# VBM683 Machine Learning 

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Slides are adapted from
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## Classification

- Input: X
- Real valued, vectors over real.
- Discrete values ( $0,1,2, \ldots$ )
- Other structures (e.g., strings, graphs, etc.)
- Output: $Y$
- Discrete (0,1,2,...)



Science News
$Y=$ Topic


## Regression

- Input: X
- Real valued, vectors over real.
- Discrete values ( $0,1,2, \ldots$ )
- Other structures (e.g., strings, graphs, etc.)
- Output: $Y$

- Real valued, vectors over real.



## What should I watch tonight?



## 1-NN for Regression



## 1-NN for Regression

## - Often bumpy (overfits)



## 9-NN for Regression

## - Often bumpy (overfits)




## Simple 1-D Regression



- Circles are data points (i.e., training examples) that are given to us
- The data points are uniform in $x$, but may be displaced in $y$

$$
t(x)=f(x)+\varepsilon
$$

with $\varepsilon$ some noise

- In green is the "true" curve that we don't know


## What is a Model?

1. Often Describe Relationship between Variables
2. Types

- Deterministic Models (no randomness)
- Probabilistic Models (with randomness)


## Deterministic Models

1. Hypothesize Exact Relationships
2. Suitable When Prediction Error is Negligible
3. Example: Body mass index (BMI) is measure of body fat based
$-B M I=\frac{\text { Weight in Kilograms }}{(\text { Height in Meters })^{2}}$

## Probabilistic Models

1. Hypothesize 2 Components

- Deterministic
- Random Error

2. Example: Systolic blood pressure of newborns Is 6 Times the Age in days + Random Error

- $S B P=6 \times$ age $(\mathrm{d})+\varepsilon$
- Random Error May Be Due to Factors Other Than age in days (e.g. Birthweight)


## Types of Probabilistic Models

## Probabilistic Models

## Regression

 Models
## Correlation Models

# Other <br> Models 

## Simple Regression

- Simple regression analysis is a statistical tool that gives us the ability to estimate the mathematical relationship between a dependent variable (usually called y) and an independent variable (usually called x).
- The dependent variable is the variable for which we want to make a prediction.
- While various non-linear forms may be used, simple linear regression models are the most common.


## Introduction

- The primary goal of quantitative analysis is to use current information about a phenomenon to predict its future behavior.
- Current information is usually in the form of a set of data.
- In a simple case, when the data form a set of pairs of numbers, we may interpret them as representing the observed values of an independent (or predictor or explanatory) variable X and a dependent ( or response or outcome) variable Y.

| lot size | Man-hours |
| :---: | :---: |
| 30 | 73 |
| 20 | 50 |
| 60 | 128 |
| 80 | 170 |
| 40 | 87 |
| 50 | 108 |
| 60 | 135 |
| 30 | 69 |
| 70 | 148 |
| 60 | 132 |

## Introduction

- The goal of the analyst who studies the data is to find a functional relation
between the response variable $y$ and the predictor variable x .

$$
y=f(x)
$$



## Pictorial Presentation of Linear Regression Model



## Types of Regression Models

## 1 Explanatory Variable

Regression Models

2+ Explanatory Variables

## Multiple

## Linear Regression Model



## Assumptions

- Linear regression assumes that...
- 1. The relationship between $X$ and $Y$ is linear
- 2. Y is distributed normally at each value of X
- 3. The variance of $Y$ at every value of $X$ is the same (homogeneity of variances)
- 4. The observations are independent


## Linear Equations



## Linear Regression Model

- 1. Relationship Between Variables Is a Linear Function

$$
\begin{aligned}
& \begin{array}{c}
\text { Population } \\
\text { Y-Intercept }
\end{array} \quad \begin{array}{c}
\text { Population } \\
\text { Slope }
\end{array} \\
& \qquad Y_{i}=\beta_{0}+\beta_{1} X_{i}+\varepsilon_{i}
\end{aligned}
$$

Dependent
(Response)
Variable (e.g., CD+ c.)

Independent (Explanatory) Variable (e.g., Years s. serocon.)

