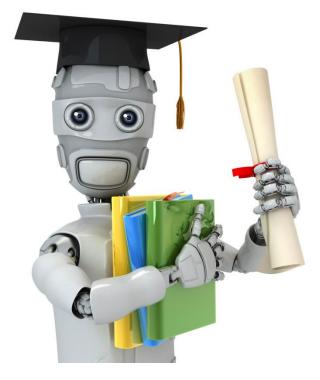


Linear regression

Fouad Hadj Selem

Machine Learning

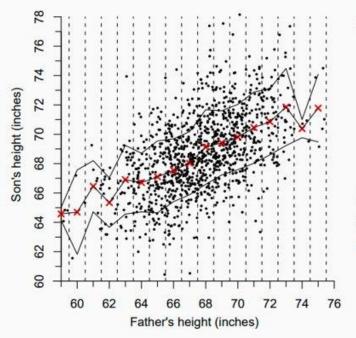


Machine Learning

Linear regression with one variable

Example 1: Pearson's Father-and-Son Data

Father-son pairs are grouped by father's height, to the nearest inch.

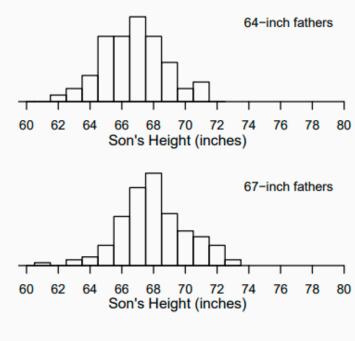


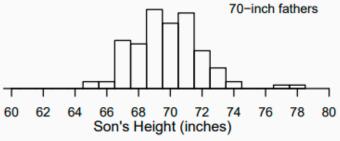
How do the

- mean of son's height (SH),
- · SD of SH, and
- distribution of SH (histogram of SH)?

within each group change with father's height (FH)?

Example 1: Pearson's Father-and-Son Data





Simple Linear Regression Model

Pearson's father-and-son data inspire the following assumptions for the simple linear regression (SLR) model:

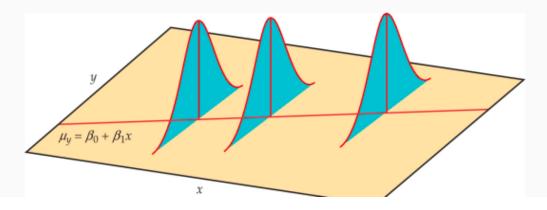
1. The means of Y is a linear function of X, i.e.,

$$E(Y|X=x) = \beta_0 + \beta_1 x$$

2. The SD of Y does not change with x, i.e.,

$$SD(Y|X=x) = \sigma$$
 for every x

3. (Optional) Within each subpopulation, the distribution of *Y* is normal.



Simple Linear Regression Model

Equivalently, the SLR model asserts the values of X and Y for individuals in a population are related as follows

$$Y = \beta_0 + \beta_1 X + \varepsilon$$
,

• the value of ε , called the **error** or the **noise**, varies from observation to observation, follows a normal distribution

$$\varepsilon \sim N(0,\sigma)$$

In the model, the line $y = \beta_0 + \beta_1 x$ is called the **population** regression line.

Data for a Simple Linear Regression Model

Suppose we have a SRS of *n* individuals from a population.

From individual i we observe the response y_i and the explanatory variable x_i :

$$(x_1, y_1), (x_2, y_2), (x_3, y_3), \dots, (x_n, y_n)$$

The SLR model states that

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$$

Recall in the previous lecture, the least square line of the data above is

$$y=b_0+b_1x$$

in which

$$b_1 = r \frac{s_y}{s_x} = \frac{\sum_i (x_i - \overline{x})(y_i - \overline{y})}{\sum_i (x_i - \overline{x})^2}, \quad b_0 = \overline{y} - b_1 \overline{x}$$

We can use b_1 to estimate β_1 and b_0 to estimate β_0 .

