

*Linear Algebra*

# ***General Linear Models and Least Squares***

Automotive Intelligence Lab.



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- General linear models
- Solving GLMs
- GLM in a simple example
- Least squares via QR
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# General Linear Models

# General Linear Model

## ■ Statistical model (data-driven model)

- ▶ A set of equations that **relates** predictors to observations.
  - Predictors: independent variable.
  - Observations: dependent variable.

## ■ Example of the model in stock market price

- ▶ Independent variable: time
- ▶ Dependent variable: stock market price

## ■ We will focus on General Linear Model, which is called as GLM.

- ▶ **Regression** is a type of GLM, for example.

# Terminology of GLM

## ■ Difference terminology between fields of statistics and linear algebras

LinAlg	Stats	Description
$Ax = b$	$X\beta = y$	General Linear Model(GLM)
$A$	$X$	<b>Design matrix</b> (columns=independent variables, predictors, regressors)
$x$	$\beta$	Regression coefficients or beta parameters
$b$	$y$	<b>Dependent variable</b> , outcome measure, <b>data</b>

Table of terms in GLMs

# Setting up a GLM

## ■ Process to set up GLM

1. **Define an equation** that relates the predictor variables to the dependent variable.
2. **Map** the observed data onto the equations.
3. **Transform** the series of equations into a matrix equation.
4. **Solve** that equation.

# Simple Example to Explain Process of GLM

- **Model:** Predicts adult height based on weight and parent's height

$$y = \beta_0 + \beta_1 w + \beta_2 h + \epsilon$$

Equation of example model

- ▶  $y$ : height of an individual
  - ▶  $w$ : weight
  - ▶  $h$ : parents' height (average of mother and father)
  - ▶  $\epsilon$ : error term (also called residual)
- 
- **Why we need error term  $\epsilon$  (residual)?**
    - ▶ Weight and parents' height cannot perfectly determine an individual's height.
    - ▶ Variance not attributable to weight and parents' height will be absorbed by residual.
      - Such as growing environment, sleeping time and so on.

# More Explanation about Previous Simple GLM

## ■ What is $\beta$ ?

- ▶ Coefficients or weights.
- ▶ Describe how to combine weight and parent's height to predict an individual's height.
- ▶  $\beta_0$ ?
  - Called an intercept or a constant.
  - Without this term, best-fit line always pass the origin.
    - It will be explained at the end of chapter.

$$y = \beta_0 + \beta_1 w + \beta_2 h + \epsilon$$

Previous GLM model

## ■ After defining equations, map the observed data onto the equations.

- ▶ Use the simple data table below.
- ▶ For simplicity, omit  $\epsilon$ .

$y$	$w$	$h$
175	70	177
181	86	190
159	63	180
165	62	172

Simple data table

$$\begin{aligned}
 175 &= \beta_0 + 70\beta_1 + 177\beta_2 \\
 181 &= \beta_0 + 86\beta_1 + 190\beta_2 \\
 159 &= \beta_0 + 63\beta_1 + 180\beta_2 \\
 165 &= \beta_0 + 62\beta_1 + 172\beta_2
 \end{aligned}
 \rightarrow
 \begin{bmatrix} 1 & 70 & 177 \\ 1 & 86 & 190 \\ 1 & 63 & 180 \\ 1 & 62 & 172 \end{bmatrix}
 \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}
 =
 \begin{bmatrix} 175 \\ 181 \\ 159 \\ 165 \end{bmatrix}$$

Transforming series of equations into a matrix equation

## ■ Of course, we can express this equation briefly as $X\beta = y$ .



# Solving GLMs



# Idea to Solve for the Vector of Unknown Coefficients $\beta$

Method 1

- Simply **left-multiply** both sides of the equation by **left-inverse of  $X$** .

$$\begin{aligned}X\beta &= y \\(X^T X)^{-1} X^T X\beta &= (X^T X)^{-1} X^T y \\ \beta &= (X^T X)^{-1} X^T y\end{aligned}$$

Solution to solve  $\beta$

- **Memorize  $\beta = (X^T X)^{-1} X^T y$** 
  - ▶ Also called **least squares solution**.
  - ▶ One of the most important mathematical equations in applied linear algebra.

# Code Exercise of Left-Multiply to Solve Least Squares

## ■ Code Exercise (11\_01)

- ▶ Simply left-multiply both sides of the equation.
- ▶ Variable  $X$ : design matrix
- ▶ Variable  $y$ : data vector

```
% Clear workspace, command window, and close all figures
clc; clear; close all;

% Define a matrix X and y
X = [7; 5; 6];
y = [4; 7; 8];

% Compute the left-inverse of X
X_leftinv = ;

% Calculate beta
beta = ;
disp("beta");
disp(beta);
```

MATLAB code to solve least squares using left-multiply

# Is the Solution Exact?

## Method 2

### ■ When is equation $X\beta = y$ exactly solvable?

- ▶ In case of  $y$  is in the column space of design matrix  $X$ .
- ▶ Then, question would be
  - Whether data vector is guaranteed to be in the Column Space of design matrix.
- ▶ Answer is "No"
  - There is no such guarantee.
  - Data vector  $y$  is almost never in the column space of  $X$ .

# Why is Data Vector Not Guaranteed?

## ■ Imagine a survey of university students.

- ▶ Researchers are trying to predict average GPA based on drinking behavior.
- ▶ Survey may contain data from 2000 students.
- ▶ But questions are only 3.
  - How much alcohol do you consume?
  - How often do you black out?
  - What is your GPA?

## ■ Data will be contained in a $2000 \times 3$ table.

- ▶ 3 questions for 2000 students.
- ▶ Column space of the **design matrix**
  - $2D$  subspace inside that  $2000D$  ambient dimensionality.
  - Question of “How much alcohol do you consume?” and “How often do you black out?”
- ▶ **Data vector**
  - $1D$  subspace inside that same ambient dimensionality.
  - Question of “What is your GPA?”

