Linear Algebra General Linear Models and Least Squares Automotive Intelligence Lab.





Contents

- General linear models
- Solving GLMs
- GLM in a simple example
- Least squares via QR
- Summary
- Code exercise





General Linear Models





General Linear Model

Statistical model

- Set of equations that relates predictors to observations.
 - Predictors: independent variable.
 - Observations: dependent variable.

Example of 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	Design matrix (columns=independent variables, predictors, regressors)	
x	β	Regression coefficients or beta parameters	
b	у	Dependent variable, outcome measure, data	

Table of terms in GLMs





Setting up a GLM

Process to set up GLM

- 1. Defining an equation that relates the predictor variables to the dependent variable.
- 2. Mapping the observed data onto the equations.
- 3. Transforming the series of equations into a matrix equation.
- 4. Solving that equation.





Simple Example to Explain Process of GLM

Model: Predicts adult height based on weight and on 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)
- ϵ : error term (also called residual)
- Why we need error term ϵ (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 β ?

- Coefficients or weights.
- Describe how to combine weight and parent's height to predict an individual's height.
- \triangleright β_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.
- \blacktriangleright For simplicity, omitting ϵ .

у	W	h
175	70	177
181	86	190
159	63	180
165	62	172

Simple data table

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 β

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

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

Solution to solve β

$$f^{T}x = f^{T}x^{T}x$$

$$f^{T}x^{T}(x^{T}x) = f^{T}x^{T}x$$

$$f^{T}x^{T}(x^{T}x) = f^{T}x^{T}x$$

- 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 square

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 = inv(X' * X) * X';

% Calculate the beta
beta = X_leftinv * y;
disp("beta");
disp(beta);