Sample v.s. Population

Note the population regression line

$$y = \beta_0 + \beta_1 x$$

is different from the least square regression line

$$y=b_0+b_1x$$

- The latter is merely the least square line for a <u>sample</u>, while the former is the least square line for the entire population.
- The values of b_0 and b_1 will change from sample to sample.

$$b_1 = r \frac{s_y}{s_x} = \frac{\sum_i (x_i - x)(y_i - y)}{\sum_i (x_i - \overline{x})^2}, \quad b_0 = \overline{y} - b_1 \overline{x}$$

We are interested in the population intercept β₀ and slope β₁,
 NOT the sample counterparts b₀ and b₁.

How Close Is b1 to β1?

Recall the slope of the least square line is

$$b_1 = \frac{\sum_i (x_i - \overline{x})(y_i - \overline{y})}{\sum_i (x_i - \overline{x})^2}$$

Under the SLR model: $y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$, replacing y_i in the formula above by $\beta_0 + \beta_1 x_i + \varepsilon_i$, we can show after some algebra that

$$b_1 = \beta_1 + \frac{\sum_i (x_i - \overline{x}) \varepsilon_i}{\sum_i (x_i - \overline{x})^2}$$

From the above, one can get the mean, the SD, and the **sampling distribution** of b_1 .

- $E(b_1) = \beta_1 \dots (b_1 \text{ is an } \mathbf{unbiased} \text{ estimate of } \beta_1)$
- SD(b₁) = ?.....(See the next slide)

Distribution of $\beta 1$

The **sampling distribution** of b_1 is normal

$$b_1 \sim N\left(\beta_1, \frac{\sigma}{\sqrt{\sum (x_i - \overline{x})^2}}\right) \Rightarrow z = \frac{b_1 - \beta_1}{\sigma / \sqrt{\sum (x_i - \overline{x})^2}} \sim N(0, 1)$$

This is (approx.) valid

- either if the errors ε_i are i.i.d. $N(0, \sigma)$
- or if the errors ε_i are independent and the sample size n is large

As σ is unknown, if replaced with s_e , the t-statistic below has a t-distribution with n-2 degrees of freedom

$$T = \frac{b_1 - \beta_1}{S_0 / \sqrt{\sum (x_i - \overline{x})^2}} = \frac{b_1 - \beta_1}{SE(b_1)} \sim t_{n-2},$$

Confidence Intervals for \$1

The $(1 - \alpha)$ confidence interval for β_1 is given as

$$b_1 \pm t^*SE(b_1)$$

where t^* is the critical value for the $t_{(n-2)}$ distribution at confidence level $1 - \alpha$.

Tests for β1

To **test the hypothesis** $H_0: \beta_1 = a$, we use the *t*-statistic

$$t = \frac{b_1 - a}{SE(b_1)} \sim t_{n-2}$$

The *p*-value can be computed using the *t*-table based on the H_a:

-	•			
H_a	$\beta_1 \neq a$	$\beta_1 < a$	$\beta_1 > a$	
P-value	- t t		1 t	

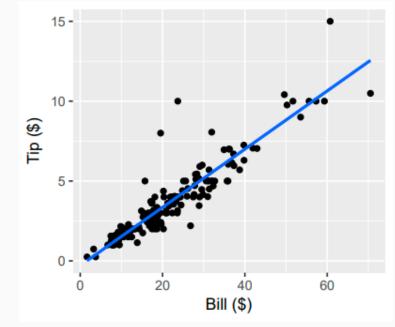
Observe that testing $H_0: \beta_1 = 0$ is equivalent to testing whether x is useful in predicting y linearly.

It is possible that *r* is small but β₁ is significantly different from
 0.

Example: Restaurant Tips

The owner of a bistro called *First Crush* in Potsdam, NY, collected 157 restaurant bills over a 2-week period that he believes provide a good sample of his customers.

He wanted to study the payment and tipping patterns of its patrons.



Regression in R

```
Regression in R is as simple as lm(y \sim x), in which "lm" stands for
"linear model"
> tips = read.table("RestaurantTips.txt",h=T)
> lm(Tip ~ Bill, data=tips)
Call:
lm(formula = Tip ~ Bill, data = tips)
Coefficients:
(Intercept)
                     Bill
                   0.1822
    -0.2923
It is better to save the model as an object,
lmtips = lm(Tip ~ Bill, data=tips)
```

and then we can get a more detailed output by viewing the summary() of

the model object. The output is shown in the next slide

Regression in R

- The column "Estimate" gives the LS estimate for the intercept $b_0 = -0.292267$ and the slope $b_1 = 0.182215$
- The column "Std. Error" gives SE(b₀) and SE(b₁):

$$SE(b_0) = 0.166160, SE(b_1) = 0.006451$$

Example: Test for the Slope β1

A general rule for waiters is to tip 15 to 20% of the pre-tax bill. That is, $\beta_0 = 0$ and β_1 is between 0.15 to 0.20.