# Meaning of Data in the Column Space of Design Matrix

- “**Data vector** in the column space” means that matrix model accounts for 100% of the variance of data.
  - ▶ This almost never happens.
  - ▶ Real world data contains **noise** and **sampling variability**.
  - ▶ Models are simplifications that don't account for all of variability.
    - GPA is determined by myriad factors that our model ignores.

# Solution to this Conundrum (수수께끼)

- Modify GLM equation to allow for a discrepancy between model predicted data and observed data.

- ▶ It can be expressed in several equivalent ways as below.

$$X\beta = y + \epsilon$$

$$X\beta - \epsilon = y$$

$$\epsilon = X\beta - y$$

three equivalent expressions

- ▶ Interpretation of the **first equation**.
  - $\epsilon$  is residual, or an error term.
  - Added to the data vector.
  - So that it fits inside the column space of the design matrix.
- ▶ Interpretation of the **second equation**.
  - Residual term is an adjustment to the design matrix.
  - So that it fits the data perfectly.
- ▶ Interpretation of the **third equation**.
  - Residual is defined as the difference between model-predicted data and observed data.

# Point of This Section

## ■ Observed data is **almost never inside** the subspace spanned by regressors.

▶ Reason why we can easily see GLM expressed as  $X\beta = \hat{y}$ , not  $X\beta = y$ .

- $\hat{y} = y + \epsilon$

## ■ Goal of the GLM


▶ To find linear combination of the regressors.

▶ **Close as possible** to the observed data.



# Geometric Perspective on Least Squares

## ■ Consider column space of design matrix $\mathcal{C}(X)$ is a subspace of $\mathbb{R}^M$ .

- ▶ It's typically a very low-dimensional subspace.
  - It means  $N \ll M$ .
  - Statistical models tend to have much more observations ( $M$ , rows) than predictors ( $N$ , columns).
- ▶ Dependent variable is vector  $y \in \mathbb{R}^M$ .
- ▶ Questions:
  - Is vector  $y$  in the column space of the design matrix? 
  - If not, what coordinate inside the column space of the design matrix is as close as possible to data vector?

# Abstracted Geometric View of GLM

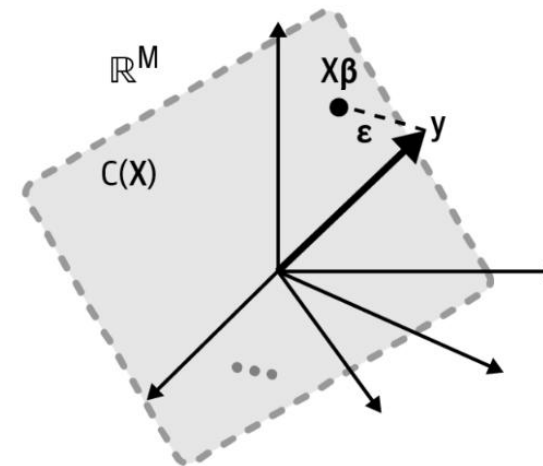
## ■ Our goal: find set of coefficients $\beta$

- ▶ Weighted combination of columns in  $X$  minimizes distance to data vector  $y$ .
- ▶ We can call projection vector  $\epsilon$ .
- ▶ How can find vector  $\epsilon$  and coefficients  $\beta$  ?
  - Use orthogonal vector projection!
- ▶ Key insight
  - Shortest distance between  $y$  and  $X$  is given by the projection vector  $y - X\beta$  that meets  $X$  at a right angle as shown in below equation.

## ■ We have rederived the same left-inverse solution which we got from the algebraic approach.

$$\begin{aligned}
 X^T \epsilon &= 0 \\
 X^T (y - X\beta) &= 0 \\
 X^T y - X^T X\beta &= 0 \\
 X^T X\beta &= X^T y \\
 \beta &= (X^T X)^{-1} X^T y
 \end{aligned}$$

Equation expansion



Abstracted geometric view of GLM

# Meaning of Least Squares

## Method 3

### ■ Why is it called “least squares”?

#### ▶ Squares

- Squared **errors** between predicted data and observed data
- There is an error term for each  $i^{th}$  predicted data point.
  - Defined as  $\epsilon_i = X_i\beta - y_i$ .
- Each data point is predicted using same set of coefficients.
  - Same weights for combining predictors in design matrix.
- So, we can capture all errors in one vector:  $\epsilon = X\beta - y$ .

#### ▶ If model is a good fit to the data,

- Errors  $\epsilon$  should be small.

#### ▶ Objective of model fitting

- Choose elements in  $\beta$  that **minimize elements in  $\epsilon$** .

# Expression of Least Squares

- ▶ If just minimizing errors,
  - It cause the model to predict values toward negative infinity.
- ▶ Instead, minimizing squared errors
  - Corresponding to their geometric squared distance to observed data  $y$ .
  - Regardless of whether prediction error itself is positive or negative.
- ▶ Same as minimizing the squared norm of the errors.
  - Hence named “least square”.
  - Leads to the following modification:

$$\|e\|^2 = \|X\beta - y\|^2$$

Expression of least squares

# View Least Squares as Optimization Problem

## ■ Find set of coefficients $\beta$ that minimizes squared errors.

- ▶ Minimization can be expressed as follows:

$$\min_{\beta} \|X\beta - y\|^2$$

Minimization

- ▶ Solution to this optimization

- Can be found by setting derivative of objective to zero.
- Applying a bit of differential calculus and a bit of algebra.

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

$$0 = X^T X\beta - X^T y$$

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

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

Solution of optimization

- ▶ Rediscover same solution that reached simply by using our linear algebra intuition!

