CIS 490 Machine Learning

Lecture 5

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Last time

- Review: Probability Theory (III)
  - Central limited theory (II)
  - Multivariate distribution
    - Joint probability
    - Marginal probability
    - Conditional probability

Reminder: Sectional Homework 1, Due Feb 4^{th}.

Adapted from Jeff Howbert, Greg Shakhnarovich

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Answers to class exercises in LS 4: Multivariate Discrete Distribution

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Example: Probability Table			**X= Model type**		
		Sedan	**Minivan**	**SUV**	**Sport**
Y= Manufacturer	**European**	**n/a**	**0.1481**	**n/a**	**n/a**
	Asian	**n/a**	**0.1111**	**n/a**	**n/a**
	American	**n/a**	**0.0741**	**n/a**	**n/a**
		Marginal	**0.3333**		
Assuming calculating the probability of selling a high volume of cars					
Joint Probability	p(X = x, Y = y) p (X = minivan, Y= European) = 0.1481				
Marginal Probability	p (X=x) = $\sum_{b= \text{all values of } Y}$ p(X=x,Y=b)				
	p(X = minivan) = 0.0741 + 0.1111 + 0.1481 = 0.3333				
Conditional probability	p(X = x | Y = y) = p(X = x, Y = y) / p(Y = y) p(Y = European | X = minivan) = 0.1481 / (0.0741 + 0.1111 + 0.1481) = 0.4433				

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Outline

- Supervised Learning (I): Two major categories
  - Regression
  - Classification

What is the difference between these two categories?

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Regression: Continuous Outcome (Y)

- Linear Regression

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Linear Regression: Simple vs Multiple linear regression

- Simple linear regression & Multiple linear regression

  You need to understand:
  - Loss function: sum of squared loss (SSL), sum of squared residual (SSR), or residual sum of squares (RSS)
  - Estimation: Least square, the best fit line
  - Accuracy checking/quality of model fit: Residual standard error (RSE), R-squared (R^2), Mean squared error (MSE),

    or use simulation (not required for this course).

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Simple linear regression

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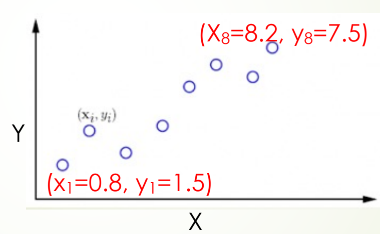
Simple linear regression (1)

- Simple linear regression: only 1 predictor/explanatory variable/attribute (X); outcome is continuous variable (Y)

Faked data:

ID	X	Y
1	0.8	1.5
2	2.1	2.5
3	3.2	2.4
4	4.1	2
5	5.2	5.3
6	6.0	6.4
7	7.2	6.1
8	8.2	7.5

Regress Y on X: Predict Y based on X



Assuming approximately linear relationship, how would you write this relationship mathematically?
(next slides)

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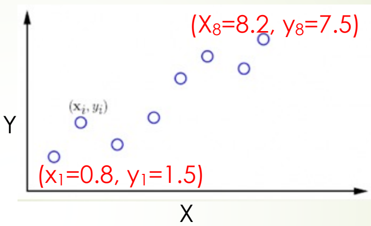
Simple linear regression (2)

$$Y = f(X) + \epsilon$$



If this unknown function *f* is approximately linear, then

$$f(X) = \beta_0 + \beta_1 X$$

How can you find Betas?

So,

$Y = \beta_0 + \beta_1 X + \epsilon$ for Population

β_0 : intercept; when X =0, Y =?

β_1 : Slope, the average increase in Y given one unit increase in X

ϵ : a mean-zero random error term

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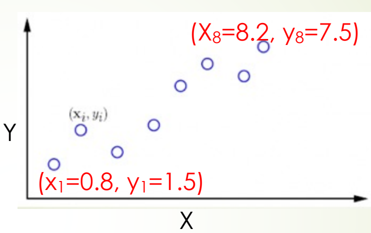
Simple linear regression (3)

ID	X	Y
1	0.8	1.5
2	2.1	2.5
3	3.2	2.4
4	4.1	2
5	5.2	5.3
6	6.0	6.4
7	7.2	6.1
8	8.2	7.5



Given this sample, how would you find the estimates for Betas, $\hat{\beta}_0$ $\hat{\beta}_1$?