- R tests $\beta_0 = 0$ for us: t-statistic = -1.759, 2-sided p-value = 0.0806
- To test H_0 : $\beta_1 = 0.2$ v.s. H_A : $\beta_1 < 0.2$. The *t*-statistic is

$$t = \frac{b_1 - 0.2}{SE(b_1)} = \frac{0.182215 - 0.2}{0.006451} = -2.757$$

with df = 155, the one-sided p-value is < 0.005.

one ta	il I	0.1	0.05	0.025	0.01	0.005
wo tai	1000	0.2	0.10	0.050	0.02	0.010
df 15	0	1.29	1.66	1.98	2.35	2.61
20	0	1.29	1.65	1.97	2.35	2.60

Conclusion: Customers of this restaurant gave less than 20% the bill as tips on average.

How to Read R Outputs for Regression?

Residual standard error: 0.9795 on 155 degrees of freedom

Multiple R-squared: 0.8373, Adjusted R-squared: 0.8363 F-statistic: 797.9 on 1 and 155 DF, p-value: < 2.2e-16

- Residual standard error: 0.9795 on 155 degrees of freedom This gives the estimate s_e of σ , which is 0.9795. df = n - 2 = 157 - 2 = 155
- Multiple R-squared: 0.8373 gives $r^2 = 0.8373$, Bill size explained 83.73% of the variation in tipping amount. The correlation between bill size and tips is $r = \sqrt{r^2} = \sqrt{0.8373} = 0.915$.
- Adjusted R-squared: Ignore this.
- F-statistic: 797.9 on 1 and 155 DF, p-value: < 2.2e-16 Skip.

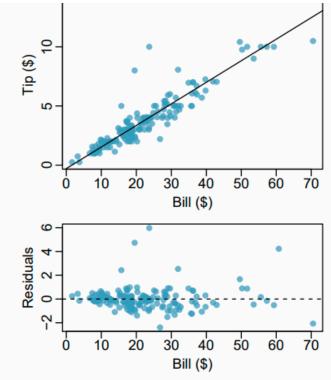
Checking Conditions for Simple Linear Regression Model?

- 1. Linearity
- 2. Constant variability
- (Optional) Nearly normal residuals

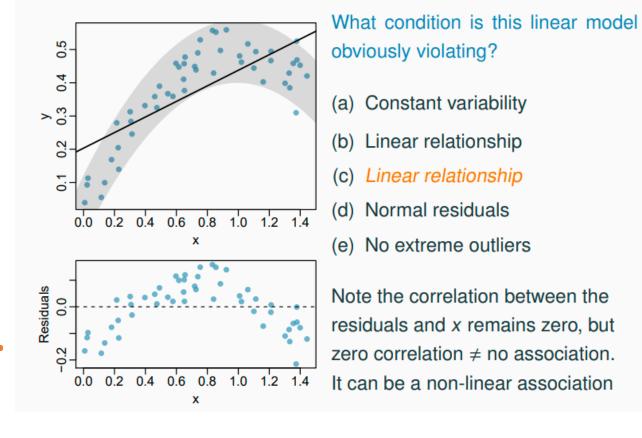
Tools for checking conditions:

Residual plot

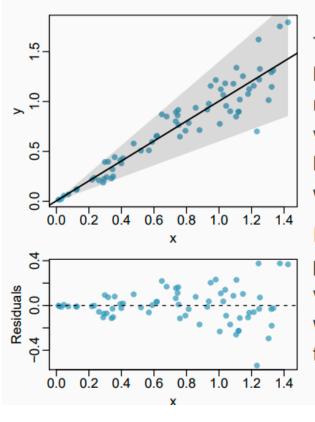
If conditions are satisfied, points should scatter evenly around the zero line in the residual plot.