- Although started from a different perspective to minimize the squared distance between the model-predicted values and the observed values.

# Visualization Intuition for Least Squares

## ■ Black squares

- ▶ Observed data

## ■ Gray dots

- ▶ Model predicted values

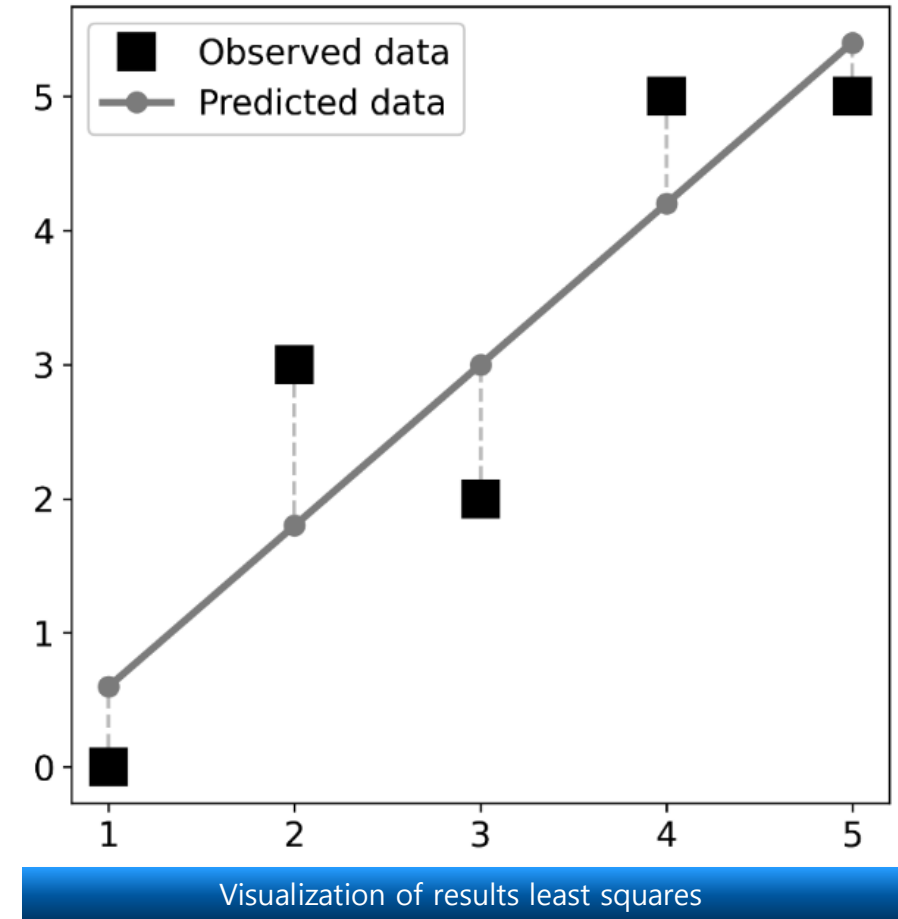
## ■ Gray dashed lines

- ▶ Distances between observed data and model predicted values

## ■ All model predicted values lie on a line.

## ■ Goal of least squares

- ▶ Find slope and intercept!
  - Minimize distance from predicted to observed data.



# All Roads Lead to Least Squares

- **You've now seen three ways.**
  - ▶ To derive least squares solution.
- **Remarkably, all approaches lead to same conclusion.**
  - ▶ Left-multiply both sides of GLM equation by left-inverse of design matrix  $X$ .
- **Different approaches have unique theoretical perspectives.**
  - ▶ Provide insight into nature and optimality of least squares.
- **But it is a beautiful thing.**
  - ▶ No matter how you begin your adventure into linear model fitting.
  - ▶ Because you end up at same conclusion.

# GLM in a Simple Example



# GLM in a Simple Example

$$X\beta = y$$

## ■ Example

- ▶ Report the number of online courses they took and their general satisfaction with life.
- ▶ Experiment which is surveyed a random set of 20 students.

■ Table 1. shows first 4 (out of 20) rows of data matrix.

■ Data is easier to visualize in scatterplot as Fig 1..

- ▶ Notice that independent variable is plotted on the x-axis.
  - While dependent variable is plotted on the y-axis.
  - That is common convention in statistics.

Number of courses	Life happiness
4	25
12	54
3	21
14	80

Table 1. Data table

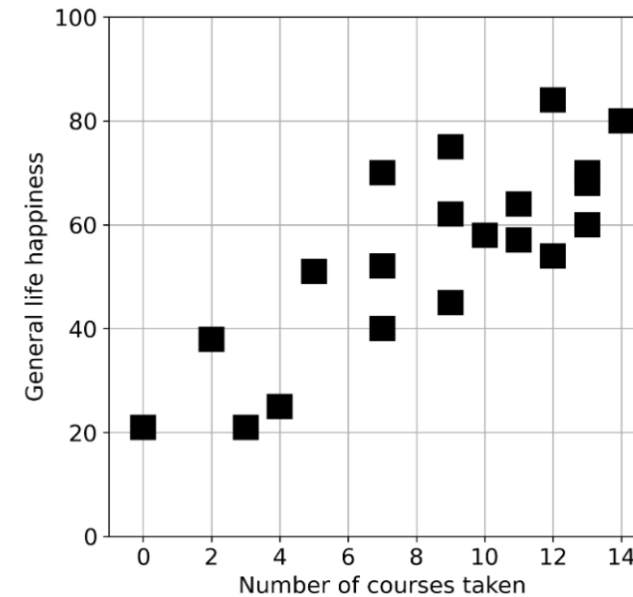


Fig 1. Fake data from fake survey

# Create Design Matrix

- Design matrix is actually only one column vector.
  - ▶ Because this is a simple model with only one predictor.
- Matrix equation  $X\beta = y$  looks like Eq 1. (Only first four data values).