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$$

Hint: How do you define a line?

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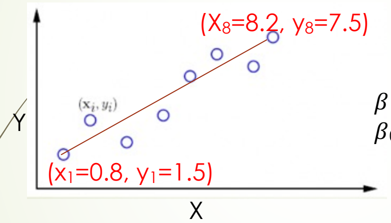
Simple linear regression (4)

- A Fit line



β_1= (7.5 -1.5)/(8.2-0.8) = 6/7.4
β_0= sum (1.5 + …+7.5)/8 = avg (Y)

Is this the best fit line?

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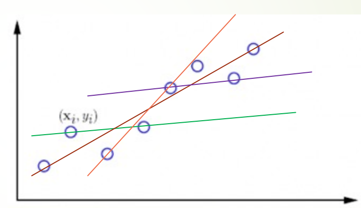
Simple linear regression (5)

- A few Fit lines based on sample data

ID	X	Y
1	0.8	1.5
2	2.1	2.5
3	3.2	2.4
4	4.1	2
5	5.2	5.3
6	6.0	6.4
7	7.2	6.1
8	8.2	7.5



Is one of them the best line?

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Simple linear regression: Loss function

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Simple linear regression-Loss function

To find the best fit line with best estimated $\hat{\beta}_0$ $\hat{\beta}_1$, we need to find the function *f*, that minimizes the sum of squared loss (SSL)

Loss function: defines the penalty for predicting $\hat{y}$ when the true value is y. (ie., penalizing errors in prediction)

- Loss function for regression:

$$L(y, \hat{y}) = (y - \hat{y})^2$$

Recall: sum of squared loss (SSL), sum of squared residual (SSR), or residual sum of squares (RSS), refer to the same thing.

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Simple linear regression—(Ordinary) Least Squares Estimation

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Simple linear regression: Ordinary) Least Squares Estimation (I)

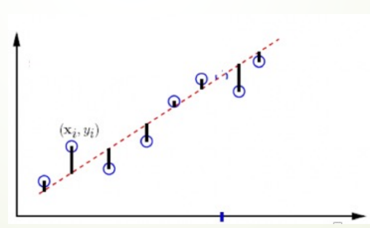
Likewise, in statistics, we call Least Squares (LSQ), or Ordinary Least Squares (OLS) to estimate $\hat{\beta}_0$ $\hat{\beta}_1$, and find the best line

Let $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$ be predication for y based on x_i

ID	X	Y
1	0.8	1.5
2	2.1	2.5
3	3.2	2.4
4	4.1	2
5	5.2	5.3
6	6.0	6.4
7	7.2	6.1
8	8.2	7.5

Step 1: Compute residual (ie, loss)

$$e_i = y_i - \hat{y}_i$$



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Simple linear regression: (Ordinary) Least Squares Estimation (II)

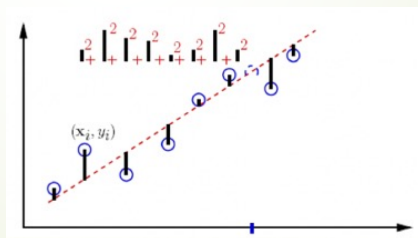
ID	X	Y
1	0.8	1.5
2	2.1	2.5
3	3.2	2.4
4	4.1	2
5	5.2	5.3
6	6.0	6.4
7	7.2	6.1
8	8.2	7.5

Step 2: Compute residual sum of squares (RSS). recall, also called as sum of squared residuals (SSR) or sum of squared loss (SSL).

$$\mathrm{RSS} = e_1^2 + e_2^2 + \cdots + e_n^2$$

Equivalently,

$$\mathrm{RSS} = (y_1 - \hat{\beta}_0 - \hat{\beta}_1 x_1)^2 + (y_2 - \hat{\beta}_0 - \hat{\beta}_1 x_2)^2 + \ldots + (y_n - \hat{\beta}_0 - \hat{\beta}_1 x_n)^2$$



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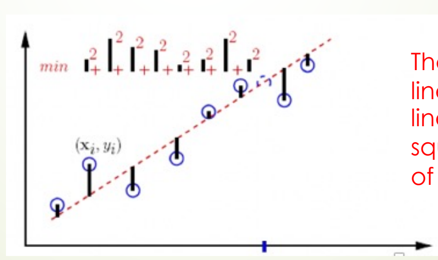
Simple linear regression: (Ordinary) Least Squares Estimation (III)

ID	X	Y
1	0.8	1.5
2	2.1	2.5
3	3.2	2.4
4	4.1	2
5	5.2	5.3
6	6.0	6.4
7	7.2	6.1
8	8.2	7.5

Step 3: use calculus to find the values of $\hat{\beta}_0$ $\hat{\beta}_1$ that give the minimum RSS/SSR/SSL.

