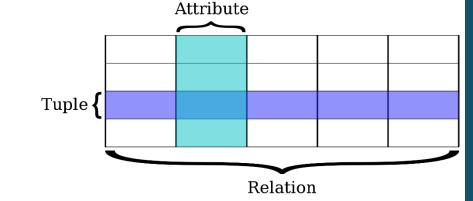
Multiple Linear Regression

Praphul Chandra



From 1 to many



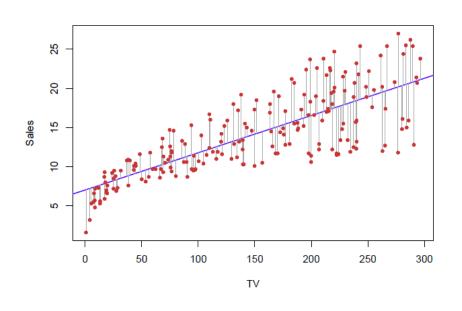
- Independent random variable.
 - Predictor variables, explanatory variables, feature, dimension, attributes
- Simple Linear Regression → Multiple Linear Regression
 - 1 independent r.v. → Multiple independent r.v.
 - Models the effect of several independent variables, x_1, x_2 etc., on one dependent variable, y
 - The different x variables are combined in a linear way and each has its own regression coefficient
 - Same assumptions: Linearity, Noise is i.i.d. Normal with mean 0 and fixed variance
- Independence assumption (new!)

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_p x_p + \varepsilon$$

- Independence among predictor variables: hence the name.
- β parameters reflect the independent contribution of each variable, x, on the value of the dependent variable, y.
- A coefficient is the slope of the linear relationship between the dependent variable (DV) and the independent contribution of the independent variable (IV),
 - i.e., that part of the IV that is independent of (or uncorrelated with) all other IVs.

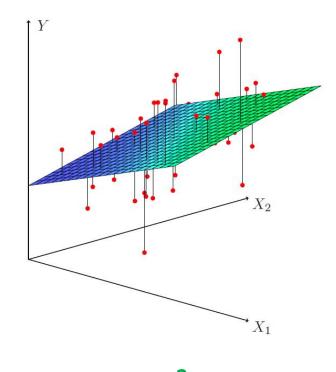


Multiple Linear Regression : Visualization



$$p=1$$

$$y = \beta_0 + \beta_1 x_1 + \varepsilon$$



$$\mathbf{p=2}$$

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \varepsilon$$





Simple LR → Multiple LR

- Multiple Linear Regression
 - Dependent variable is numeric
 - Fit a line plane / hyper-plane
- Line Hyperplane Fitting
 - More than p+1 data points → Over-specified problem
 - Criteria: Minimize error (sum of squared residuals)
- Optimization problem
 - Solve (using matrix manipulation)
 - Find coefficients (line) which minimizes the Residual Sum of Squares
- Use estimated coefficients ("model") to make predictions



Multiple Linear Regression: Math

$$y = \beta_0 + \beta_1 x + \epsilon$$
$$\epsilon \sim N(0, \sigma^2)$$

$$RSS = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2$$

$$\min_{\beta} RSS$$

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

$$\hat{\beta_0} = \bar{y} - \hat{\beta_1} \bar{x}$$

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

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_p x_p + \epsilon$$
$$\epsilon \sim N(0, \sigma^2)$$