$$\begin{bmatrix} 4 \\ 12 \\ 3 \\ 14 \end{bmatrix} [\beta] = \begin{bmatrix} 25 \\ 54 \\ 21 \\ 80 \end{bmatrix}$$

Eq 1. Matrix equation  $X\beta = y$

# Code Exercise of Creating Design Matrix

## Code Exercise (11\_02)

- ▶ Follow the previous slide.
- ▶ The matrix equation looks like a form of  $X\beta = y$ .

```
% Clear workspace, command window, and close all figures
clc; clear; close all;

% Define a matrix number of courses and life happiness
X = [4,12,3,14,13,12,9,11,7,13,11,9,2,5,7,10,0,9,7,13]'; % number of course
y = [25,54,21,80,68,84,62,57,40,60,64,45,38,51,52,58,21,75,70,70]'; % life happiness

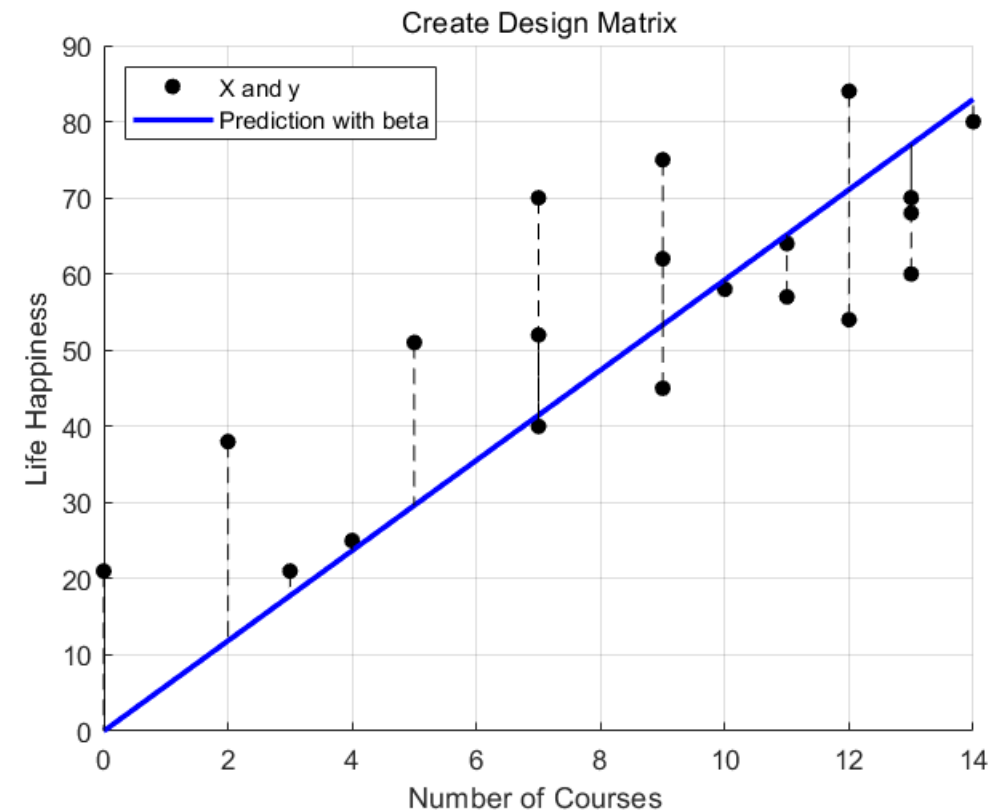
% Compute the left-inverse of X
X_leftinv = ;

% Calculate beta
beta = ;
disp("beta");
disp(beta);

% Calculate y_pred with beta
y_pred = ;

% Plot
figure;
hold on;
grid on;
scatter(X, y, 'k', 'filled'); % X and y
plot(X, y_pred, 'b', 'LineWidth', 2); % Plot predicted line with beta
for i = 1:length(X)
    plot([X(i) X(i)], [y(i) y_pred(i)], 'k--'); % Plot residuals as dashed lines
end
title('Create Design Matrix');
xlabel('Number of Courses ');
ylabel('Life Happiness');
legend('X and y', 'Prediction with beta', 'Location', 'northwest');
hold off;
```

MATLAB code of creating design matrix



Result of code

# Meaning of Least Squares Formula's Result

■ Following least squares formula tells  $\beta = 5.92$ .

■ What does this number mean?

▶ It means Slope in formula.

- For each additional course that someone takes, their self-reported life happiness increases by 5.92 points.

■ Let's see how that result looks in plot as Fig 1..

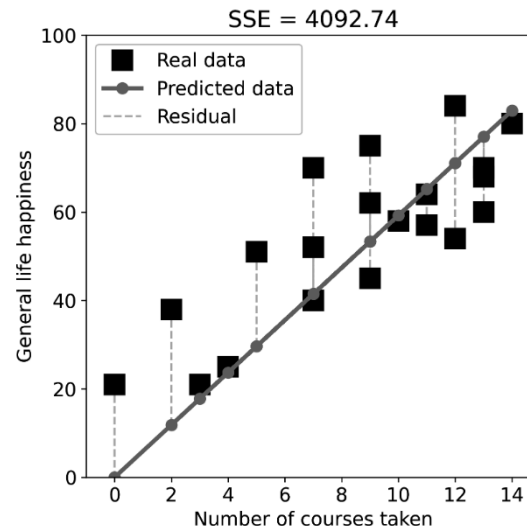
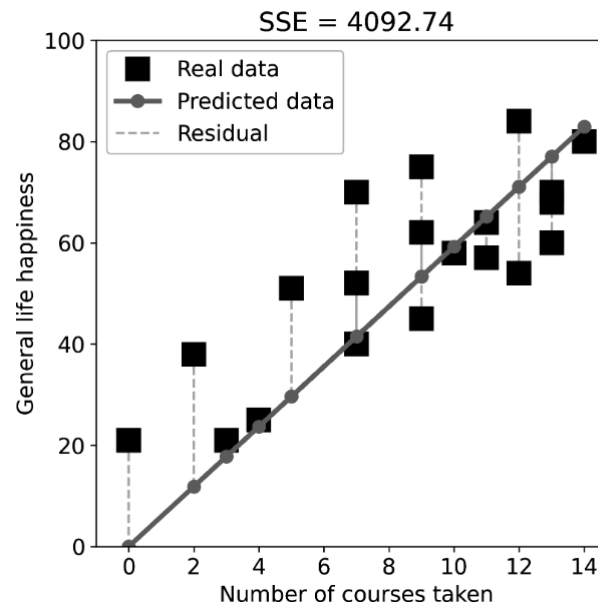


