STAC67: Regression Analysis

Lecture 8

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Chapter 5: Matrix Approach to Simple Linear Regression Analysis

Matrix

- Definition: A matrix is a rectangular array of numbers or symbolic elements
- The dimension of a matrix is its number of rows and columns, often denoted as $r \times c$ (r rows by c columns)
- Can be represented in full form or abbreviated form:

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1c} \\ a_{21} & a_{22} & \dots & a_{2c} \\ \vdots & \vdots & \vdots & \vdots \\ a_{r1} & a_{r2} & \dots & a_{rc} \end{bmatrix} = [a_{ij}], \quad i = 1, \dots, r; j = 1, \dots, c$$

Special Types of Matrics

Squre Matrix: number of rows = number of columns (r = c)

Vector: matrix with one column (column vector) or one row (row vector)

$$\mathbf{D} = \left[egin{array}{c|c} d_1 \\ d_2 \\ d_3 \end{array} \right], \quad \mathbf{E}' = [17 \ 31], \quad \mathbf{F}' = [f_1 \ f_2 \ f_3]$$

Special Types of Matrices

Transponse: matrix formed by interchanging rows and columns of matrix (use "prime" to denote transpose)

$$\mathbf{G}_{2\times3} = \begin{bmatrix} 6 & 15 & 22 \\ 8 & 13 & 25 \end{bmatrix}, \quad \mathbf{G}_{3\times2}' = \begin{bmatrix} 6 & 8 \\ 15 & 13 \\ 22 & 25 \end{bmatrix}$$

Regression Example

Response Vector:
$$\mathbf{Y}_{n \times 1} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix}$$
, $\mathbf{Y}'_{1 \times n} = [Y_1 \ Y_2 \ \dots \ Y_n]$

Design Matrix:
$$\mathbf{X}_{n \times 2} = \begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots \\ 1 & X_n \end{bmatrix}$$
, $\mathbf{X'}_{2 \times n} = \begin{bmatrix} 1 & 1 & \dots & 1 \\ X_1 & X_2 & \dots & X_n \end{bmatrix}$

Matrix Addition and Subtraction

- Addition/subtraction: add (or subtract) the corresponding elements of the two matrices, defined if and only if the matrices are of the same order.
- Addition is commutative, i.e. $\mathbf{A} + \mathbf{B} = \mathbf{B} + \mathbf{A}$.
- Regression Example

$$\mathbf{Y}_{n \times 1} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix}, \quad \mathbf{E}(\mathbf{Y})_{n \times 1} = \begin{bmatrix} E(Y_1) \\ E(Y_2) \\ \vdots \\ E(Y_n) \end{bmatrix}, \quad \epsilon_{n \times 1} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

$$\mathbf{Y}_{n\times 1} = \mathbf{E}(\mathbf{Y}) + \underset{n\times 1}{\epsilon} \quad since \quad \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} E(Y_1) \\ E(Y_2) \\ \vdots \\ E(Y_n) \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix} = \begin{bmatrix} E(Y_1) + \epsilon_1 \\ E(Y_2) + \epsilon_2 \\ \vdots \\ E(Y_n) + \epsilon_n \end{bmatrix}$$

Matrix Multiplication

Multiplication of a Matrix by a Scalar (single number)

$$k = 3$$
, $\mathbf{A} = \begin{bmatrix} 2 & 1 \\ -2 & 7 \end{bmatrix} \Rightarrow k\mathbf{A} = \begin{bmatrix} 3(2) & 3(1) \\ 3(-2) & 3(7) \end{bmatrix} = \begin{bmatrix} 6 & 3 \\ -6 & 21 \end{bmatrix}$

Multiplication of a Matrix by a Matrix (# cols(A) = #rows(B))

If $c_A = r_B = c$:

$$m{A}_{r_A imes c_A r_B imes c_B} = [ab_{ij}] = \left[\sum_{k=1}^c a_{ik} b_{kj}\right] \quad i = 1, \dots, r_A; j = 1, \dots, c_B$$