MATLAB code to solve the least square using left-multiply
```



Is the Solution Exact?

- 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?

GPA= BX2+B xBlack out 20007H [\$ black] [B] = [Gi] Design Matrix

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

- ➤ 3 questions for 2000 students.
- Column space of the design matrix
 - 2*D* subspace inside that 2000*D* ambient dimensionality.
 - Question of "How much alcohol do you consume?" and "How often do you black out?"
- Data vector
 - 1*D* 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

- Modify GLM equation to allow for a discrepancy between model predicted data and observed data.
 - lt 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.
 - \bullet ϵ is residual, or an error term.
 - Add 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 $X\beta = \hat{y}$.
 - $\bullet \ \widehat{y} = y + \epsilon$
- 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 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 many more observations (M, row) 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? $\boxed{100}$
 - If not, what coordinate inside the column space of the design matrix is as close as possible to data vector?

$$\begin{bmatrix} C_1 & C_2 \\ 2600 \times 2 \end{bmatrix} \begin{bmatrix} 2 \\ \times \\ 1 \end{bmatrix} = \begin{bmatrix} 2500 \times 1 \end{bmatrix}$$





Abstracted geometric view of GLM

$$2 \cdot 0 \cdot \begin{bmatrix} 1 & 1 \\ 0 & \zeta \\ 1 & 1 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} 1 \\ 3 \\ 1 \end{bmatrix}$$

- lacksquare Our goal: find set of coefficients $oldsymbol{eta}$.
 - \blacktriangleright Weighted combination of columns in X minimizes distance to data vector y.
 - \blacktriangleright We can call projection vector ϵ .
 - \blacktriangleright How can find vector ϵ and coefficients β ?
 - 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 form the algebraic approach.

$$X^{T} \epsilon = 0$$

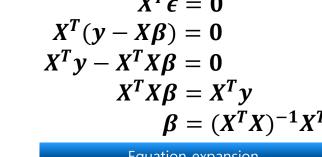
$$X^{T} (y - X\beta) = 0$$

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

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

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

Equation expansion







Meaning of Least Squares

- Why is it called "least squares"?
 - Squares
 - Squared errors between predicted data and observed data
 - There is an error term for each ith 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 ϵ should be small.
 - Objective of model fitting
 - Choose elements in β that minimize elements in ϵ .





Expression of Least Squares

- Why is it called "least squares"?
 - ► If just minimizing errors,
 - It cause the model to predict values toward negative infinity.
 - ► Instead, minimizing squared errors
 - Correspond 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 name "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 β 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 which is minimize the squared distance between the model-predicted values and the observed values.

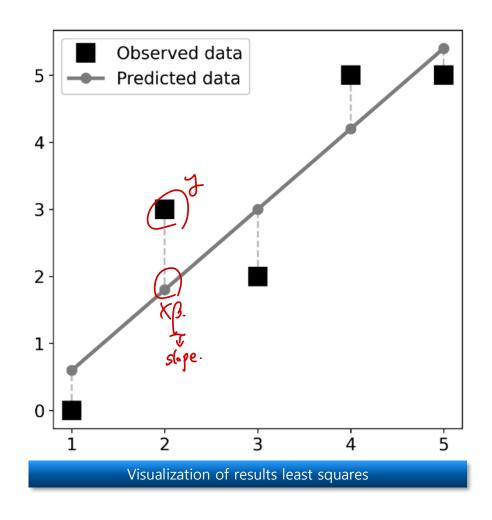




Visualization Intuition for Least Squares

Black squares

- J=a.
- 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!
 - Minimizes distances 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 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 Simple Example

Example

- Report the number of online courses they taken and their general satisfaction with life.
- ► Fake experiment which is surveyed random set of 20 of fake 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 plotter 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			

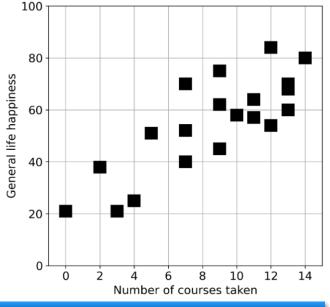


Fig 1. Fake data from fake survey





Create Design Matrix

- Design matrix is actually only only 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 $X\beta = y$



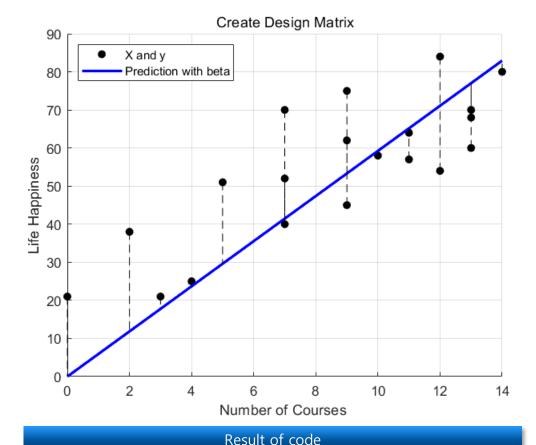
Code Exercise of Creating Design Matrix

■ Code Exercise (11_02)

- ► Follow the previous slide.
- ightharpoonup 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 = inv(X' * X) * X';
% Calculate the beta
beta = X_leftinv * y;
disp("beta");
disp(beta);
y_pred = beta * X;
% 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



Meaning of Least Squares Formula's Result

- Following least squares formula tells $\beta = 5.92$.
- What does this number mean?
 - ► It means 5 op@ 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..

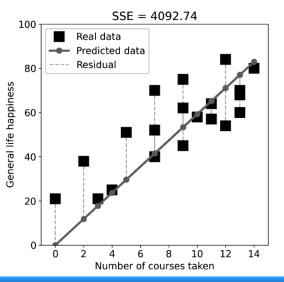


Fig 1. Observed and predicted data (SSE=sum of squared errors)





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?

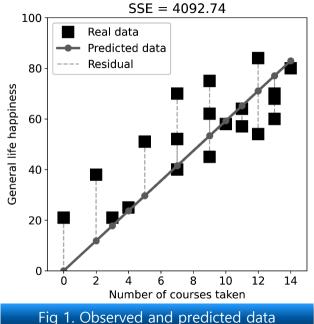


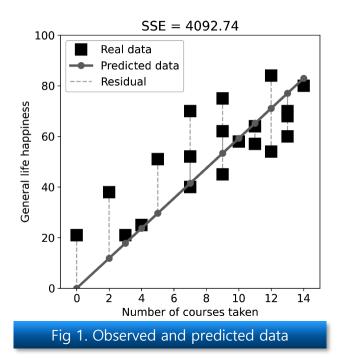
Fig 1. Observed and predicted data





Problem in Fig 1.

- Design matrix contains no intercept
 - ightharpoonup 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.







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.
- Statistical interpretation of intercept
 - Expected numerical value of observations
 - When predictors are set to ₹e_V
- 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
                                                                          % Plot
clc; clear; close all;
                                                                          figure;
                                                                          hold on;
% Define a matrix number of courses and life happiness
                                                                          grid on;
number_of_course = [4,12,3,14,13,12,9,11,7,13,11,9,2,5,7,10,0,9,7,13]';
                                                                          scatter(number_of_course, y, 'k', 'filled'); % X and y
                                                                          plot(number_of_course, y_pred, 'b', 'LineWidth', 2); % Plot predicted
life_happiness =
[25,54,21,80,68,84,62,57,40,60,64,45,38,51,52,58,21,75,70,70]';
                                                                          line with beta
                                                                          for i = 1:length(X)
% Define a new design matrix X that contains the intercept term and
                                                                              plot([number_of_course(i) number_of_course(i)], [y(i) y_pred(i)],
                                                                          'k--'); % Plot residuals as dashed lines
% dependent variable matrix y
X = [ones(20,1) number_of_course]; % Use number_of_course
                                                                          end
y = [life_happiness];
                                                                          title('Add Intercept Term');
                                                                          xlabel('Number of Courses ');
% Compute the left-inverse of X
                                                                          ylabel('Life Happiness');
                                                                          legend('X and y', 'Prediction with beta', 'Location', 'northwest');
X_{leftinv} = inv(X' * X) * X';
                                                                          hold off;
% Calculate the beta
beta = X leftinv * y;  % [beta0 beta1]
beta = flip(beta);
                       % [beta1 beta0]
y_pred = polyval(beta, number_of_course); % Predict y values using
beta
```

