Handling multicollinearity with PCR and PLSR

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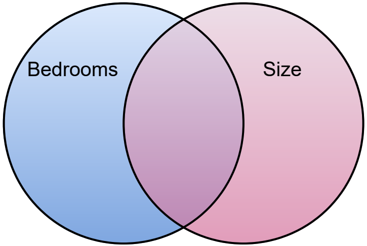
Outline

1. What is Multicollinearity
2. Why is it a problem
3. How to measure collinearity
4. Principal Component Regression (PCR)
5. Partial Least Squares Regression (PLSR)
6. Discussion/Conclusion

What is Multicollinearity

- When **two or more predictor variables** in a regression model are **highly correlated**
  - When predicting a **house's price** using different predictor variables like the **size** of the house, the **number of bedrooms**, and the **age** of the house.
  - **Size** and **number of bedrooms** are highly related to each other, you have **multicollinearity**.



Source: Penn State

Multicollinearity - 3D plot

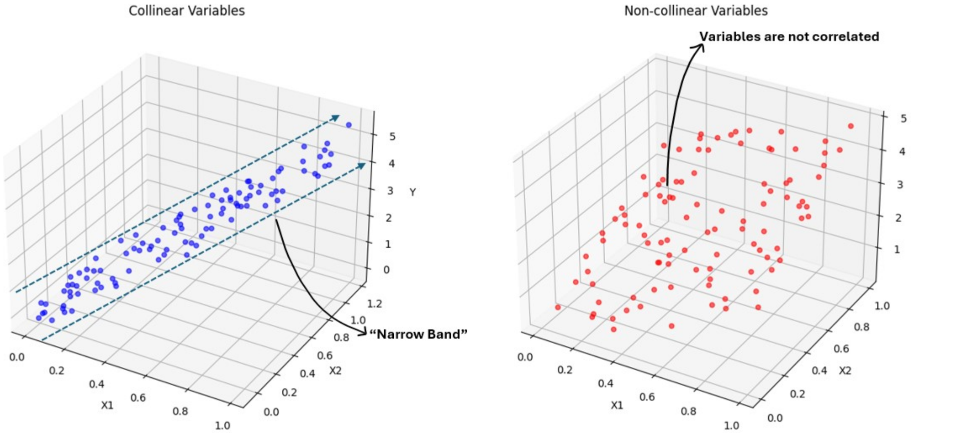


Figure: On the left, predictors that are highly correlated form a "Narrow Band". On the right, data without multicollinearity are dispersed and uncorrelated.

Fit the hyperplane to the data using MLR method

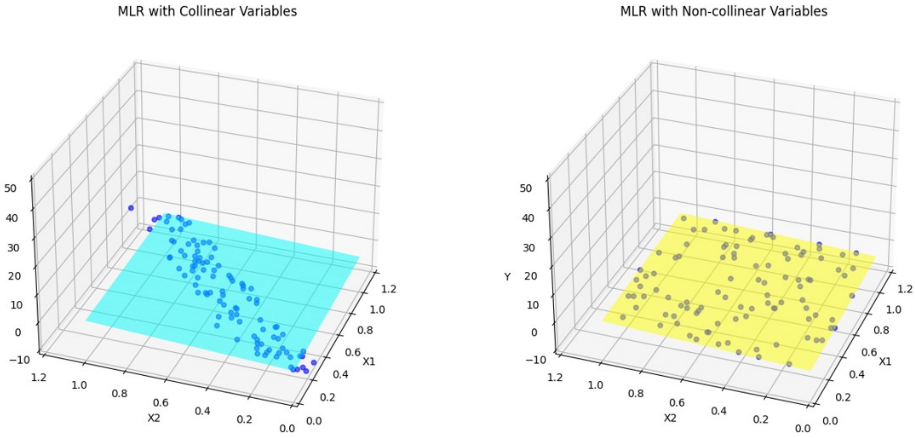


Figure: MLR fitting on both data, everything seems alright ...