Fig 1. Observed and predicted data (SSE=sum of squared errors)

# Feeling of Unease While Looking at Fig 1.

- If you experience feeling of unease while looking at Fig 1.,
  - ▶ Then, that's good signal!
    - It means you are thinking critically and noticed that **model doesn't do great job at minimizing errors.**
  - ▶ You can easily imagine pushing left side of best-fit line up to get better fit.
- What's the problem here in term of mathematics?



$$y = ax$$
$$y = ax + b$$

Fig 1. Observed and predicted data

# Problem in Fig 1.

## ■ Design matrix contains no intercept

► Equation of the best-fit line is  $y = mx$ .

- Which means  $x = 0, y = 0$ .
- That constraint doesn't make sense for this problem.
  - Because it means anyone who doesn't take courses is completely devoid of life satisfaction.

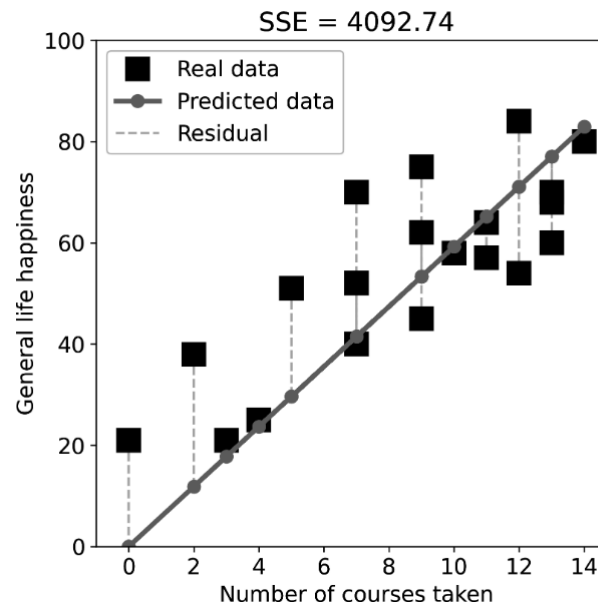


Fig 1. Observed and predicted data

# Add Intercept Term

■ In form of  $y = mx + b$ .

▶  $b$  is **intercept** term.

- Allows the best-fit line to cross the  $y$ -axis at any value.

↪  $\frac{1}{2}$ 항

$$y = \beta_2 x + \beta_1$$

$$y = \beta_1 + \beta_2 x + \beta_3 \dots$$

■ **Statistical interpretation of intercept**

▶ Expected numerical value of observations when predictors are set to zero.

■ **Adding intercept term to design matrix as below Eq 1.**

▶ Only showing first four rows.

■ **Code doesn't change with one exception of creating design matrix.**

$$\begin{bmatrix} 1 & 4 \\ 1 & 12 \\ 1 & 3 \\ 1 & 14 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} = \begin{bmatrix} 25 \\ 54 \\ 21 \\ 80 \end{bmatrix}$$