$$RSS = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2$$

 $\min_{\beta} RSS$

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

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \dots + \hat{\beta}_p x_p$$

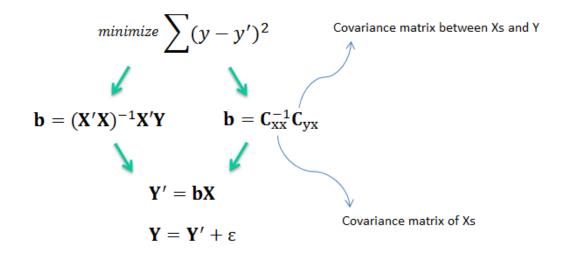


 $\bar{y} = \frac{1}{n} \sum_{i=1}^{n} y_i$

 $\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i$

Estimating the coefficients

$$\begin{split} &\frac{\partial}{\partial \hat{\beta}} \left(\mathrm{SSE} \Big(\hat{\alpha}, \hat{\beta} \Big) \right) = -2 \sum_{i=1}^{n} \left[\left(y_{i} - \bar{y} \right) - \hat{\beta} \left(x_{i} - \bar{x} \right) \right] \left(x_{i} - \bar{x} \right) = 0 \\ &\Rightarrow \sum_{i=1}^{n} \left(y_{i} - \bar{y} \right) \left(x_{i} - \bar{x} \right) - \hat{\beta} \sum_{i=1}^{n} \left(x_{i} - \bar{x} \right)^{2} = 0 \\ &\Rightarrow \hat{\beta} = \frac{\sum_{i=1}^{n} \left(y_{i} - \bar{y} \right) \left(x_{i} - \bar{x} \right)}{\sum_{i=1}^{n} \left(x_{i} - \bar{x} \right)^{2}} = \frac{\mathrm{Cov}(x, y)}{\mathrm{Var}(x)} \end{split}$$





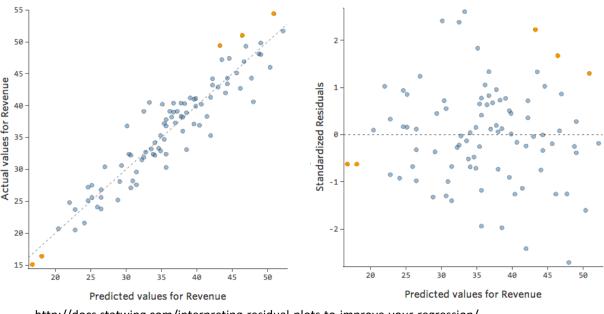
More is better Or is it?

- More is better
 - More explanatory variables → More (potential) explanation → Higher R² (Better Fit)
- But
 - Multi-collinearity
 - Model comparison
 - Feature selection
- Assumptions (as in simple linear regression)
 - Linearity
 - Homoscedasticity (constant variance)
 - Independence of errors
 - Normality of errors



Linear correlation between x and y?

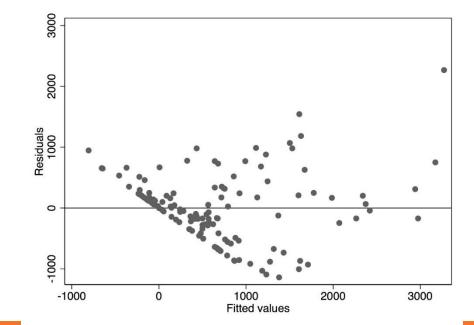
- Is there a non-linear relationship?
 - Linear \rightarrow Plot between y & $(\beta_0 + \beta_1 x)$ would be linear
 - Linear → Errors (Residuals) will not show any pattern
- Residual Plots
 - Graphical tool for identifying non-linearity
 - Plot residuals vs. fitted values
- Interpretation
 - No discernible pattern → Linearity
 - U shape → Non-linearity
- What next?
 - Feature Transformations (later)