- $ab_{ij} = \text{sum of the products of the c elements of } i^{th} \text{ row of } \mathbf{A} \text{ and } j^{th} \text{ column of } \mathbf{B}$

$$\mathbf{A} \mathbf{B}_{(3\times 2)(2\times 2)} = \begin{bmatrix} 2 & 5 \\ 3 & -1 \\ 0 & 7 \end{bmatrix} \begin{bmatrix} 3 & -1 \\ 2 & 4 \end{bmatrix} = \begin{bmatrix} 16 & 18 \\ 7 & -7 \\ 14 & 28 \end{bmatrix}$$

Matrix Multiplication Example

• Simultaneous Equations: $a_{11}x_1 + a_{12}x_2 = y_1$ $a_{21}x_1 + a_{22}x_2 = y_2$ $\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$

• Sum of Squares:
$$4^2 + (-2)^2 + 3^2 = \begin{bmatrix} 4 & -2 & 3 \end{bmatrix} \begin{vmatrix} 4 \\ -2 \\ 3 \end{vmatrix} = [29]$$

• Regression Equation (Expected Values):—Regression Coef - Vector

$$\text{Design Morthix} \begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots & \vdots \\ 1 & X_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} \beta_0 + \beta_1 X_1 \\ \beta_0 + \beta_1 X_2 \\ \vdots \\ \beta_0 + \beta_1 X_n \end{bmatrix}$$

Matrix Multiplication Examples

 Matrices used in simple linear regression (that generalize to multiple regression):

$$\mathbf{Y}'\mathbf{Y} = \begin{bmatrix} Y_1 & Y_2 & \dots & Y_n \end{bmatrix} \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \sum_{\mathbf{Y}'_i} \mathbf{Y}_i$$

$$\mathbf{X}'\mathbf{X} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ X_1 & X_2 & \cdots & X_n \end{bmatrix} \begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots & \vdots \\ 1 & X_n \end{bmatrix} = \begin{bmatrix} \mathbf{X} & \mathbf{X} & \mathbf{X} & \mathbf{X} \\ \mathbf{X} & \mathbf{X} & \mathbf{X} & \mathbf{X} \end{bmatrix}$$

$$\mathbf{X}'\mathbf{Y} = \begin{bmatrix} 1 & 1 & \dots & 1 \\ X_1 & X_2 & \dots & X_n \end{bmatrix} \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} \mathbf{Y}_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix}$$

Special Matrix Types

- Symmetric Matrix: Squre matrix with a transpose equal to itself: $\mathbf{A} = \mathbf{A}'$
- Diagonal Matrix: Squre matrix with all off-diagonal elements equal to 0:
- **Identity Matrix**: Diagonal matrix with all diagonal elements equal to 1 (acts like multiplying a scalar by 1)

$$\mathbf{A}_{3\times3} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$
 $\mathbf{A}_{3\times3} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$
 $\Rightarrow \mathbf{IA} = \mathbf{AI} = \mathbf{AI}$

• 1-Vector and Matrix and Zero Vector:

$$\mathbf{1}_{r\times 1} = \begin{bmatrix} 1\\1\\\vdots\\1 \end{bmatrix} \quad \mathbf{J}_{r\times r} = \begin{bmatrix} 1&\dots&1\\\vdots&\ddots&\vdots\\1&\dots&1 \end{bmatrix} \quad \mathbf{0}_{r\times 1} = \begin{bmatrix} 0\\0\\\vdots\\0 \end{bmatrix}$$

Linear Dependence and Rank of a Matrix

- Linear Dependence: When a linear function of the columns (rows) of a matrix produces a zero vector (one or more columns (rows) can be written as linear function of the other columns (rows))
- Rank of a matrix: Number of linearly independent columns (rows) of the matrix. Rank cannot exceed the minimum of the number of rows or columns of the matrix. $rank(\mathbf{A}) \leq min(r_A, c_A)$
- A matrix is full rank if $rank(A) = min(r_A, c_A)$
- Matrix Inversion

In matrix form if A is a square matrix and full rank (all rows and columns are linearly independent), then A has an inverse: A^{-1} such that:

$$A^{-1}A = AA^{-1} = I$$

Computing an Inverse of 2 X 2 Matrix

$$A_{2\times 2} = \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = \text{full rank (columns/rows are linear indepenent)}$$

