COMP 680
Statistics for Computing and Data Science
Week 11: Linear Regression

Su Chen, Assistant Teaching Professor,
Rice D2K Lab

Outline

Regression

- Regression is the general label for investigating relationship between (two) variables
  - the term first coined by Francis Galton (1822 - 1911)
  - study of human differences and inheritance of intelligence

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- Start with two (numerical) variables:
  - dependent variable Y: outcome, response, label ...
  - independent variable X: covariate, predictor, feature ...
  - regress Y on X to understand how Y depends on X

A Regression Model

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- Mathematical model and the regression function $f(x)$:

$$y_i = f(x_i) + \epsilon_i, \quad i = 1, 2, \cdots n$$

  - the regression function: quantifies the relationship between X and Y
  - the error terms ϵ_i: captures measurement errors and other discrepancies

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- Captures measurement errors and other discrepancies:
- Most common is Gaussian errors:

$$\epsilon_i \overset{\text{i.i.d.}}{\sim} \mathrm{N}(0, \sigma^2)$$

- $\boldsymbol{\epsilon}$ are independent of the regression function f
- $\boldsymbol{\epsilon}$ are independent of each other
- $\mathbb{E}[\boldsymbol{\epsilon}] = 0, \quad \mathbb{V}[\boldsymbol{\epsilon}] = \sigma^2$

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  - finite and fixed number of parameters
  - less flexible but more interpretable
  - what is the simplest f?
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- Nonparametric models:
  - no fixed number of parameters
  - more flexible but less interpretable
  - need more data to estimate

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$$\epsilon_i \overset{\text{i.i.d.}}{\sim} \mathrm{N}(0, \sigma^2) \Rightarrow Y|X = x \overset{\text{i.i.d.}}{\sim} \mathrm{N}(\beta_0 + \beta_1 x, \sigma^2)$$

The Conditional Distribution

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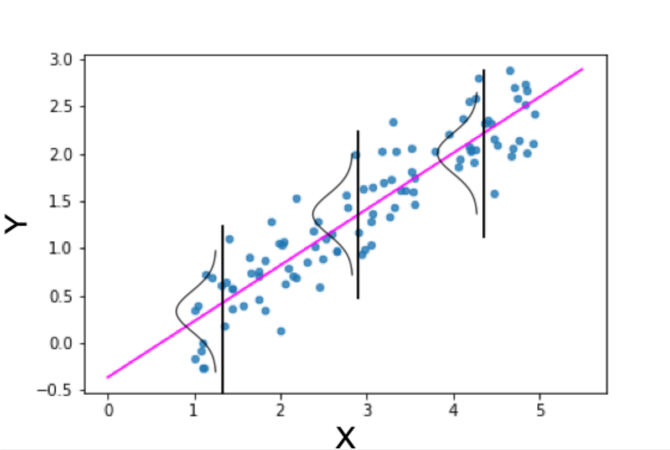
- The "true" regression function $f(x) = \beta_0 + \beta_1 x$
  - aka population regression line
  - unknown population parameters β_0 and β_1

Simple Linear Regression

The population regression line:



Simple Linear Regression

- Fitting the models means estimate β_0 and β_1 from the observed data
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  - $\hat{\beta}_0$ and $\hat{\beta}_1$ are statistics with sampling distribution!
- What can a regression model do?
  - prediction: for a given value of X : $\hat{y}_i = \mathbb{E}[Y|X = x_i] = \hat{\beta}_0 + \hat{\beta}_1 x_i$
  - inference: sampling distributions and CI for β
  - interpretation: understand how Y depends on X
- Recall the 3 types of questions:

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- Idea: minimize difference between $\hat{y}_i$ and y_i, i.e., the Residual Sum of Square (RSS):

$$\hat{\beta}_0^{\text{OLS}}, \hat{\beta}_1^{\text{OLS}} = \arg\min \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \arg\min \sum_{i=1}^{n} (\beta_0 + \beta_1 x_i - y_i)^2$$

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- Residual $r_i = y_i - \hat{y}_i$ represents the estimate of the error term ϵ_i
  - the OLS line minimize RSS