## Meaning of Regression Coefficients

- General regression model

1. $\beta_{0}$, and $\beta_{1}$ are parameters
2. X is a known constant
3. Deviations $\varepsilon$ are independent $\mathrm{N}\left(\mathrm{o}, \sigma^{2}\right)$

- The values of the regression parameters $\beta_{0}$, and $\beta_{1}$ are not known. We estimate them from data.
- $\beta_{1}$ indicates the change in the mean response per unit increase in $X$.


## Population Linear Regression Model



## Estimating Parameters: Least Squares Method

## Scatter plot

- 1. Plot of All $\left(X_{i}, Y_{i}\right)$ Pairs
- 2. Suggests How Well Model Will Fit



## Thinking Challenge

How would you draw a line through the points? How do you determine which line 'fits best'?


## Thinking Challenge

How would you draw a line through the points? How do you determine which line 'fits best'?


Intercept unchanged

## Thinking Challenge

How would you draw a line through the points? How do you determine which line 'fits best'?

Slope unchanged


## Thinking Challenge

How would you draw a line through the points? How do you determine which line 'fits best'?


## What is the best fitting line

| $\boldsymbol{i}$ | $x_{i}$ | $y_{i}$ | $\hat{y}_{i}$ |
| :--- | :--- | :--- | :--- |
| 1 | 63 | 127 | 120.1 |
| 2 | 64 | 121 | 126.3 |
| 3 | 66 | 142 | 138.5 |
| 4 | 69 | 157 | 157.0 |
| 5 | 69 | 162 | 157.0 |
| 6 | 71 | 156 | 169.2 |
| 7 | 71 | 169 | 169.2 |
| 8 | 72 | 165 | 175.4 |
| 9 | 73 | 181 | 181.5 |
| 10 | 75 | 208 | 193.8 |



$$
\hat{y}_{i}=b_{0}+b_{1} x_{i}
$$

- $y_{i}$ denotes the observed response for experimental unit $i$
- $x_{i}$ denotes the predictor value for experimental unit $i$
- $\hat{y}_{i}$ is the predicted response (or fitted value) for experimental unit $i$


## Prediction Error



| $\boldsymbol{w}=\mathbf{- 3 3 1 . 2}+\mathbf{7 . 1} \boldsymbol{l}$ (the dashed line) |  |  |  |  |  |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $\boldsymbol{i}$ | $x_{i}$ | $y_{i}$ | $\hat{y}_{\boldsymbol{i}}$ | $\left(y_{i}-\hat{y}_{i}\right)$ | $\left(y_{i}-\hat{y}_{i}\right)^{\mathbf{2}}$ |
| 1 | 63 | 127 | 116.1 | 10.9 | 118.81 |
| 2 | 64 | 121 | 123.2 | -2.2 | 4.84 |
| 3 | 66 | 142 | 137.4 | 4.6 | 21.16 |
| 4 | 69 | 157 | 158.7 | -1.7 | 2.89 |
| 5 | 69 | 162 | 158.7 | 3.3 | 10.89 |
| 6 | 71 | 156 | 172.9 | -16.9 | 285.61 |
| 7 | 71 | 169 | 172.9 | -3.9 | 15.21 |
| 8 | 72 | 165 | 180.0 | -15.0 | 225.00 |
| 9 | 73 | 181 | 187.1 | -6.1 | 37.21 |
| 10 | 75 | 208 | 201.3 | 6.7 | 44.89 |
|  |  |  |  |  |  |
|  |  |  |  |  | $\mathbf{7 6 6 . 5}$ |


| $w=-\mathbf{2 6 6 . 5 3}+6.1376 \boldsymbol{l}$ (the solid line) |  |  |  |  |  |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $\boldsymbol{i}$ | $x_{i}$ | $y_{i}$ | $\hat{y}_{i}$ | $\left(y_{i}-\hat{y}_{i}\right)$ | $\left(y_{i}-\hat{y}_{i}\right)^{2}$ |
| 1 | 63 | 127 | 120.139 | 6.8612 | 47.076 |
| 2 | 64 | 121 | 126.276 | -5.2764 | 27.840 |
| 3 | 66 | 142 | 138.552 | 3.4484 | 11.891 |
| 4 | 69 | 157 | 156.964 | 0.0356 | 0.001 |
| 5 | 69 | 162 | 156.964 | 5.0356 | 25.357 |
| 6 | 71 | 156 | 169.240 | -13.2396 | 175.287 |
| 7 | 71 | 169 | 169.240 | -0.2396 | 0.057 |
| 8 | 72 | 165 | 175.377 | -10.3772 | 107.686 |
| 9 | 73 | 181 | 181.515 | -0.5148 | 0.265 |
| 10 | 75 | 208 | 193.790 | 14.2100 | 201.924 |
|  |  |  |  |  |  |
|  |  |  |  |  | $\mathbf{5 9 7 . 4}$ |