Eq 1. Adding intercept term at design matrix

# Code Exercise to Add Intercept Term

## Code Exercise (11\_03)

- ▶ Code is same with **Code Exercise (11\_02)** with one exception.
- ▶ The difference is design matrix.
- ▶ Add intercept term in design matrix following the previous slide.

```
% Clear workspace, command window, and close all figures
clc; clear; close all;

% Define a matrix number of courses and life happiness
number_of_course = [4,12,3,14,13,12,9,11,7,13,11,9,2,5,7,10,0,9,7,13]';
life_happiness = [25,54,21,80,68,84,62,57,40,60,64,45,38,51,52,58,21,75,70,70]';

% Define a new design matrix X that contains the intercept term and
% dependent variable matrix y
X = ; % Use number_of_course
y = ;

% Compute the left-inverse of X
X_leftinv = ;

% Calculate the beta
beta = ; % [beta0 beta1]
beta = flip(beta); % [beta1 beta0]
y_pred = polyval(beta, number_of_course); % Predict y values using
beta

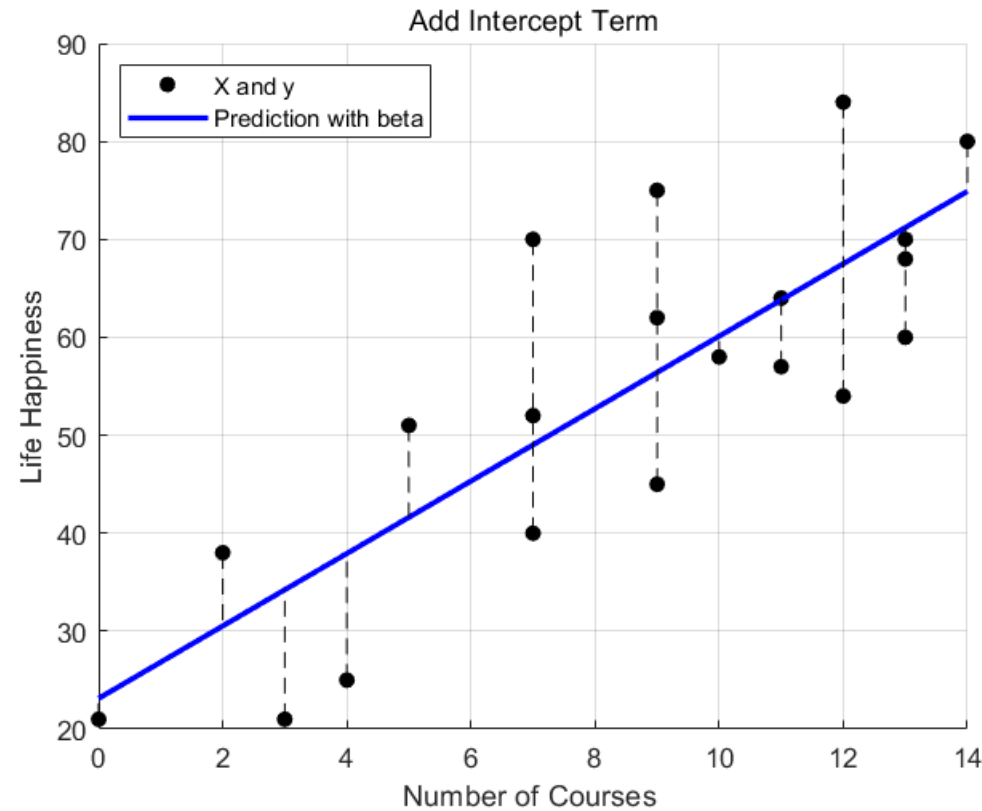
% Plot
figure;
hold on;
grid on;
scatter(number_of_course, y, 'k', 'filled'); % X and y
plot(number_of_course, y_pred, 'b', 'LineWidth', 2); % Plot predicted
line with beta
for i = 1:length(X)
    plot([number_of_course(i) number_of_course(i)], [y(i) y_pred(i)],
    'k--'); % Plot residuals as dashed lines
end
title('Add Intercept Term');
xlabel('Number of Courses ');
ylabel('Life Happiness');
legend('X and y', 'Prediction with beta', 'Location', 'northwest');
hold off;
```

MATLAB code to add Intercept term



# Visual result of Code Exercise

## Code Exercise (11\_03)



Visual result of code exercise (11\_03)

# Result of Including Intercept Term

- Now,  $\beta$  is two-element vector [23.1, 3.7].
  - ▶ Expected level of happiness for someone who has taken zero courses is 23.1.
  - ▶ For each additional course someone takes, their happiness increase by 3.7 points.
- You will agree that Fig 2. looks much better than Fig 1..
  - ▶ And SSE is around half of what it was when we excluded intercept.

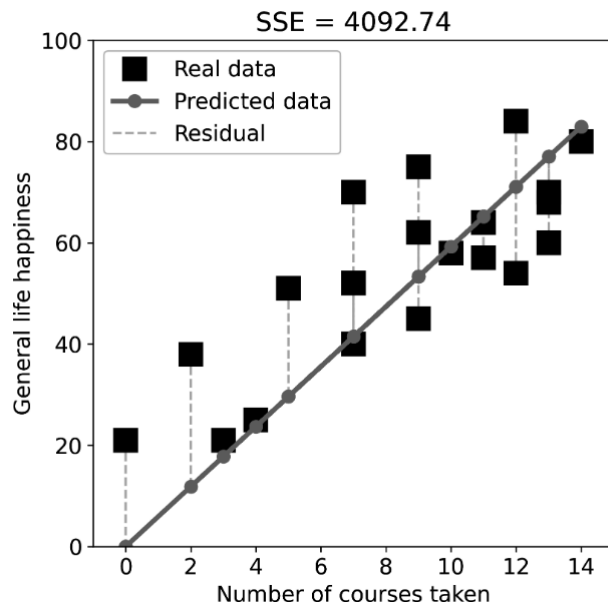


Fig 1. Observed and predicted data

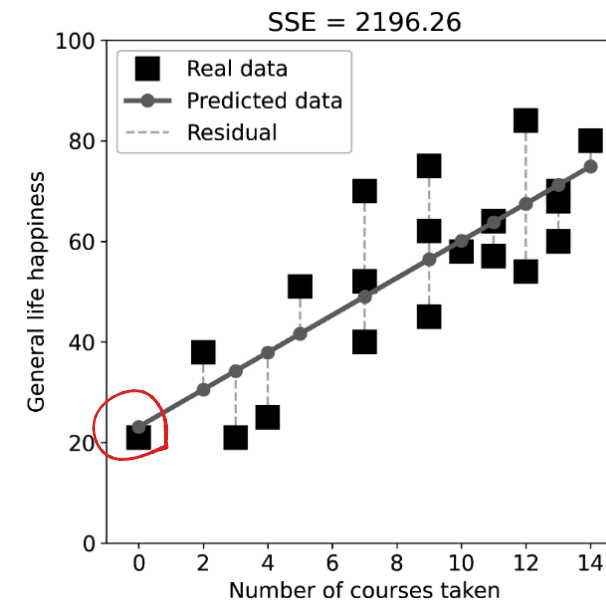


Fig 2. Observed and predicted data, with an intercept term

# Least Squares via QR

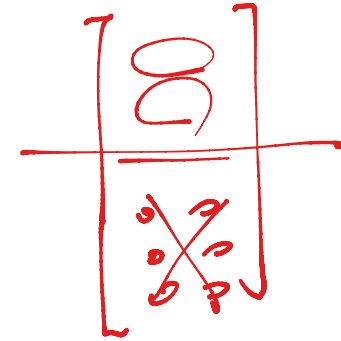
# Problem of Left-Inverse

- Left-inverse method is theoretically reasonable but risks **numerical instability**.
  - ▶ Because of computing **matrix inverse** which can be numerically unstable.
  - ▶ Matrix  $X^T X$  itself can introduce difficulties.
    - Multiplying matrix by its transpose has implications.
      - Properties such as norm and condition number which you will learn more later.
    - Matrices with high condition number can be numerically unstable.
      - Thus, design matrix with high condition number will become even less numerically stable when squared.