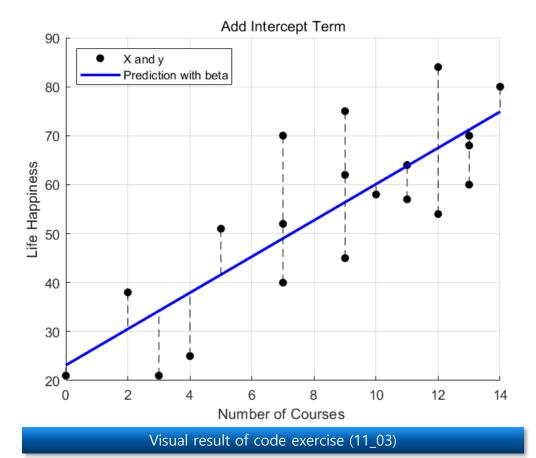




MATLAB code to add Intercept term

Visual result of Code Exercise

■ Code Exercise (11_03)

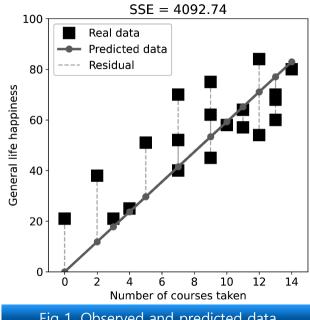






Result of Including Intercept Term

- Now, β 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.





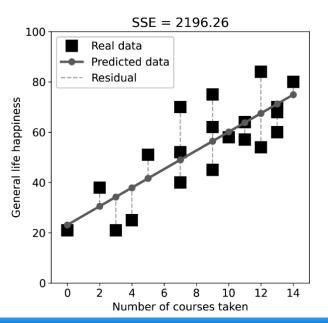


Fig 2. Observed and predicted data, with an intercept term





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.
 - \blacktriangleright Matrix X^TX itself can introduce difficulties.
 - Multiplying matrix by its transpose has implications.
 - For properties such as norm and condition number which you will learn more about condition number 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

- Observe following sequence of equations as Eq 1...
- ► Eq 1. is slightly simplified.
 - From actual low-level numerical implementations.

$$X\beta = y$$
 $QR\beta = y$
 $R\beta = Q^{T}y$
 $\beta = R^{-1}Q^{T}y$

Eq 1. Sequence of equation





Example of How to Stable

- \blacksquare R is same shape as X.
 - ► Tall (and therefore noninvertible)
 - ► Although only first *N* rows are nonzero
 - Rows N + 1 through M do not contribute to the solution.
 - In matrix multiplication, rows of zeros produce results of zeros.
 - Those rows can be removed.
 - From \mathbf{R} and from $\mathbf{Q}^T \mathbf{y}$.
- Row swaps
 - ► Implemented via matrices.
 - Might be used to increase numerical stability.

$$X\beta = y$$
 $QR\beta = y$
 $R\beta = Q^{T}y$
 $\beta = R^{-1}Q^{T}y$

Eq 1. Sequence of equation





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.
 - Row reduce to obtain RREF.
 - Extract solution from final column of augmented matrix.

$$X\beta = y$$
 $QR\beta = y$
 $R\beta = Q^{T}y$
 $\beta = R^{-1}Q^{T}y$

Eq 1. Sequence of equation





Conclusion of Least Squares Via QR Decomposition

- QR decomposition solves least squares problem
 - ▶ Without squaring X^TX .
 - ► Without explicitly inverting a matrix.
- \blacksquare Main risk of numerical instability comes from computing Q.
 - ► This is fairly numerically stable.
 - When implemented via Householder reflections.