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} \qquad \hat{\beta}_1 = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

where $\bar{y} \equiv \frac{1}{n}\sum_{i=1}^{n} y_i$ and $\bar{x} \equiv \frac{1}{n}\sum_{i=1}^{n} x_i$ are the sample means



The dashed red line is the best fit line with least squares estimates of $\hat{\beta}_0$ $\hat{\beta}_1$

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Suppl.: Simple linear regression:(Ordinary) Least Squares Estimation (III) deviation of betas

SSR, the quantity to minimize.

$$
\begin{aligned}
SSR &= \sum_{i=1}^{n}(y_i - (\beta_0 + \beta_1 x_i))^2 \\
&= \sum_{i=1}^{n}\left(y_i^2 - 2y_i(\beta_0 + \beta_1 x_i) + \beta_0^2 + 2\beta_0\beta_1 x_i + \beta_1^2 x_i^2\right)
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial SSR}{\partial \beta_0} &= \sum_{i=1}^{n}(-2y_i + 2\beta_0 + 2\beta_1 x_i) \\
0 &= \sum_{i=1}^{n}\left(-y_i + \hat\beta_0 + \hat\beta_1 x_i\right) \\
0 &= -n\bar y + n\hat\beta_0 + \hat\beta_1 n\bar x \\
\hat\beta_0 &= \bar y - \hat\beta_1 \bar x \\
\frac{\partial SSR}{\partial \beta_1} &= \sum_{i=1}^{n}\left(-2x_i y_i + 2\beta_0 x_i + 2\beta_1 x_i^2\right) \\
0 &= -\sum_{i=1}^{n} x_i y_i + \hat\beta_0 \sum_{i=1}^{n} x_i + \hat\beta_1 \sum_{i=1}^{n} x_i^2 \\
0 &= -\sum_{i=1}^{n} x_i y_i + (\bar y - \hat\beta_1 \bar x)\sum_{i=1}^{n} x_i + \hat\beta_1 \sum_{i=1}^{n} x_i^2 \\
\hat\beta_1 &= \frac{\sum_{i=1}^{n} x_i(y_i - \bar y)}{\sum_{i=1}^{n} x_i(x_i - \bar x)}
\end{aligned}
$$

See details in Section 9.4 of Chapter 9 Simple Linear Regression at http://www.stat.cmu.edu/~hseltman/309/Book/chapter9.pd

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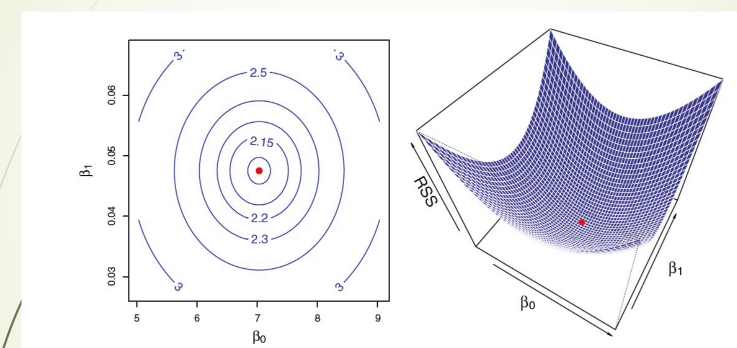
Example: the least squares estimates $\hat\beta_0$ $\hat\beta_1$ for Advertising data (ISLR_chpt3)



Contour and three-dimensional plots of the RSS on the Advertising data, using sales as the response and TV as the predictor. The red dots correspond to the least squares estimates: $\hat\beta_0$ =7.03. $\hat\beta_1$ =0.0475

Recall: ISLR refers to the book called An introduction to statistical learning with application in R

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Multiple linear regression

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Multiple linear regression (1)

- Multiple linear regression: Multiple dimensions (i.e., multiple X, called multiple regression)

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p + \epsilon,$$

- Predict the response Y on the basis of a set of values for the predictors $X_1, X_2, \ldots, X_p$, where p = number of predictors

Multiple linear regression (2)

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- Multiple linear regression:
  - Find the Least squares plane ("the best fit plane", e.g. 2-Dimensions/Predictors) ; hyperplane, if *d*-Dimensions.