Example



Checking Conditions : Constant Variability?

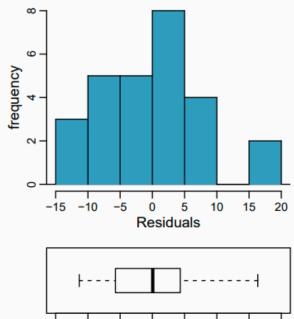


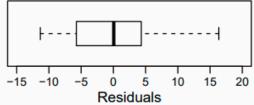
The variability of points around the least-squares line should be roughly constant, implying the variability of residuals around the 0 line should be roughly constant as well, called *homoscedasticity*.

If not, called *heterocedasticity*, predictions made in areas of larger variability will be worse. May try weighted least-square method or transforming the response.

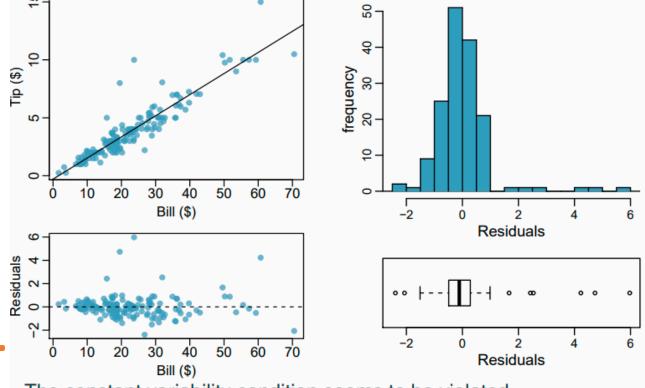
Conditions: Nearly **Normal** Residuals?

- Less relevant than the first two conditions
- Diagnosis: Check the histogram or boxplot of residuals
- If the linearity or constant variability condition is clearly violated, there is no need to check the normality of residuals.



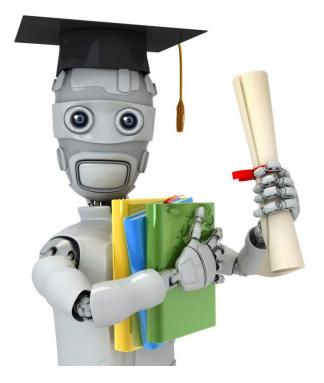


Checking Conditions for the Restaurant Tip Data



The constant variability condition seems to be violated.

The size of residual seems to increase with Bill.



Machine Learning

Linear regression with multiple variables

Multiple regression

- Simple linear regression: Bivariate two variables: y and x
- Multiple linear regression: Multiple variables: y and x_1, x_2, \cdots
- ullet Suppose we have n independent observations

$$(oldsymbol{x}_1^ op, Y_1), \dots, (oldsymbol{x}_n^ op, Y_n),$$

where x_i is a (p-1)-vector of known (explanatory) values.

 A natural extension of simple linear regression is to consider the model with more than one predictor variables

$$Y_i = \beta_0 + \beta_1 x_{i1} + \ldots + \beta_k x_{i,p-1} + \epsilon_i, \ \ i = 1, \ldots, n,$$

where $\epsilon_i \sim NID(0, \sigma^2)$ and p is the number of regression parameters to estimate.

• Equivalently, we can write in matrix notation

$$Y = X\beta + \epsilon, \quad \epsilon \sim N(\mathbf{0}, \sigma^2 \mathbf{I}_n),$$

where

$$\mathbf{X} = egin{pmatrix} 1 & oldsymbol{x}_1^ op \ 1 & oldsymbol{x}_2^ op \ dots & dots \ 1 & oldsymbol{x}_n^ op \end{pmatrix}, \quad oldsymbol{eta} = egin{pmatrix} eta_0 \ eta_1 \ dots \ eta_{p-1} \end{pmatrix}, \quad oldsymbol{\epsilon} = egin{pmatrix} \epsilon_1 \ \epsilon_2 \ dots \ eta_n \end{pmatrix}$$

Regression parameter estimation?

Still minimise residual sum of squares to get:

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^{\top}\mathbf{X})^{-1}\mathbf{X}^{\top}\boldsymbol{Y}$$

if $(\mathbf{X}^{\top}\mathbf{X})^{-1}$ exists.