$$
\begin{aligned}
e_{i} & =y_{i}-\hat{y}_{i} \\
Q & =\sum_{i=1}^{n}\left(y_{i}-\hat{y}_{i}\right)^{2}
\end{aligned}
$$

## Least Squares

- 1. 'Best Fit' Means Difference Between Actual Y Values \& Predicted Y Values Are a Minimum. But Positive Differences Off-Set Negative. So square errors!

- 2. LS Minimizes the Sum of the Squared Differences (errors) (SSE)


## Least Squares Graphically

$$
\text { LS minimizes } \sum_{i=1}^{n} \hat{\varepsilon}_{i}^{2}=\hat{\varepsilon}_{1}^{2}+\hat{\varepsilon}_{2}^{2}+\hat{\varepsilon}_{3}^{2}+\hat{\varepsilon}_{4}^{2}
$$

$$
\left\{\begin{array}{l}
\hat{y}_{2}=\hat{\boldsymbol{\beta}}_{0}+\hat{\boldsymbol{\beta}}_{1} \boldsymbol{X}_{\mathbf{2}}+\hat{\varepsilon}_{2} \\
\hat{\varepsilon}_{2}
\end{array}\right.
$$

## Coefficient Equations

- Prediction equation

$$
\hat{y}_{i}=\hat{\beta}_{0}+\hat{\beta}_{1} x_{i}
$$

- Sample slope

$$
\hat{\beta}_{1}=\frac{S S_{x y}}{S S_{x x}}=\frac{\sum\left(x_{i}-\bar{x}\right)\left(y_{i}-\bar{y}\right)}{\sum\left(x_{i}-\bar{x}\right)^{2}}
$$

- Sample Y - intercept

$$
\hat{\beta}_{0}=\bar{y}-\hat{\beta}_{1} \bar{x}
$$

## Derivation of Parameters (1)

- Least Squares (L-S):

Minimize squared error

$$
\begin{aligned}
& \sum_{i=1}^{n} \varepsilon_{i}^{2}=\sum_{i=1}^{n}\left(y_{i}-\beta_{0}-\beta_{1} x_{i}\right)^{2} \\
& 0=\frac{\partial \sum \varepsilon_{i}^{2}}{\partial \beta_{0}}=\frac{\partial \sum\left(y_{i}-\beta_{0}-\beta_{1} x_{i}\right)^{2}}{\partial \beta_{0}} \\
& =-2\left(n \bar{y}-n \beta_{0}-n \beta_{1} \bar{x}\right) \\
& \hat{\beta}_{0}=\bar{y}-\hat{\beta}_{1} \bar{x}
\end{aligned}
$$

## Derivation of Parameters (1)

- Least Squares (L-S):

Minimize squared error

$$
\begin{aligned}
& 0=\frac{\partial \sum \varepsilon_{i}^{2}}{\partial \beta_{1}}= \frac{\partial \sum\left(y_{i}-\beta_{0}-\beta_{1} x_{i}\right)^{2}}{\partial \beta_{1}} \\
&=-2 \sum x_{i}\left(y_{i}-\beta_{0}-\beta_{1} x_{i}\right) \\
&=-2 \sum x_{i}\left(y_{i}-\bar{y}+\beta_{1} \bar{x}-\beta_{1} x_{i}\right) \\
& \beta_{1} \sum x_{i}\left(x_{i}-\bar{x}\right)=\sum x_{i}\left(y_{i}-\bar{y}\right) \\
& \beta_{1} \sum\left(x_{i}-\bar{x}\right)\left(x_{i}-\bar{x}\right)=\sum\left(x_{i}-\bar{x}\right)\left(y_{i}-\bar{y}\right) \\
& \hat{\beta}_{1}=\frac{S S_{x y}}{S S_{x x}}
\end{aligned}
$$