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  - minimize loss function in ML: mean square loss = RSS / n
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  - however, no inference!
- Approach as a statistical problem:
  - maximum likelihood estimates
  - leads to equivalent solutions - why?

$$\hat{\beta}_0^{\text{MLE}}, \hat{\beta}_1^{\text{MLE}} \iff \hat{\beta}_0^{\text{OLS}}, \hat{\beta}_1^{\text{OLS}}$$

The Coefficients

- Closed form solutions:

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(x_i - \bar{x}_n)(y_i - \bar{y}_n)}{\sum_{i=1}^{n}(x_i - \bar{x}_n)^2} = r_{X,Y} \cdot \frac{s_Y}{s_X}$$
$$\hat{\beta}_0 = \bar{y}_n - \hat{\beta}_1 \bar{x}_n$$

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$$\hat{\beta}_0 = \bar{y}_n - \hat{\beta}_1 \bar{x}_n$$

- slope $\hat{\beta}_1$ is rescaled Pearson correlation coefficient $r_{X,Y}$
  - describe the linear association between X and Y
  - depends on unit of X and Y

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$$\hat{\beta}_1 \sim \mathrm{N}\left(\beta_1, \quad \sigma^2 \frac{1}{\sum_{i=1}^{n}(x_i - \bar{x}_n)^2}\right)$$

$$\hat{\beta}_0 \sim \mathrm{N}\left(\beta_0, \quad \sigma^2 \left[\frac{1}{n} + \frac{\bar{x}_n^2}{\sum_{i=1}^{n}(x_i - \bar{x}_n)^2}\right]\right)$$

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- What about σ^2? usually unknown...
  - nuisance parameter, can be estimated from data
  - replace σ^2 with $\hat{\sigma}^2 = \mathrm{RSS}/(n-2)$: the above Normal $\rightarrow$ t distribution!

Inference

- Confidence intervals for β_j and $j = 0, 1$
  - $[\hat{\beta}_j + t_{\alpha/2, df=n-2} \cdot \mathrm{SE}(\hat{\beta}_j), \quad \hat{\beta}_j + t_{1-\alpha/2, df=n-2} \cdot \mathrm{SE}(\hat{\beta}_j)]$
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- Hypothesis testing on regression slope is standard:
  - H_0: $\beta_1 = 0$ vs. H_1: $\beta_1 \neq 0$: one-sample t-test
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- for two-sided test, the following are equivalent:
  - reject H_0: $\beta_1 = 0$ at α level
  - $1 - \alpha$ CI for β_1 does NOT include 0

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- $\hat{\beta}_1$: the average change in Y when X increase by 1 unit
  - only if we reject H_0: $\beta_1 = 0$!
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  - $\hat{\beta}_1$ depends on the units!
  - the t-statistic is the “standardized” slope
- $\hat{\beta}_0$: the average value of Y when X is 0
  - not meaningful if X cannot be 0 - extrapolate is dangerous!
  - can choose model with no intercept

Outline

Multiple Covariates

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  - independent Gaussian error $\epsilon_i \overset{\text{i.i.d.}}{\sim} \mathrm{N}(0, \sigma^2)$
- The regression function is linear in the parameters $\boldsymbol{\beta}$
  - for 2 covariates, the linear function is a plane
  - for more than 2 covariates, a hyperplane

Matrix Notation

$$
\begin{pmatrix} y_1 \\ y_2 \\ \cdots \\ y_n \end{pmatrix} = \begin{pmatrix} \beta_0 \\ \beta_0 \\ \cdots \\ \beta_0 \end{pmatrix} + \begin{pmatrix} x_{1,1} & x_{1,2} & \cdots x_{1,p} \\ x_{2,1} & x_{2,2} & \cdots x_{2,p} \\ \cdots & \cdots & \cdots \\ x_{n,1} & x_{n,2} & \cdots x_{n,p} \end{pmatrix} \times \begin{pmatrix} \beta_1 \\ \beta_2 \\ \cdots \\ \beta_p \end{pmatrix} + \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \cdots \\ \epsilon_n \end{pmatrix}
$$

$$
= \begin{pmatrix} 1 & x_{1,1} & x_{1,2} & \cdots x_{1,p} \\ 1 & x_{2,1} & x_{2,2} & \cdots x_{2,p} \\ \cdots & \cdots & \cdots & \cdots \\ 1 & x_{n,1} & x_{n,2} & \cdots x_{n,p} \end{pmatrix} \times \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \cdots \\ \beta_p \end{pmatrix} + \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \cdots \\ \epsilon_n \end{pmatrix}
$$

$$
\boldsymbol{y}_{n\times 1} = \boldsymbol{X}_{n\times p}\boldsymbol{\beta}_{p\times 1} + \boldsymbol{\epsilon}_{n\times 1}
$$

Use p for number of parameters from now on.