Assumptions of the linear model

Assumptions

$$E(Y \mid X) = \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p$$
$$Var(Y \mid X) = \sigma^2$$

- 1. Errors $\varepsilon_i \sim N(0, \sigma^2)$.
- 2. Error variances are equal.
- 3. Errors are independent.
- 4. Y has a linear dependence on X.

T-test

Hypothesis concerning one of the terms

$$H_0: \beta_i = b_i$$
$$H_1: \beta_i \neq b_i$$

t-test statistic:
$$t = \frac{\hat{\beta}_i - b_i}{\sqrt{c_{ii}MSE}} \sim t(n - p - 1)$$

The confidence interval for β_i is $b_i \pm t_{\alpha/2} \sqrt{c_{ii}MSE}$

If H₀ is true, $t \sim t(n-p-1)$, so we reject H₀ at level α if $|t| > 2t_{\alpha/2}(n-p-1)$

> summary(lm(Fuel~.,data=fueldata))
Call:

 $lm(formula = Fuel \sim ., data = fueldata)$

Residuals: Min 1Q Median 3Q Max -163.145 -33.039 5.895 31.989 183.499

3.145 -33.039 5.895 31.989 183.499

Coefficients: Estimate Std. Error t value Pr(>|t|) (Intercept) 154.1928 194.9062 0.791 0.432938 2.0301 -2.083 0.042873 -4.2280 Tax 3.672 0.000626 *** Dlic 0.4719 0.12852.1936 -2.797 0.007508 ** -6.1353Income 18.5453 6.4722 2.865 0.006259 ** logMiles

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 " 0.1 ' ' 1

F-test

Hypothesis test for the reduced model

$$H_0: \beta_{r+1} = \cdots \beta_p = 0$$

$$H_1: not \ H_0$$

F test statistic:
$$F = (\frac{SSE_R - SSE_F}{p - r})/(\frac{SSE_F}{n - p - 1})$$

If H0 is true, $F \sim F(p-r,n-p-1)$ so we reject H0 at level α if $F > F_{\alpha}(p-r,n-p-1)$

From this test, we conclude that the hypotheses are plausible or not. And we say that which model is adequate.

```
> summary(lm(Fuel~,,data=fueldata))
```

Call:

lm(formula = Fuel ~ ., data = fueldata)

Residuals:

Min 1Q Median 3Q Max -163.145 -33.039 5.895 31.989 183.499

Coefficients:

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 ". 0.1 ' ' 1

Residual standard error: 64.89 on 46 degrees of freedom Multiple R-squared: 0.5105, Adjusted R-squared: 0.4679 F-statistic: 11.99 on 4 and 46 DF, p-value: 9.33e-07

checking model conditions using graphs

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_p x_p$$

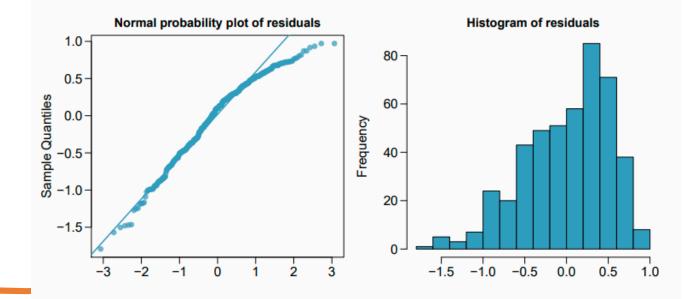
The model depends on the following conditions

- residuals are nearly normal (primary concern relates to residuals that are outliers)
- 2. residuals have constant variability
- 3. residuals are independent
- 4. each variable is linearly related to the outcome

We often use graphical methods to check the validity of these conditions, which we will go through in detail in the following slides.

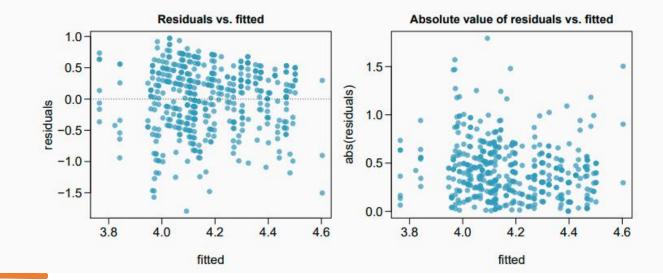
Nearly Normal Residuals

normal probability plot and/or histogram of residuals:



Does this condition appear to be satisfied?