## Computation Table

| $X_{i}$ | $Y_{i}$ | $X_{i}^{2}$ | $Y_{i}^{2}$ | $X_{i} Y_{i}$ |
| :---: | :---: | :---: | :---: | :---: |
| $X_{1}$ | $Y_{1}$ | $X_{1}{ }^{2}$ | $Y_{1}{ }^{2}$ | $X_{1} Y_{1}$ |
| $X_{2}$ | $Y_{2}$ | $X_{2}{ }^{2}$ | $Y_{2}{ }^{2}$ | $X_{2} Y_{2}$ |
| $:$ | $:$ | $:$ | $:$ | $:$ |
| $X_{n}$ | $Y_{n}$ | $X_{n}{ }^{2}$ | $Y_{n}{ }^{2}$ | $X_{n} Y_{n}$ |
| $\Sigma X_{i}$ | $\Sigma Y_{i}$ | $\Sigma X_{i}^{2}$ | $\Sigma Y_{i}^{2}$ | $\Sigma X_{i} Y_{i}$ |

## Interpretation of Coefficients

- 1. Slope $\left(\beta_{1}\right)$
- Estimated $Y$ Changes by $\beta_{1}$ for Each 1 Unit Increase in $X$
- If $\beta_{1}=2$, then $Y$ Is Expected to Increase by 2 for Each 1 Unit Increase in $X$
- 2. Y -Intercept $\left(\beta_{0}\right)$
- Average Value of $Y$ When $X=0$
- If $\beta_{0}=4$, then Average $Y$ Is Expected to Be 4 When $X$ Is 0


## Parameter Estimation Example

- Obstetrics: What is the relationship between Mother's Estriol level \& Birthweight using the following data?
$\frac{\text { Estriol }}{(\mathrm{mg} / 24 \mathrm{~h})}$
1
2
3
4
5


## Birthweight

( $\mathrm{g} / 1000$ ) 1
1
2
2
4


## Scatterplot

## Birthweight vs. Estriol level



## Parameter Estimation Solution Table

| $X_{i}$ | $Y_{i}$ | $X_{i}^{2}$ | $Y_{i}^{2}$ | $X_{i} Y_{i}$ |
| :---: | :---: | :---: | :---: | :---: |
| 1 | 1 | 1 | 1 | 1 |
| 2 | 1 | 4 | 1 | 2 |
| 3 | 2 | 9 | 4 | 6 |
| 4 | 2 | 16 | 4 | 8 |
| 5 | 4 | 25 | 16 | 20 |
| 15 | 10 | 55 | 26 | 37 |

## Parameter Estimation Solution

$$
\begin{aligned}
& \hat{\beta}_{1}=\frac{\sum_{i=1}^{n} X_{i} Y_{i}-\frac{\left(\sum_{i=1}^{n} X_{i}\right)\left(\sum_{i=1}^{n} Y_{i}\right)}{n}}{\sum_{i=1}^{n} X_{i}^{2}-\frac{\left(\sum_{i=1}^{n} X_{i}\right)^{2}}{n}}=\frac{37-\frac{(15)(10)}{5}}{55-\frac{(15)^{2}}{5}}=0.70 \\
& \hat{\beta}_{0}=\bar{Y}-\hat{\beta}_{1} \bar{X}=2-(0.70)(3)=-0.10
\end{aligned}
$$

## How to estimate parameters

We minimize the equation for the sum of the squared prediction errors:

$$
Q=\sum_{i=1}^{n}\left(y_{i}-\left(b_{0}+b_{1} x_{i}\right)\right)^{2}
$$

(that is, take the derivative with respect to $b_{0}$ and $b_{1}$, set to 0 , and solve for $b_{0}$ and $b_{1}$ ) and get the "least squares estimates" for $b_{0}$ and $b_{1}$ :

$$
b_{1}=\frac{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)\left(y_{i}-\bar{y}\right)}{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}} \quad b_{0}=\bar{y}-b_{1} \bar{x}
$$


the least squares line passes through the point $(\bar{x}, \bar{y})$, since when $x=\bar{x}$, then $y=b_{0}+b_{1} \bar{x}=\bar{y}-b_{1} \bar{x}+b_{1} \bar{x}=\bar{y}$.