# Stable Way to Solve Least Squares Problem

- QR decomposition for Tall (and therefore noninvertible) matrix.

	$X$	$Q$	$Q^T Q$	$Q Q^T$	$R$
Tall "full"	$M > N$ $r = K$	$M \times M$ $r = M$	$I_M$	$I_M$	$M \times N$ $r = k$



- Observe following sequence of equations as Eq 1.

- ▶  $R$  is same shape as  $X$ .
- ▶ Although only first  $N$  rows are nonzero.
  - Rows  $N + 1$  through  $M$  do not contribute to the solution.
- ▶ Those rows can be removed from  $R$  and  $Q^T y$ .

$$X \rightarrow QR$$

$$\begin{aligned}
 X\beta &= y \\
 QR\beta &= y \\
 R\beta &= Q^T y \\
 \beta &= R^{-1} Q^T y
 \end{aligned}$$

Eq 1. Sequence of equation

$$Q^T = Q^T$$

# Code Exercise of QR decomposition to Solve Least Squares

## ■ Code Exercise (11\_04)

- ▶ With **Code Exercise (11\_01)**, you solved least squares problem with left-inverse of X.
- ▶ Now, solve least squares problem with QR decomposition and compare the beta coefficients of two methods.
- ▶ Refer to page 37.

```
% Clear workspace, command window, and close all figures
clc; clear; close all;

% Matrix A
nNumOfVariables = 3;
nNumOfData = 10;

X = randi(20, [nNumOfData, nNumOfVariables]);
y = randi(20, [nNumOfData, 1]);

%%%%%%%%% TODO %%%%%%%%%%
% Compare beta from leftinv and QR decomposition

% Beta from LeftInv
Beta_from_LeftInv = ;

% Beta from QR decomposition
[Q,R] = ; % Full QR decomposition
Q_t_y = ;
Beta_from_QR = ;
%%%%%%%%% %%%%%%%%%%
```

```
% Display the results
disp("X")
disp(X);
disp("y")
disp(y);

disp("Q")
disp(Q);
disp("R")
disp(R);
disp("Q*R")
disp(Q*R);

disp("Beta_from_LeftInv")
disp(Beta_from_LeftInv);

disp("Beta_from_QR")
disp(Beta_from_QR);
```

MATLAB code to solve least squares with QR decomposition

# Best Part of Eq 1.

## ■ Unnecessary to invert $R$ .

- ▶ Matrix is upper triangular
- ▶ Therefore, solution can be obtained via back substitution.
  - As solving simultaneous equations via Gauss-Jordan method.
    - Augment coefficients matrix by constants.
    - Reduce row to obtain RREF.
    - Extract solution from final column of augmented matrix.

$$\begin{aligned}
 X\beta &= y \\
 QR\beta &= y \\
 R\beta &= Q^T y \\
 \beta &= R^{-1} Q^T y
 \end{aligned}$$

Eq 1. Sequence of equation

# Summary



# Summary

## ■ GLM is a statistical framework.

- ▶ To understand our rich and beautiful universe.
- ▶ Works by setting up simultaneous equations.
  - Like that you learned about in previous lecture.

## ■ Different terms between linear algebra and statistics

- ▶ Once you learn terminological mappings, statistics becomes easier.
  - Because you already know math.

## ■ Least squares method of solving equations via left-inverse

- ▶ Foundation of many statistical analysis
- ▶ You will often see least squares solution “hidden” inside seemingly complicated formulas.

## ■ Least squares formula

- ▶ Derived via algebra, geometry or calculus.
- ▶ Multiple ways of understanding and interpreting least squares

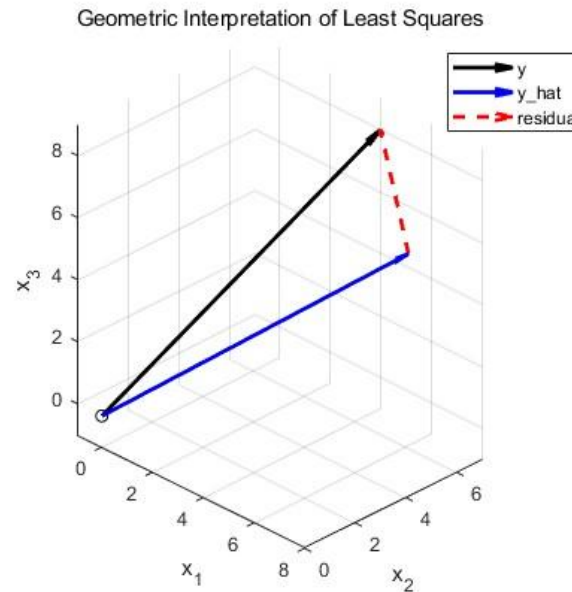
# Summary

- **Multiplying observed data vector by left-inverse**
  - ▶ Right way to think about least squares
- **In practice, other methods are more numerically stable.**
  - ▶ Such as LU and QR decomposition