Checking Constant Variance scatterplot of residuals and/or absolute value of residuals vs. fitted (predicted):



Checking Constant Variance

- When we did simple linear regression (one explanatory variable) we checked the constant variance condition using a plot of residuals vs. x.
- With multiple linear regression (2+ explanatory variables) we checked the constant variance condition using a plot of residuals vs. fitted.

Why are we using different plots?

In multiple linear regression there are many explanatory variables, so a plot of residuals vs. one of them wouldn't give us the complete picture.

Residuals are Independent ?

- Checking for independent residuals allows us to indirectly check for independent observations.
- If observations and residuals are independent, we would not expect to see an increasing or decreasing trend in the scatterplot of residuals vs. order of data collection.
- This condition is often violated when we have time series data. Such data require more advanced time series regression techniques for proper analysis.

scatterplot of residuals vs. order of data collection:



• Fact:
$$\hat{\sigma}^2 = \frac{SSE}{n - (p + 1)} (= MSE)$$
 is an unbiased estimator of σ^2 .

• If *e* is normally distributed,
$$\frac{SSE}{\sigma^2} = \frac{(n-(p+1))\hat{\sigma}^2}{\sigma^2} \sim \chi^2(n-(p+1))$$

Coefficient of Determination

Define SSreg=SYY-SSE (SYY= the sum of squares of Y)
As with the simple regression, the coefficient of determination is

$$R^2 = \frac{SS_{reg}}{SYY} = 1 - \frac{SSE}{SYY}$$

It is also called the multiple correlation coefficient because it is the maximum of the correlation between Y and any linear combination of the terms in the mean function.

Coefficient of Determination

1. square the correlation coefficient of *x* and *y* (how we have been calculating it)

2. square the correlation coefficient of y and \hat{y}

 R^2 can be calculated in three ways:

3. based on definition:

$$R^2 = \frac{\text{explained variability in } y}{\text{total variability in } y}$$

For single-predictor linear regression, having three ways to calculate the same value may seem like overkill. However, in multiple linear regression, we can't calculate R^2 as the square of the correlation between x and y because we have multiple xs.

have multiple xs.

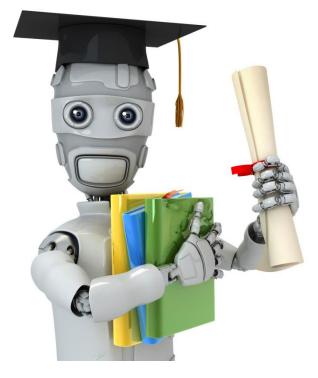
And next we'll learn another measure of explained variability, adjusted R^2 , that requires the use of the third approach, ratio of explained and unexplained variability.

Adjusted Coefficient

$$R_{adj}^2 = 1 - \left(\frac{SS_{Error}}{SS_{Total}} \times \frac{n-1}{n-p-1}\right)$$

where n is the number of cases and p is the number of predictors (explanatory variables) in the model.

- Because p is never negative, R_{adj}^2 will always be smaller than R^2 .
- R_{adj}^2 applies a penalty for the number of predictors included in the model.
- Therefore, we choose models with higher R_{adi}^2 over others.
- When any variable is added to the model R^2 increases.
- But if the added variable doesn't really provide any new information, or is completely unrelated, adjusted R² does not increase.