Determinant of $\mathbf{A} = |\mathbf{A}| = a_{11}a_{22} - a_{12}a_{21}$

Note: If \boldsymbol{A} is not full rank then $|\boldsymbol{A}| = 0$

• **Regression Example**: find the expression for $(X'X)^{-1}$

Thus
$$(x'x)^{-1} = \frac{1}{\sqrt{S \times x}}$$
, $\begin{bmatrix} \frac{1}{2}x^{2} & -\frac{1}{2}x^{2} \\ \frac{1}{2}x^{2} & \frac{1}{2}x^{2} \end{bmatrix} = \frac{1}{\sqrt{S \times x}}$, $\begin{bmatrix} \frac{1}{2}x^{2} & -\frac{1}{2}x^{2} \\ -\frac{1}{2}x^{2} & \frac{1}{2}x^{2} \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{S \times x}} & -\frac{1}{2}x^{2} \\ -\frac{1}{2}x^{2} & \frac{1}{2}x^{2} \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{S \times x}} & -\frac{1}{2}x^{2} \\ -\frac{1}{2}x^{2} & \frac{1}{2}x^{2} \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{S \times x}} & -\frac{1}{2}x^{2} \\ -\frac{1}{2}x^{2} & \frac{1}{2}x^{2} \end{bmatrix}$

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Useful Matrix Results

Addition Rules:

$$A + B = B + A$$
, $(A + B) + C = A + (B + C)$

Multiplcation Rules:

$$(AB)C = A(BC), \quad C(A+C) = CA+CB, \quad k(A+B) = kA+kB, k = scalar$$

Transpose Rules:

$$(A')' = A, (A+B)' = A' + B', (AB)' = B'A', (ABC)' = C'B'A'$$

Inverse Rules (Full Rank, Square Matrices)

$$(\mathbf{A}\mathbf{B})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}, (\mathbf{A}\mathbf{B}\mathbf{C})^{-1} = \mathbf{C}^{-1}\mathbf{B}^{-1}\mathbf{A}^{-1}, (\mathbf{A}^{-1})^{-1} = \mathbf{A}, (\mathbf{A}')^{-1} = (\mathbf{A}^{-1})'$$

Useful Matrix Resuls

• Properties of the determinant:

• Properties of the trace:

def (c Anxn) = c det (A)

Random Vectors and Matrices

- Shown for case of n = 3, generalies to any n:
- Random variables: $Y_1, Y_2, Y_3 \Rightarrow \mathbf{Y} = \begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \end{bmatrix}$ with expectation: $\mathbf{E}(\mathbf{Y}) = \begin{bmatrix} E(Y_1) \\ E(Y_2) \\ E(Y_3) \end{bmatrix}$
- Variance-covariance Matrix:

$$\sigma^{2} \mathbf{Y} = E \left[(\mathbf{Y} - E(\mathbf{Y}))(\mathbf{Y} - E(\mathbf{Y}))' \right] =$$

$$E \left[\begin{bmatrix} Y_{1} - E(Y_{1}) \\ Y_{2} - E(Y_{2}) \\ Y_{3} - E(Y_{3}) \end{bmatrix} \left[Y_{1} - E(Y_{1}) \quad Y_{2} - E(Y_{2}) \quad Y_{3} - E(Y_{3}) \right] \right] =$$

$$\begin{bmatrix} (\circ \vee (Y_{1}, Y_{1}) & \cdots & C_{0} \vee (Y_{2}, Y_{3}) \\ \vdots & \vdots & \vdots & \vdots \\ (Y_{2}, Y_{1}) & \cdots & C_{0} \vee (Y_{2}, Y_{3}) \end{bmatrix}$$

$$= \begin{bmatrix} 6^{2} & \circ & \circ \\ \circ & 6^{2} & \circ \\ \circ & 6^{2} & \circ \\ \circ & 6^{2} & \circ \end{bmatrix}$$

$$= \begin{bmatrix} 6^{2} & \circ & \circ \\ \circ & 6^{2} & \circ \\ \circ & 6^{2} & \circ \\ \circ & 6^{2} & \circ \end{bmatrix}$$

$$= \begin{bmatrix} 6^{2} & \circ & \circ \\ \circ & 6^{2} & \circ \\ \circ & 6^{2} & \circ \\ \circ & 6^{2} & \circ \end{bmatrix}$$

$$= \begin{bmatrix} 6^{2} & \circ & \circ \\ \circ & 6^{2} & \circ \\ \circ & 6^{2} & \circ \\ \circ & 6^{2} & \circ \end{bmatrix}$$

$$= \begin{bmatrix} 6^{2} & \circ & \circ \\ \circ & 6^{2} & \circ \\ \circ & 6^{2} & \circ \\ \circ & 6^{2} & \circ \end{bmatrix}$$