Small data adjustment: Unstable hyperplane fitting

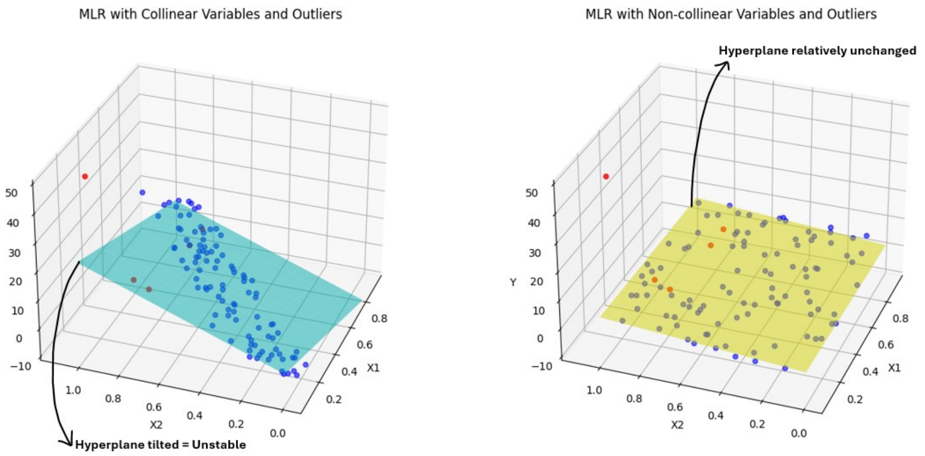
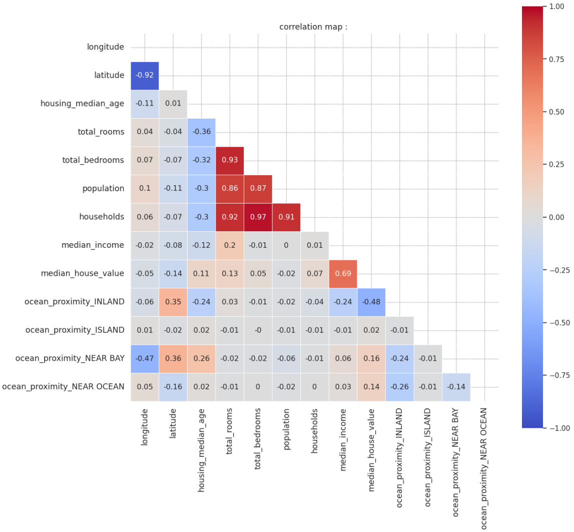


Figure: MLR is quite unstable when implemented to data with multicollinearity.

Why is it a problem

- **Inflated Standard Errors**
  - Makes it difficult to determine which predictors are significant.
- **Unstable Coefficients**
  - Coefficients change drastically with small data adjustments.
  - Coefficient change:
    - Data with multicollinearity, $[X_1, X_2] = [23.493,\ 21.637]$
    - Data without multicollinearity, $[X_1, X_2] = [3.518,\ 2.049]$
- **Complicates Interpretation**
  - Hard to identify each predictor's unique impact.

Python notebook here!
Source: Medium


correlation map :
longitude
latitude -0.92
housing_median_age -0.11 0.01
total_rooms 0.04 -0.04 -0.36
total_bedrooms 0.07 -0.07 -0.32 0.93
population 0.1 -0.11 -0.3 0.86 0.87
households 0.06 -0.07 -0.3 0.92 0.97 0.91
median_income -0.02 -0.08 -0.12 0.2 -0.01 0 0.01
median_house_value -0.05 -0.14 0.11 0.13 0.05 -0.02 0.07 0.69
ocean_proximity_INLAND -0.06 0.35 -0.24 0.03 -0.01 -0.02 -0.04 -0.24 -0.48
ocean_proximity_ISLAND 0.01 -0.02 0.02 -0.01 -0 -0.01 -0.01 -0.01 0.02 -0.01
ocean_proximity_NEAR BAY -0.47 0.36 0.26 -0.02 -0.02 -0.06 -0.01 0.06 0.16 -0.24 -0.01
ocean_proximity_NEAR OCEAN 0.05 -0.16 0.02 -0.01 0 -0.02 0 0.03 0.14 -0.26 -0.01 -0.14
longitude
latitude
housing_median_age
total_rooms
total_bedrooms
population
households
median_income
median_house_value
ocean_proximity_INLAND
ocean_proximity_ISLAND
ocean_proximity_NEAR BAY
ocean_proximity_NEAR OCEAN
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00

How to handle it?