Machine Learning

Model selection

Backward-Elimination

- 1. R_{adj}^2 approach:
 - Start with the full model
 - Drop one variable at a time and record R²_{adj} of each smaller model
 - Pick the model with the highest increase in R_{adj}^2
 - Repeat until none of the models yield an increase in R^2_{adj}
- 2. p-value approach:
 - Start with the full model
 - Drop the variable with the highest p-value and refit a smaller model
 - Repeat until all variables left in the model are significant

Example Backward-**Elimination:** R2 Approac Step

Full

beauty

0.00

gender

male

0.00

Step 1	beauty	gender	age	formal	lower	native	students	tenure
		male		yes	yes	non english		tenure track
	0.00	0.00	0.01	0.04	0.38	0.03	0.34	0.02
Step 2	beauty	gender	age	formal		native	students	tenure
		male		yes		non english		tenure track
	0.00	0.00	0.01	0.05		0.02	0.44	0.01
Step 3	beauty	gender	age	formal		native		tenure
		male		yes		non english		tenure track
	0.00	0.00	0.01	0.06		0.02		0.01
Step 4	beauty	gender	age			native		tenure
		male				non english		tenure track
	0.00	0.00	0.01			0.06		0.01
Step 5	beauty	gender	age					tenure
		male						tenure track
	0.00	0.00	0.01					0.01

lower

yes

0.29

formal

yes

0.04

age

0.01

Variables included & p-value

non english

native

0.06

minority

yes

0.35

students

0.30

tenure

0.02

tenure track

tenur

0.0

0.0

0.0 tenur

0.0 tenur

0.0

tenur

tenure 0.0

tenur

tenure

tenure

tenure

tenur

tenure

tenure

Best model: beauty + gender + age + tenure

Example BackwardElimination: p_value Approach

Step	Variables included	R _{adj}
Full	beauty + gender + age + formal + lower + native + minority + students + tenure	0.0839
Step 1	gender + age + formal + lower + native + minority + students + tenure	0.0642
	beauty + age + formal + lower + native + minority + students + tenure	0.0557
	beauty + gender + formal + lower + native + minority + students + tenure	0.0706
	beauty + gender + age + lower + native + minority + students + tenure	0.0777
	beauty + gender + age + formal + native + minority + students + tenure	0.0837
	beauty + gender + age + formal + lower + minority + students + tenure	0.0788
	beauty + gender + age + formal + lower + native + students + tenure	0.0842
	beauty + gender + age + formal + lower + native + minority + tenure	0.0838
	beauty + gender + age + formal + lower + native + minority + students	0.0733
Step 2	gender + age + formal + lower + native + students + tenure	0.0647
	beauty + age + formal + lower + native + students + tenure	0.0543
	beauty + gender + formal + lower + native + students + tenure	0.0708
	beauty + gender + age + lower + native + students + tenure	0.0776
	beauty + gender + age + formal + native + students + tenure	0.0846
	beauty + gender + age + formal + lower + native + tenure	0.0844
	beauty + gender + age + formal + lower + native + students	0.0725
Step 3	gender + age + formal + native + students + tenure	0.0653
	beauty + age + formal + native + students + tenure	0.0534
	beauty + gender + formal + native + students + tenure	0.0707
	beauty + gender + age + native + students + tenure	0.0786
	beauty + gender + age + formal + students + tenure	0.0756
	beauty + gender + age + formal + native + tenure	0.0855
	beauty + gender + age + formal + native + students	0.0713
Step 4	gender + age + formal + native + tenure	0.0667
	beauty + age + formal + native + tenure	0.0553
	beauty + gender + formal + native + tenure	0.0723
	beauty + gender + age + native + tenure	0.0806

Best model: beauty + gender + age + formal + native + tenure

Forwardselection

- 1. R_{adj}^2 approach:
 - Start with regressions of response vs. each explanatory variable
 - Pick the model with the highest R_{adj}^2
 - Add the remaining variables one at a time to the existing model, and once again pick the model with the highest R²_{adj}
 - Repeat until the addition of any of the remanning variables does not result in a higher R_{adi}^2
- 2. p value approach:
 - Start with regressions of response vs. each explanatory variable
 - Pick the variable with the lowest significant p-value
 - Add the remaining variables one at a time to the existing model, and pick the variable with the lowest significant p-value
 - Repeat until any of the remaining variables does not have a significant p-value

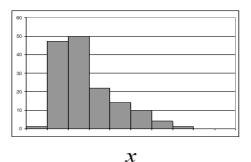
Moving Beyond Linearity (in the features)

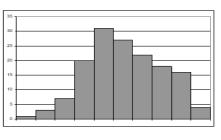
Common intrinsically linear models and required transformations