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- Recall multivariate normal - Gaussian distribution
  - p-dimensional random vector: mean vector and $p \times p$ covariate matrix
  - marginal of Gaussian: each dimension is normal!

Inference

- Sampling distribution for $\hat{\boldsymbol{\beta}}$ is Gaussian:

$$\hat{\boldsymbol{\beta}} \sim \text{MVN}\left(\boldsymbol{\beta}, \quad (\boldsymbol{X}^T\boldsymbol{X})^{-1}\sigma^2\right)$$

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- Hypothesis testing and CI for each $\hat{\beta}_j$
    - use $\hat{\sigma}^2$
    - t-test
    - t-CI

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$$\hat{\beta} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y} \implies \hat{\boldsymbol{y}} = \boldsymbol{X}\hat{\beta} = \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y} = \boldsymbol{H}\boldsymbol{y}$$

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- The intercept:
  - the average value of Y when all covariates are 0
  - may not be interpretable if any covariate cannot be 0
- More covariates $\Rightarrow$ more complex and less interpretable model
  - is the goal making inference or making prediction?
  - variable/model selection

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  - slope in multiple regression $\propto$ partial correlation
- The "correlation" between X_j and Y after taking out the effects of other covariates
- It is possible that X_j and Y are positively correlated but $\hat{\beta}_j$ is negative and significant!
  - example?

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   - X need to be full rank
3. Gaussian errors:
   - errors have 0 mean
   - errors are independent: no auto-correlation
   - errors have constant variance: homoscedasticity
   - implies the conditional distribution of Y given X is Gaussian!

Gauss-Markov Theorem

Under the previous assumptions, the OLS solution $\hat{\beta}$ is the Best Linear Unbiased Estimate (BLUE)!

- smallest variance among unbiased estimates
  - $\mathrm{SE}(\hat{\beta}^{\mathrm{OLS}}) \leq \mathrm{SE}(\hat{\beta})$
  - in general MLE is efficient

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  - in general MLE is efficient
- OLS does not necessarily have the smallest MSE!
  - recall MSE $=$ bias^2 $+$ variance
  - Ridge and Lasso estimate are both biased

Outline

Categorical Covariates

- Design matrix X is numerical, what about categorical variables?
- Example: gender, ethnicity, education level...
- Common mistake: code categories with 1, 2, 3, ...
  - what is wrong with that?

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- Common mistake: code categories with 1, 2, 3, ...
  - what is wrong with that?
- Correct way: dummy variable coding
  - K categories $\rightarrow K - 1$ dummy variables
  - adds $K - 1$ columns to $\boldsymbol{X}$
  - why not K dummy variables?

Categorical Covariates

Example: investigate difference in credit card balance between males and females. We create 1 dummy variable:

$$x_i = \begin{cases} 1 & \text{if ith person is female} \\ 0 & \text{if ith person is male} \end{cases}$$

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$$x_i = \begin{cases} 1 & \text{if ith person is female} \\ 0 & \text{if ith person is male} \end{cases}$$

Resulting model:

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i = \begin{cases} \beta_0 + \beta_1 + \epsilon_i & \text{if ith person is female} \\ \beta_0 + \epsilon_i & \text{if ith person is male} \end{cases}$$

Interpretation?