Two solutions are:

- Principal Component Regression (PCR)
- Partial Least Squares Regression (PLSR)

Principal Component Regression

- Handles multicollinearity by **combining variables into principal components**
- *Example:* MLR with two variables, v_1 and v_2, can become PCR using one principal component, PC_1
  - PC_1 is some linear combination of v_1 and v_2. $PC_1 = \alpha_1 v_1 + \alpha_2 v_2$

MLR

$\hat{y} = \beta_0 + \beta_1 v_1 + \beta_2 v_2$

PCR

$\hat{y} = \beta_0 + \beta_1 PC_1$

- **Using** Principal Components ensures *non-collinearity* as components are orthogonal
- **Select** the number of Principal Components by using validation methods (next week) e.g. Root mean square error of prediction
- **Substitute** in $PC_1 = \alpha_1 v_1 + \alpha_2 v_2$ obtained from PCA to obtain variable coefficients

Principal Component Regression - Example: Predict student's abilities in untested areas

- **Dataset overview**: 234 students, 36 questions, numerical full rank but high condition number (105.3) indicating multicollinearity
- **Limitations of using total score**: Oversimplifies student abilities. Ignores variance among individual question performances
- **Challenges with individual predictors**: High multicollinearity among questions leads to unstable regression coefficients. Difficult to interpret due to overlapping content areas

Candidate ID	Q1	Q2	...	Q36	Score (0-100)	Prediction in untested area
$\vdots$	$\vdots$			$\vdots$	$\vdots$	$\vdots$

$\rightarrow$ PCR might be a better predictor of individual's student abilities in untested areas

Data: Exam scores in TTK4105 spring 2024

Principal Component Regression - Problems

Values, α are chosen to optimise PCA (i.e maximum variance) and NOT to optimise prediction, $\hat{y}$. Therefore:

Problem

Resulting variable parameters ($\beta_1 \alpha_1$ etc) don't necessarily have meaning in the context of our **dependent variable** i.e. y

We need a way to optimise for the dependent variable so that learned parameters have meaning.

Solution

Partial Least Squares Regression

Partial Least Squares Regression

- Another way to ensure non-collinearity and lower dimensionality of predictor variables
- The method is the same as PCR, but in this case latent variable LV_1 is chosen to optimise for the dependent variable: $LV_1 = \alpha_1 v_2 + \alpha_2 v_2$

MLR

$\hat{y} = \beta_0 + \beta_1 v_1 + \beta_2 v_2$

PLSR

$\hat{y} = \beta_0 + \beta_1 LV_1$

- **Choose** different algorithms to find optimal set of latent variable components $\boldsymbol{\alpha}$
- **Continue** as you would with PCR

Partial Least Square Regression - Example: Predicting housing value based on house specification

- **Dataset overview**: 20640 house listed, 13 variables explaining housing specification
- **Multicollinearity indication**: 6 variables with high VIF scores, indicating multicollinearity
- **Objective**: PLSR is applied to improve the predictive accuracy of housing value despite the highly correlated variables
- **Results**: PLSR outperformed both PCR and MLR in terms of R-squared accuracy, achieving values of 0.626, 0.621, and 0.57, respectively.

Long	Lat	Housing age	...	No. of bedrooms	Ocean proximity	**House value**
⋮	⋮			⋮	⋮	⋮

Partial Least Square Regression - Problems

- **Higher Risk of Overlooking 'Real' Correlations**
  - *Example:* PLSR may cause the unique impact of important variables (e.g., house size) to disappear if they are highly correlated with others (e.g., number of bedrooms), as PLSR combines them into a single latent variable.
- **Sensitivity to the relative scaling of the descriptor variables**
  - **Normalization** only addresses scaling issue, but not distribution
  - PLSR can still be **sensitive if variables have different shapes of distribution**
  - *Example:* If one variable is **normally distributed** (e.g., house size) and another is **highly skewed** (e.g., distance to city center), the **skewed variable** can disproportionately influence the model

Source: Partial Least Squares (PLS): Its strengths and limitations

Conclusion/Discussion

- For handling multicollinearity, **PLSR** is generally preferred over **PCR** when your objective is **prediction**, as it directly links the predictor variables to the response while still reducing dimensionality