True relationship	Transformation	Linearized model
$y = \beta_0 x^{\beta_1}$	$y' = \log y, x' = \log x$	$y' = \log \beta_0 + \beta_1 x'$
$y = \beta_0 e^{\beta_1 x}$	$y' = \log y$	$y' = \log \beta_0 + \beta_1 x$
$y = \beta_0 + \beta_1 \log x$	$x' = \log x$	$y = \log \beta_0 + \beta_1 x'$
$y = \frac{x}{\beta_0 x - \beta_1}$	$y' = \frac{1}{y}, x' = \frac{1}{x}$	$y' = \beta_0 - \beta_1 x'$

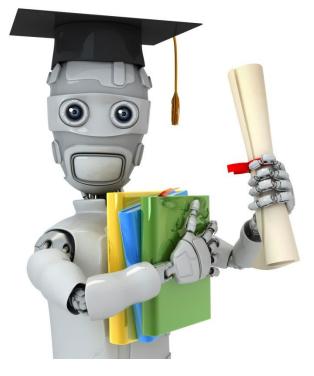
The effect of the ln transformation

- It spreads out values that are close to zero
- Compacts values that are large





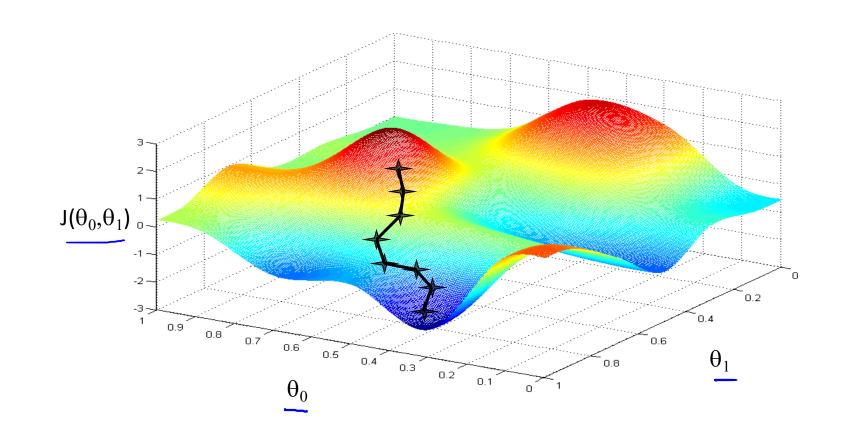
$$x^{(new)} = \ln(x)$$

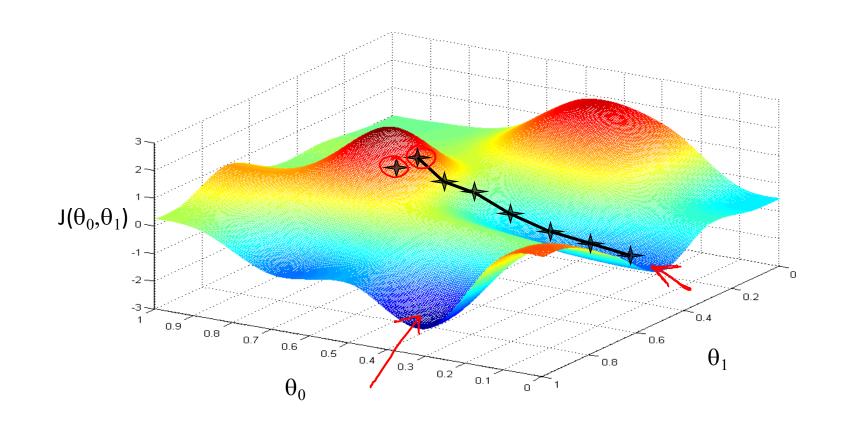


Machine Learning

See you next chapter

Thanks:)





Gradient descent algorithm

repeat until convergence {
$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1) \qquad \text{(for } j = 0 \text{ and } j = 1\text{)}$$
 }

Correct: Simultaneous update

$$temp0 := \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$$

$$temp1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$$

$$\theta_0 := temp0$$

$$\theta_1 := temp1$$

Incorrect:

$$temp0 := \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$$

$$\theta_0 := temp0$$

$$temp1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$$

$$\theta_1 := temp1$$