Categorical Covariates

Results for gender model:

	Coefficient	Std. Error	t-statistic	p-value
Intercept	509.80	33.13	15.389	< 0.0001
gender [female]	19.73	46.05	0.429	0.6690

Categorical Covariates

- For the ethnicity variable we create 2 dummy variables:
- The first one could be:

$$x_{i1} = \begin{cases} 1 & \text{if ith person is Asian} \\ 0 & \text{if ith person is not Asian} \end{cases}$$

- The second one could be:

$$x_{i2} = \begin{cases} 1 & \text{if ith person is Caucasian} \\ 0 & \text{if ith person is not Caucasian} \end{cases}$$

Categorical Covariates

- Then both of these variables can be used in the regression equation:
-

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \epsilon_i = \begin{cases} \beta_0 + \beta_1 + \epsilon_i & \text{if ith person is Asian} \\ \beta_0 + \beta_2 + \epsilon_i & \text{if ith person is Caucasia} \\ \beta_0 + \epsilon_i & \text{if ith person is African} \end{cases}$$

- The category with no dummy variable – African American in this example – is the baseline .

Categorical Covariates

	Coefficient	Std. Error	t-statistic	p-value
Intercept	531.00	46.32	11.464	< 0.0001
Ethnicity [Asian]	-18.69	65.02	-0.287	0.7740
Ethnicity [Caucasian]	-12.50	56.68	-0.221	0.8260

Interaction

- Relax the additive assumption: interactions and nonlinearity
- Example: predict credit card balance using income and student status (binary)
- Model without interaction:

$$
\begin{aligned}
\text{balance}_i &= \beta_0 + \beta_1 \cdot \text{income}_i + \begin{cases} \beta_2 & \text{if } i\text{th person is a student} \\ 0 & \text{if } i\text{th person is not a student} \end{cases} \\
&= \beta_1 \cdot \text{income}_i + \begin{cases} \beta_0 + \beta_2 & \text{if } i\text{th person is a student} \\ \beta_0 & \text{if } i\text{th person is not a student} \end{cases}
\end{aligned}
$$

- Different intercept, same slope!

Interaction Term

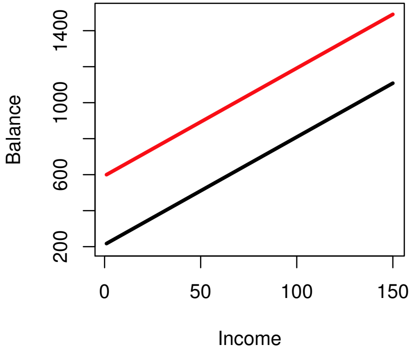
- Model with interaction:

$$\begin{aligned} \text{balance}_i &= \beta_0 + \beta_1 \cdot \text{income}_i + \beta_2 \cdot \text{student}_i + \beta_3 \cdot \text{income}_i \times \text{student}_i \\ &= \beta_0 + \beta_1 \cdot \text{income}_i + \begin{cases} \beta_2 + \beta_3 \cdot \text{income}_i & \text{if student} \\ 0 & \text{if not student} \end{cases} \\ &= \begin{cases} (\beta_0 + \beta_2) + (\beta_1 + \beta_3) \cdot \text{income}_i & \text{if student} \\ \beta_0 + \beta_1 \cdot \text{income}_i & \text{if not student} \end{cases} \end{aligned}$$

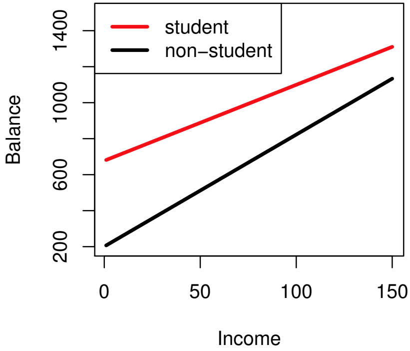
- Different intercept, different slope!

Interaction Term

- no interaction between income and student



- with an interaction between income and student



Polynomial Term

- Polynomial regression on Auto data:

$$mpg = \beta_0 + \beta_1 \cdot horsepower + \beta_2 \cdot horsepower^2 + \epsilon$$

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- Results may provide a better fit than just linear terms:

	Coefficient	Std. Error	t-statistic	p-value
Intercept	56.9001	1.8004	31.6	< 0.0001
horsepower	-0.4662	0.0311	-15.0	< 0.0001
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- But coefficients lose interpretability - why?

