X}$ is a good estimator for μ under normal distribution and $\mathrm{Var}[\bar{X}_n] = \sigma^2/n$.
- If

$$X_i = \begin{cases} N(\mu, \sigma^2) & w.p.\ 1-\delta \\ f(x) & w.p.\ \delta \end{cases}$$

  and $f(x)$ has mean θ and variance τ^2.
- Then $\mathrm{Var}[\bar{X}] = (1-\delta)\sigma^2/n + \sigma\tau^2/n + \delta(1-\delta)(\theta-\mu)^2/n$.
- If $\theta \approx \mu$ and $\sigma \approx \tau$, then we are good.
- If f is Cauchy distribution, then $\mathrm{Var}[\bar{X}] = \infty$.

Median vs Mean

One can check that the median minimizes $\sum |x_i - a|$.

- Median is more robust than the mean. How about its performance?
- For $X \sim F$, we can show that $\sqrt{n}(X_{(n/2)} - \mu)$ is asymptotically normal with mean 0 and variance $1/(2f(\mu))^2$.
- The median is the obtained as the estimator of $\beta_1 = \mu$ in the robust regression for the location model $p = 1$, $X = (1, \cdots, 1)^\top$, $\beta_1 = \mu$. Robust regression is more robust than least square linear regression.
- There is a trade-off between robustness and the performance when the assumed model is correct. The median is not efficient compared to the mean.

Something in-between

Is there an estimator between the mean and the median?

- Huber estimator: minimize $\sum \rho(x_i - a)$ where

$$\rho(x) = \begin{cases} x^2/2 & |x| \le k \\ k|x| - k^2/2 & |x| \ge k \end{cases}$$

  Here ρ is differentiable.
- By tuning the parameter k, this estimator can be more "median-like" or "mean-like".
- We should expect this estimator to be asymptotically normal, because two ends (mean and median) are both so. This is indeed the case.

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Lecture notes by Prof. Kunsch and Meinshausen.