Simple Linear Regression in Matrix form

- Simple Linear regression Model: $Y_i = \beta_0 + \beta_1 X_i + \epsilon_i$, i = 1, ..., n

• Define:
$$y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$
 response vector $\hat{B} = \begin{bmatrix} B_0 \\ B_1 \end{bmatrix}$ repression cost vector

$$X = \begin{bmatrix} 1 & X_1 \\ \vdots & \vdots \\ 1 & X_n \end{bmatrix}$$
 design $X = \begin{bmatrix} 2 & 1 \\ \vdots & \vdots \\ 2 & \vdots \\ 2 & \vdots \end{bmatrix}$ error vector

• Assuming constant variance and independence of error term, ϵ_i :

$$\sigma^{2}(\underline{Y}) = \sigma^{2}(\underline{\epsilon}) = G^{2} I_{1m} \text{ as shown above}$$

$$E(\underline{Y}) = E(\underline{XB} + \underline{\hat{\epsilon}}) = \underline{XB}$$

• Further, assuming normal distribution for error tersm,
$$\epsilon_i$$
: $\frac{1}{2} \sim N(0, 6^2 \text{T}) \qquad \forall \sim N(\times \text{R}, 6^2 \text{T})$

Estimating Parameters by Least Squares

Mimimizing the sum of squares of errors:

$$Q(\underline{\beta}) = \sum_{i=1}^{n} \epsilon_{i}^{2} = \underline{\epsilon}' \underline{\epsilon} = (\underline{Y} - \mathbf{X}\underline{\beta})' (\underline{Y} - \mathbf{X}\underline{\beta})$$

- Normal equations:

$$\begin{bmatrix} n & \sum_{i} X_i \\ \sum_{i} X_i & \sum_{i} X_i^2 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} \sum_{i} Y_i \\ \sum_{i} X_i Y_i \end{bmatrix}, \text{ or } (\mathbf{X}'\mathbf{X})\underline{\beta} = \mathbf{X}'\underline{y};$$

The soltion of
$$\beta$$
 is given by:
$$\widehat{\beta} = (x'x)^{-1}x'\hat{y}$$

Note: (X'X) should be invertable, full rank.

• Find $(\mathbf{X}'\mathbf{X})^{-1}$.

• Find $(X'X)^{-1}(X'y)$. Check whether these estiamtes agrees with $\hat{\beta}_0, \hat{\beta}_1$

Fitted Values and Residuals

$$\hat{e} = \begin{bmatrix} e_1 \\ \vdots \\ e_n \end{bmatrix} = \begin{bmatrix} Y_1 - \hat{Y}_1 \\ \vdots \\ Y_n - \hat{Y}_n \end{bmatrix} = Y - \hat{Y} = Y - X \hat{\beta}$$

$$\hat{Y} = X \hat{\beta} = X(X'X)^{-1} X' Y = HY, \quad H = X(X'X)^{-1} X'$$
Tabled the last or projection matrix. Note that H is identically

- H is called the **hat** or **projection** matrix. Note that H is idempotent matrix (HH = H) $V_{\alpha}(y) (I - H)^{I}$

$$\hat{e} = \hat{Y} - H\hat{Y} = (I - H)\hat{Y}
\hat{\sigma}^{2} = \frac{1}{n-2} \sum_{i=1}^{n} e_{i}^{2} = \frac{1}{n-2} \hat{e}' \hat{e}
(X'X)\hat{\beta} = X'\hat{Y}
\hat{X} = \hat{A} =$$