# Code Exercises

# Abstracted Geometric View of GLM

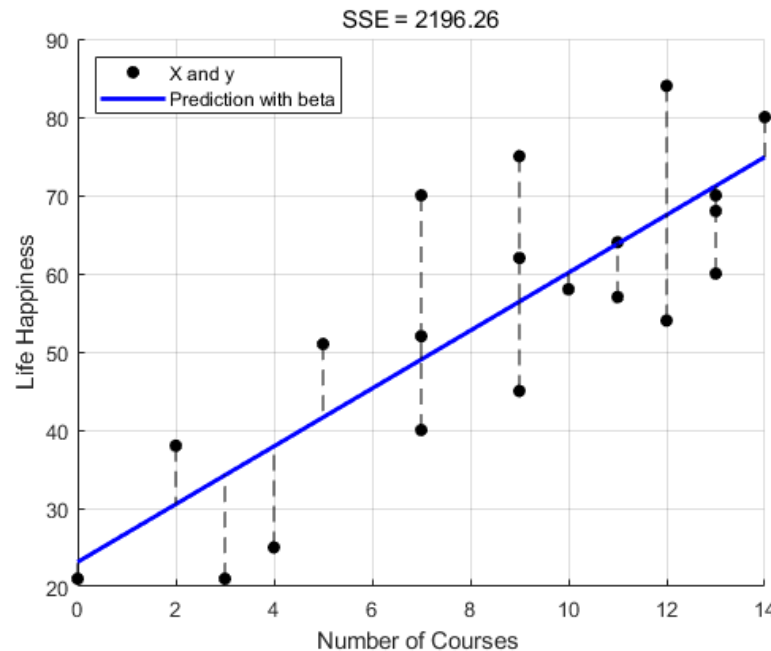
- Write code that displays  $y$  vector, predicted  $y$  vector, and residual vector to visualize GLM.
  - ▶ Variable  $X$ : design matrix
  - ▶ Variable  $y$ : data vector
- Refer to page 18.



Result of the code

# SSE Calculation

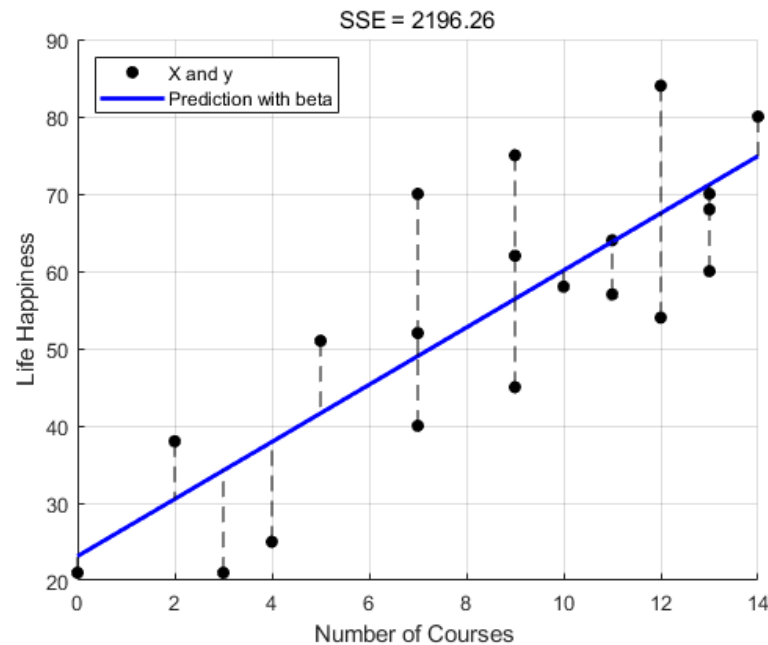
- **Code Exercise (11\_03)** introduced the best fit line  $y = mx + b$ .
- Write code that calculates SSE(Sum of Squares Error) between real data and predicted data.



Result of the code

# SSE Calculation using QR Decomposition

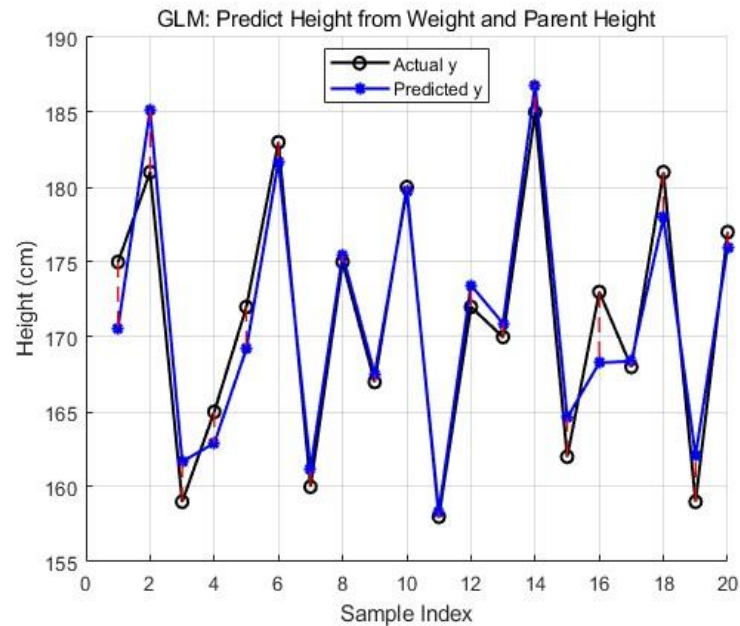
- You can also calculate beta using QR Decomposition.
- Write code that calculates SSE(Sum of Squares Error) between real data and predicted data using QR Decomposition.
- Hint: Calculate Economy-sized QR.
- Hint: Use ' $\backslash$ ' for get inverse of matrix R.



Result of the code

# Extension of Design Matrix

- Write code that predicts individuals' height based on their weight and parents' height.
- Refer to page 7,8.



Result of the code



**THANK YOU  
FOR YOUR ATTENTION**