## Estimating the intercept and slope: least squares estimation

** Least Squares Estimation
A little calculus....
What are we trying to estimate? $\beta$, the slope, from

What's the constraint? We are trying to minimize the squared distance (hence the "least squares") between the observations themselves and the predicted values, or (also called the "residuals", or leftover unexplained variability)

$$
\text { Differencei }=y i-(\beta x+\alpha) \quad \text { Differencei }^{2}=(y i-(\beta x+\alpha))^{2}
$$

Find the $\beta$ that gives the minimum sum of the squared differences. How do you maximize a function? Take the derivative; set it equal to zero; and solve. Typical max/min problem from calculus....

$$
\begin{aligned}
& \frac{d}{d \beta} \sum_{i=1}^{n}\left(y_{i}-\left(\beta x_{i}+\alpha\right)\right)^{2}=2\left(\sum_{i=1}^{n}\left(y_{i}-\beta x_{i}-\alpha\right)\left(-x_{i}\right)\right) \\
& \mathrm{F} \quad 2\left(\sum_{i=1}^{n}\left(-y_{i} x_{i}+\beta x_{i}^{2}+\alpha x_{i}\right)\right)=0 \ldots
\end{aligned}
$$

The standard error of $Y$ given $X$ is the average variability around the regression line at any given value of $X$. It is assumed to be equal at all values of $X$.



## Regression Picture



## Regression Line

- If the scatter plot of our sample data suggests a linear relationship between two variables i.e.
we can summarize the relationship by drawing a straight line on the plot.
- Least squares method give us the "best" estimated line for our set of sample data.


## Regression Line

- We will write an estimated regression line based on sample data as
- The method of least squares chooses the values for $\mathrm{b}_{0}$, and $\mathrm{b}_{1}$ to minimize the sum $\hat{y} b_{\text {of }}^{+} b_{\text {s }} x$ squared errors

$$
S S E=\sum_{i=1}^{n}\left(y_{i}-\hat{y}_{i}\right)^{2}=\sum_{i=1}^{n}\left(y-b_{0}-b_{1} x\right)^{2}
$$

## Regression Line

- Using calculus, we obtain estimating formulas:

Or

$$
\begin{gathered}
b_{1}=\frac{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)\left(y_{i}-\bar{y}\right)}{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}=\frac{n \sum_{i=1}^{n} x_{i} y_{i}-\sum_{i=1}^{n} x_{i} \sum_{i=1}^{n} y_{i}}{n \sum_{i=1}^{n} x_{i}^{2}-\left(\sum_{i=1}^{n} x_{i}\right)^{2}} \\
b_{1}=r \frac{S_{y}}{S_{x}} \\
b_{0}=\bar{y}-b_{1} \bar{x}
\end{gathered}
$$

## Probabilistic Models

## Probabilistic Models

Regression Models

Correlation Models

# Other Models 

## Correlation vs. regression

- Both variables are treated the same in correlation; in regression there is a predictor and a response
- In regression the x variable is assumed non-random or measured without error
- Correlation is used in looking for relationships, regression for prediction


## Correlation Models

- 1. Answer 'How Strong Is the Linear Relationship Between 2 Variables?'
- 2. Coefficient of Correlation Used
- Population Correlation Coefficient Denoted $\rho$ (Rho)
- Values Range from -1 to +1
- Measures Degree of Association
- 3. Used Mainly for Understanding


## Covariance

$$
\operatorname{cov}(x, y)=\frac{\sum_{i=1}^{n}\left(x_{i}-\bar{X}\right)\left(y_{i}-\bar{Y}\right)}{n-1}
$$

# Interpreting Covariance 

$\operatorname{cov}(X, Y)>0 \rightarrow X$ and $Y$ are positively correlated $\operatorname{cov}(X, Y)<0 \rightarrow X$ and $Y$ are inversely correlated $\operatorname{cov}(X, Y)=0 \rightarrow X$ and $Y$ are independent