Inferences in Linear Regression

$$\hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'Y$$

$$E(\hat{\beta}) = E((\mathbf{x}'\mathbf{x})'\mathbf{x}'\mathbf{y}) = (\mathbf{x}'\mathbf{x})'\mathbf{x}'\mathbf{x} \hat{\beta} = \hat{\mathbf{x}}$$

$$\sigma^{2}(\hat{\beta}) = (\mathbf{x}'\mathbf{x})'\mathbf{x}' \hat{\delta}^{2} + \mathbf{x}(\mathbf{x}'\mathbf{x})'' = \hat{\delta}^{2}(\mathbf{x}'\mathbf{x})^{-1}$$

$$\hat{\sigma}^{2}(\hat{\beta}) = MSE(\mathbf{x}'\mathbf{x})''$$

Reall:

$$(\mathbf{X}'\mathbf{X})^{-1}\sigma^{2} = \begin{bmatrix} V\omega(\hat{\mathbf{G}}_{1}) & Gov(\mathcal{B}_{2},\mathcal{B}_{1}) \\ Gov(\hat{\mathcal{B}}_{1},\mathcal{B}_{1}) & V\omega(\hat{\mathcal{B}}_{1}) \end{bmatrix} = \begin{bmatrix} \frac{1}{n} + \frac{\chi}{S_{xx}} & \frac{-\chi}{S_{xx}} \\ \frac{-\chi}{S_{xx}} & \frac{1}{S_{xx}} \end{bmatrix} b^{2}$$

- The diagonal elements of this matrix gives $Var(\hat{\beta}_0)$ and $Var(\hat{\beta}_1)$.
- Off diagonal elements gives $Cov(\hat{\beta}_0, \hat{\beta}_1)$

Chapter 6: Mutiple Regression I

Models with Multiple Predictors

- Most Practical Problems have more than one potential predictor variable
- Goal is to determine effects (if any) of each predictor, controlling for others
- Can include polynomial terms to allow for nonlinear relations
- Can include product terms to allow for interactions when effect of one variable depends on level of another variable
- Can include "dummy" variables for categorical predictors
- First-Order Model with 2 Numeric Predictors

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \epsilon \Rightarrow E(Y) = \beta_0 + \beta_1 X_1 + \beta_2 X_2$$

Example - Multiple Regression with Two predictor Variable

- This dataset, which can be found at <u>UCI Machine Learning Repository</u> contains a response variable **mpg** which stores the city fuel efficiency of cars, as well as several predictor variables for the attributes of the vehicles. we would like to model the fuel efficiency (mpg) of a car as a function of its weight (**wt**) and model year (**year**).

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \epsilon_i, \quad i = 1, 2, \dots, n, \quad where \ \epsilon_i \sim N(0, \sigma^2)$$

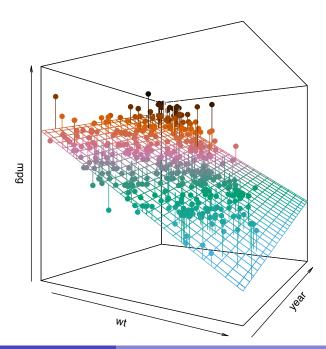
```
##
## Call:
## lm(formula = mpg ~ wt + year, data = autompg)
##
## Residuals:
             1Q Median
     Min
## -8.852 -2.292 -0.100 2.039 14.325
##
## Coefficients:
##
                Estimate Std. Error t value Pr(>|t|)
## (Intercept) -1.464e+01 4.023e+00 -3.638 0.000312 ***
              -6.635e-03 2.149e-04 -30.881 < 2e-16 ***
## wt
              7.614e-01 4.973e-02 15.312 < 2e-16 ***
## vear
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
```

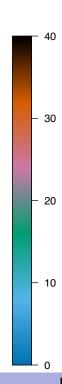
3-dimensional image

• what happens if we fit two simple regressions?

```
## 46.198395049 -0.007643021
## (Intercept) year
## -70.155395 1.231997
```

(Intercept)





Interpretation of regression parameters

- ① Change of E(Y) per unit corresponding to a unit change in X_j , $j=1,\ldots,p$ when other predictor variables are held constant.
- 2 β_2 : effect of X_2 after adjusting for X_1
- 3 β_1 : effect of X_1 after **adjusting** for the effect of X_2
- If X_1 and X_2 are **uncorrelated** then the estimates will be the same as the estimates in the simple models but in general, this is not true.
- Consider the following sequence of model:
- **1** Fit a simple linear model between Y and X_1 , and find the residual, e_1 .
- 2 Fit a regression with X_2 as a response and X_1 as a covariate and find the residual, e_2 .
- **3** Fit a regression with e_1 as a response and e_2 as a covariate.

Fit a simple regression between Y and X1 and find e1