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \cdots + \hat{\beta}_p X_p$$

Choose $\beta_0, \beta_1, \ldots, \beta_p$. to minimize the SSR using the same Least squares approach.

$$\begin{aligned} \text{RSS} &= \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \\ &= \sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{i1} - \hat{\beta}_2 x_{i2} - \cdots - \hat{\beta}_p x_{ip})^2 \end{aligned}$$

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

where **X** is the matrix with all ones in the first column (for the intercept)

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Example: Least squares plane

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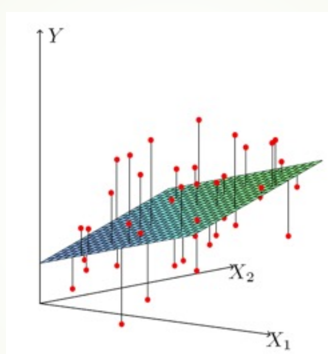

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linear regression: Accuracy Checking/Quality of Model Fit

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Linear regression Accuracy Checking

Faked example:

Quantity	Value
Residual standard error	1.69
R^2	0.897
F-statistic	570

- **Residual Standard Error (RSE)**: an estimate of the standard deviation of error term ϵ. Roughly speaking, it is the average amount that the response will deviate from the true regression line

$$\mathrm{RSE} = \sqrt{\frac{1}{n-p-1}\mathrm{RSS}}.$$

Simple linear regression: p =1. $\mathrm{RSE} = \sqrt{\frac{1}{n-2}\mathrm{RSS}}$

The RSE is considered a measure of the lack of fit of the model to the data: the smaller the better.

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Linear regression Accuracy Checking

Faked example:

Quantity	Value
Residual standard error	1.69
R^2	0.897
F-statistic	570

$$R^2 = \frac{\mathrm{TSS} - \mathrm{RSS}}{\mathrm{TSS}} = 1 - \frac{\mathrm{RSS}}{\mathrm{TSS}}$$

where $\mathrm{TSS} = \sum(y_i - \bar{y})^2$ is the *total sum of squares*.

- R^2 : the fraction of variance in Y explained by X, it is the square of the correlation between the response and the fitted linear model. E.g., 89.7% of variance in Y is explained by X in this example.
  R^2 : the larger the better.
  In the **simple** linear regression setting, $R^2 = r^2$ (r: correlation coefficient)

Adjusted R^2: adjusted for the number of predictors in the model: the larger the better.

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Linear regression Accuracy Checking

Faked example:

Quantity	Value
Residual standard error	1.69
R^2	0.897
F-statistic	570

$$F = \frac{(\mathrm{TSS} - \mathrm{RSS})/p}{\mathrm{RSS}/(n-p-1)}$$

- F-statistics: assess multiple coefficients simultaneously; compare the fitted model with the intercept model; if significant, the fitted model is better.

  e.g. 570 is significantly larger than 1 and at least one of X must be related to the outcome/response.

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Linear regression Accuracy Checking

- Mean Squared Error:

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{f}(x_i))^2$$

That is, MSE = RSS/n

- Root Mean Squared Error (RMSE)= Sqrt (MSE)

Note: MSE and RMSE Generic criteria for regression (Y is a continuous variable)

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Reading assignments:

- Review Lecture 5 Slides, and read
  - Simple linear regression: Section 9.4-9.5 (Must); Section 9.6-9.7 (Encouraged) http://www.stat.cmu.edu/~hseltman/309/Book/chapter9.pdf,
  - ISLR Chapter 3.1 and 3.2:

ISLR: An Introduction To Statistical Learning, (2013) Gareth James, Daniela Witten, Trevor Hastie, Robert Tibshirani, 2013, ISBN: 9781461471387 (online) and 9781461471370.

Will use ISLR to refer to this book from now on.

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