# Correlation coefficient 

- Pearson's Correlation Coefficient is standardized covariance (unitless):

$$
r=\frac{\operatorname{covariance}(x, y)}{\sqrt{\operatorname{var} x} \sqrt{\operatorname{var} y}}
$$

## Correlation

- Measures the relative strength of the linear relationship between two variables
- Unit-less
- Ranges between -1 and 1
- The closer to -1 , the stronger the negative linear relationship
- The closer to 1 , the stronger the positive linear relationship
- The closer to 0 , the weaker any positive linear relationship


## Sample Coefficient of Correlation

- 1. Pearson Product Moment Coefficient of Correlation between $x$ and $y$ :

$$
r=\frac{\sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)\left(Y_{i}-\bar{Y}\right)}{\sqrt{\sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}} \cdot \sqrt{\sum_{i=1}^{n}\left(Y_{i}-\bar{Y}\right)^{2}}}=\frac{S S_{x y}}{\sqrt{S S_{x x} S S_{y y}}}
$$

## Coefficient of Correlation Values



# Coefficient of Correlation Values 



## Coefficient of Correlation Values



Increasing degree of negative correlation

## Coefficient of Correlation Values

## Perfect <br> Negative <br> Correlation <br> Correlation <br>  <br> $\stackrel{7}{7}$ <br> $-1.0 \quad-.5$ <br> 0 <br> $+.5 \quad+1.0$

## Coefficient of Correlation Values



Increasing degree of positive correlation

## Coefficient of Correlation Values



## Scatter Plots of Data with

 Various Correlation Coefficients
-Slide from: Statistics for Managers Using Microsoft® Excel 4th Edition, 2004 Prentice-Hall

## Linear Correlation


-Slide from: Statistics for Managers Using Microsoft® Excel 4th Edition, 2004 Prentice-Hall

## Linear Correlation


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-Slide from: Statistics for Managers Using Microsoft®® Excel 4th Edition, 2004 Prentice-Hall

## Calculating by hand...

$$
\hat{r}=\frac{\operatorname{covariance}(x, y)}{\sqrt{\operatorname{var} x} \sqrt{\operatorname{var} y}}=\frac{\frac{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)\left(y_{i}-\bar{y}\right)}{n-1}}{\sqrt{\frac{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}{n-1} \sqrt{\frac{\sum_{i=1}^{n}\left(y_{i}-\bar{y}\right)^{2}}{n-1}}}}
$$

## Simpler calculation formula...

Numerator of covariance

$$
\hat{r}=\frac{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)\left(y_{i}-\bar{y}\right)}{\sqrt{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}} \sqrt{\sum_{i=1}^{n}\left(y_{i}-\bar{y}\right)^{2}}}=\square \xrightarrow[r-1]{\sqrt{n-1}=\frac{S S_{x y}}{\sqrt{S S_{x} S S_{y}}}} \begin{gathered}
\\
\sum^{n}\left(x_{i}-\bar{x}\right)\left(y_{i}-\bar{y}\right)
\end{gathered} \quad \xrightarrow[\text { Numerators of variance }]{ }
$$

## Least Square estimation

Slope (beta coefficient $\hat{\beta}=\frac{\operatorname{Cov}(x, y)}{\operatorname{Var}(x)}$

Intercept Calculate : $\hat{\alpha}=\overline{\mathrm{y}}-\hat{\beta} \overline{\mathrm{x}}$

Regression line always goes throu( $\overline{10}$ th $\overline{\bar{y}}$ doint:

## Relationship with correlation

## $\hat{r}=\hat{\beta} \frac{S D_{x}}{S D_{y}}$

In correlation, the two variables are treated as equals. In regression, one variable is considered independent (=predictor) variable $(X)$ and the other the dependent (=outcome) variable $Y$.