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- Bayesian information criterion (BIC)
  - -2 log likelihood + $p(\log n)$
  - penalize large model more

Model Diagnostic - Residual Plot

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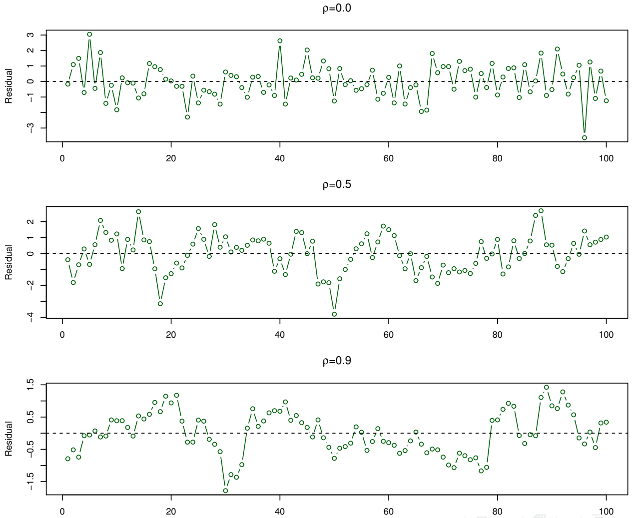
Good:

- scattered around 0
- no clear pattern
- normal distribution

Bad:

- auto-correlation
- heteroscedasticity
- non-linearity

Residual Plot



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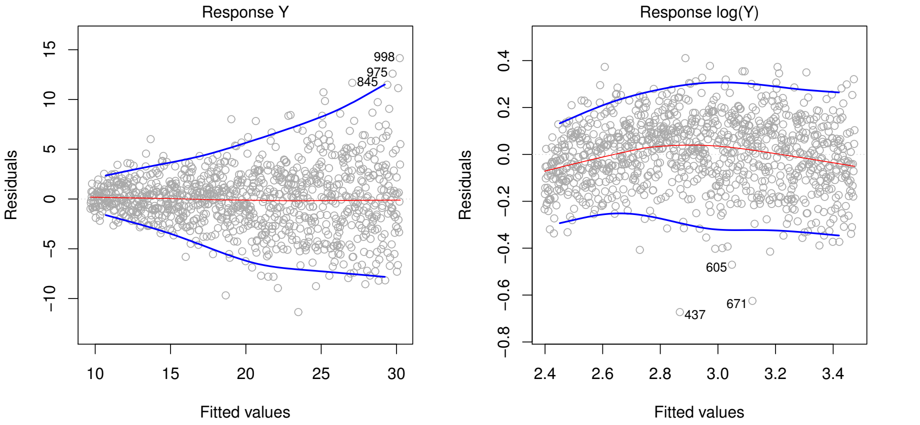

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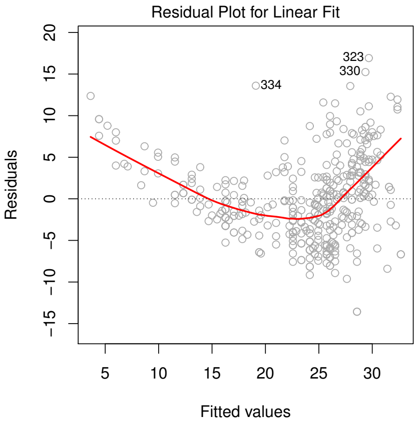

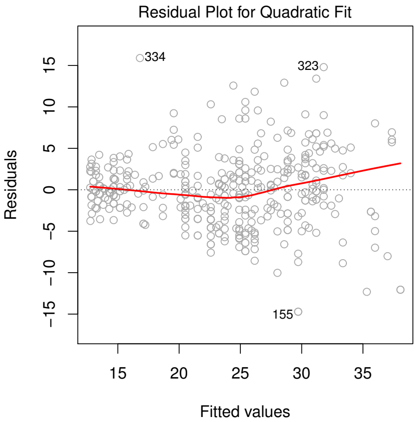

Model Diagnostic - Multicollinearity

- Refers to two or more covariates highly correlated
- Cause issues
  - numerical stability
  - coefficients SE inflated
  - interpretability
- Identify:
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- Identify:
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- Solution:
  - variable selection
  - feature engineering

Outline