Summary





Summary

- GLM is statistical framework.
 - For understanding our rich and beautiful universe.
 - Works by setting up simultaneous of equations.
 - Like that you learned about in previous lecture.

■ Different term 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 analyses
- 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



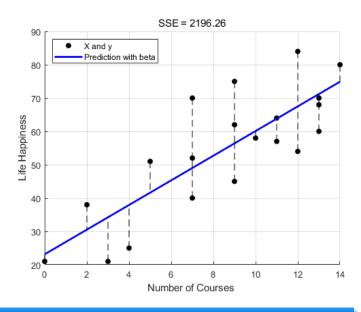


SSE Calculation

- In Code Exercise (11_03), There are introducing best fit line y = mx + b.
- Write code that calculate SSE(Sum of Squares Error) between real data and predicted data

```
% Clear workspace, command window, and close all figures
                                                                         % Plot
clc; clear; close all;
                                                                         figure;
                                                                         hold on;
% Define a matrix number of courses and life happiness
                                                                         grid on;
number of course = [4,12,3,14,13,12,9,11,7,13,11,9,2,5,7,10,0,9,7,13];
                                                                         scatter(number of course, y, 'k', 'filled'); % X and y
% Define a new design matrix X that contains the intercept term and
                                                                         plot(number of course, y pred, 'b', 'LineWidth', 2); % Plot predicted
% dependent variable matrix v
                                                                         line with beta
                                                                         for i = 1:length(X)
X = [ones(20,1) number of course]; % Use number of course
y = [25,54,21,80,68,84,62,57,40,60,64,45,38,51,52,58,21,75,70,70]';
                                                                             plot([number_of_course(i) number_of_course(i)], [y(i) y_pred(i)],
                                                                         'k--'); % Plot residuals as dashed lines
% Compute the left-inverse of X
                                                                         end
X_{int} = inv(X' * X) * X';
                                                                         xlabel('Number of Courses ');
                                                                         vlabel('Life Happiness');
% Calculate the beta
                                                                         title(sprintf('SSE = %.2f', sse));
beta = X leftinv * y;
                      % [beta0 beta1]
                                                                         legend('X and y', 'Prediction with beta', 'Location', 'northwest');
beta = flip(beta);
                       % [beta1 beta0]
                                                                         hold off;
y_pred = polyval(beta, number_of_course); % Predict y values using
beta
sse = ;
```

Sample code



Result of the code

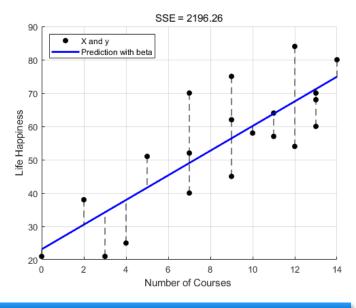




SSE Calculation using QR Decomposition

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

```
% Clear workspace, command window, and close all figures
                                                                          % Plot
clc; clear; close all;
                                                                          figure;
                                                                         hold on;
% Define a matrix number of courses and life happiness
                                                                          grid on;
number of course = [4,12,3,14,13,12,9,11,7,13,11,9,2,5,7,10,0,9,7,13];
                                                                         scatter(number of course, y, 'k', 'filled'); % X and y
                                                                          plot(number_of_course, y_pred, 'b', 'LineWidth', 2); % Plot predicted
% Define a new design matrix X that contains the intercept term and
                                                                         line with beta
% dependent variable matrix v
                                                                          for i = 1:length(X)
X = [ones(20,1) number of course]; % Use number of course
                                                                              plot([number_of_course(i) number_of_course(i)], [y(i) y_pred(i)],
y = [25,54,21,80,68,84,62,57,40,60,64,45,38,51,52,58,21,75,70,70]';
                                                                          'k--'); % Plot residuals as dashed lines
% QR decomposition of X
                                                                         title(sprintf('SSE = %.2f', sse));
% Calculate the beta
                                                                         xlabel('Number of Courses');
% Calculate sum of squared errors (SSE)
                                                                         ylabel('Life Happiness');
                                                                         legend('X and y', 'Prediction with beta', 'Location', 'northwest');
                                                                         hold off:
```



Sample code

Result of the code





THANK YOU FOR YOUR ATTENTION