## Residual Analysis. cneck assumptions

$$
e_{i}=Y_{i}-\hat{Y}_{i}
$$

- The residual for observation $\mathrm{i}, \mathrm{e}_{\mathrm{i}}$, is the difference between its observed and predicted value
- Residuals are highly useful for studying whether a given regression model is appropriate for the data at hand.
- Check the assumptions of regression by examining the residuals
- Examine for linearity assumption
- Examine for constant variance for all levels of X (homoscedasticity)
- Evaluate normal distribution assumption
- Evaluate independence assumption
- Graphical Analysis of Residuals
- Can plot residuals vs. X


## observed - predicted



## Residual Analysis for Linearity


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## Residual Analysis for Homoscedasticity




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## Residual Analysis for Independence


-Slide from: Statistics for Managers Using Microsoft ${ }^{(8)}$ Excel 4th Edition, 2004 Prentice-Hall

Example: weekly advertising expenditure

| $y$ | $x$ | $y$-hat | Residual (e) |
| :---: | :---: | :---: | :---: |
| 1250 | 41 | 1270.8 | -20.8 |
| 1380 | 54 | 1411.2 | -31.2 |
| 1425 | 63 | 1508.4 | -83.4 |
| 1425 | 54 | 1411.2 | 13.8 |
| 1450 | 48 | 1346.4 | 103.6 |
| 1300 | 46 | 1324.8 | -24.8 |
| 1400 | 62 | 1497.6 | -97.6 |
| 1510 | 61 | 1486.8 | 23.2 |
| 1575 | 64 | 1519.2 | 55.8 |
| 1650 | 71 | 1594.8 | 55.2 |

## Estimation of the variance of the error terms, $\sigma^{2}$

- The variance $\sigma^{2}$ of the error terms $\varepsilon_{\mathrm{i}}$ in the regression model needs to be estimated for a variety of purposes.
- It gives an indication of the variability of the probability distributions of $y$.
- It is needed for making inference concerning regression function and the prediction of $y$.


## Regression Standard Error

- To estimate $\sigma$ we work with the variance and take the square root to obtain the standard deviation.
- For simple linear regression the estimate of $\sigma^{2}$ is the average squared residual.
- To estimate $\sigma$, usiè ${ }^{2}=\frac{1}{n-2} \sum e_{i}^{2}=\frac{1}{n-2} \sum\left(y_{i}-\hat{y}_{i}\right)^{2}$
- $s$ estimates the standard deviation $\sigma$ of the error term $\varepsilon$ in the statistical model for simple linear regression.


## Regression Standard Error

| $y$ | $\times$ | y-hat | Residual (e) | square(e) |
| :---: | :---: | :---: | :---: | :---: |
| 1250 | 41 | 1270.8 | -20.8 | 432.64 |
| 1380 | 54 | 1411.2 | -31.2 | 973.44 |
| 1425 | 63 | 1508.4 | -83.4 | 6955.56 |
| 1425 | 54 | 1411.2 | 13.8 | 190.44 |
| 1450 | 48 | 1346.4 | 103.6 | 10732.96 |
| 1300 | 46 | 1324.8 | -24.8 | 615.04 |
| 1400 | 62 | 1497.6 | -97.6 | 9525.76 |
| 1510 | 61 | 1486.8 | 23.2 | 538.24 |
| 1575 | 64 | 1519.2 | 55.8 | 3113.64 |
| 1650 | 71 | 1594.8 | 55.2 | 3047.04 |
| $y$-hat $=828+10.8 x$ |  |  | total | 36124.76 |
|  |  |  | $S_{y . x}$ | 67.19818 |

## Residual plots

- The points in this residual plot have a curve pattern, so a straight line fits poorly



## Residual plots

- The points in this plot show more spread for larger values of the explanatory variable $x$, so prediction will be less accurate when $x$ is large.



## Variable transformations

- If the residual plot suggests that the variance is not constant, a transformation can be used to stabilize the variance.
- If the residual plot suggests a non linear relationship between $x$ and $y$, a transformation may reduce it to one that is approximately linear.
- Common linearizing transformations are:
- Variance stabilizing ${ }_{1}^{1}$ rathsformations are:

$$
\frac{1}{y}, \log (y), \quad \sqrt{y}, \quad y^{2}
$$

## 2 predictors: age and vit D...



## Different 3D view...



## Fit a plane rather than a line...



On the plane, the slope for vitamin $D$ is the same at every age; thus, the slope for vitamin D represents the effect of vitamin $D$ when age is held constant.