Residuals

http://docs.statwing.com/interpreting-residual-plots-to-improve-your-regression/

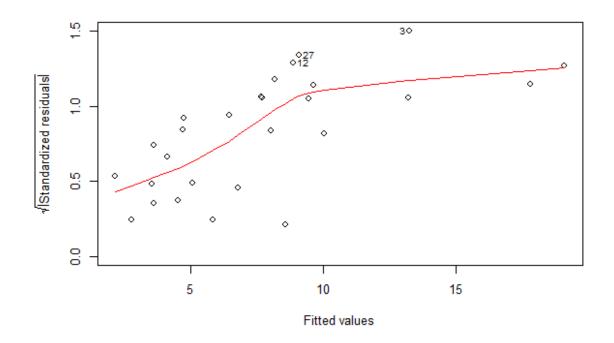
Predicted vs Actual

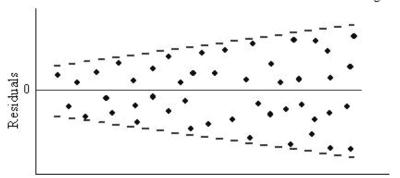


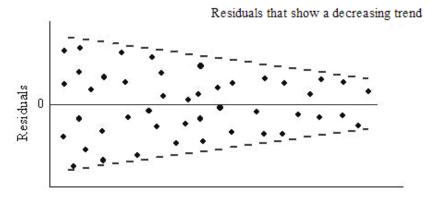


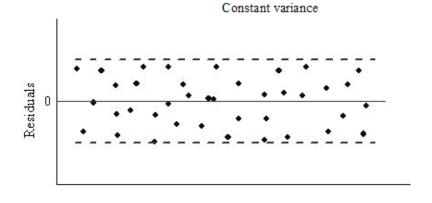
Noise has fixed variance

- The error terms have constant variances: homoscedasticity
 - What if variance depends on the predictor variable?
 - Need to check for heteroscedasticity
- What next?
 - Feature Transformations (later)





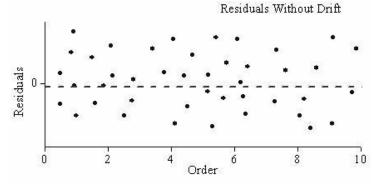


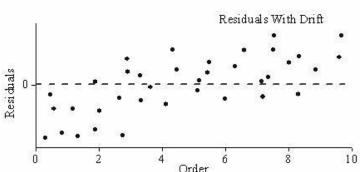


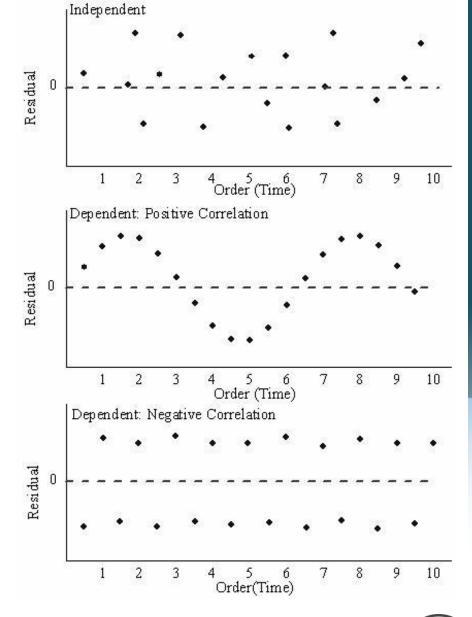


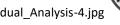
Noise (residuals) independent (i.i.d.)?

- Are error terms correlated?
 - Are "successive" residuals correlated?
 - ϵ_i is positive provides no information about the sign of ϵ_{i+1}
- Successive?
 - Temporal
 - Any sequence... (e.g. spatial)
- Source
 - Sampling error!
 - Design of Experiment error!



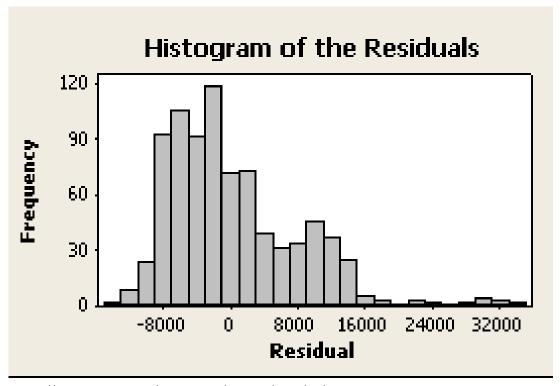






Noise (residuals) normally distributed?

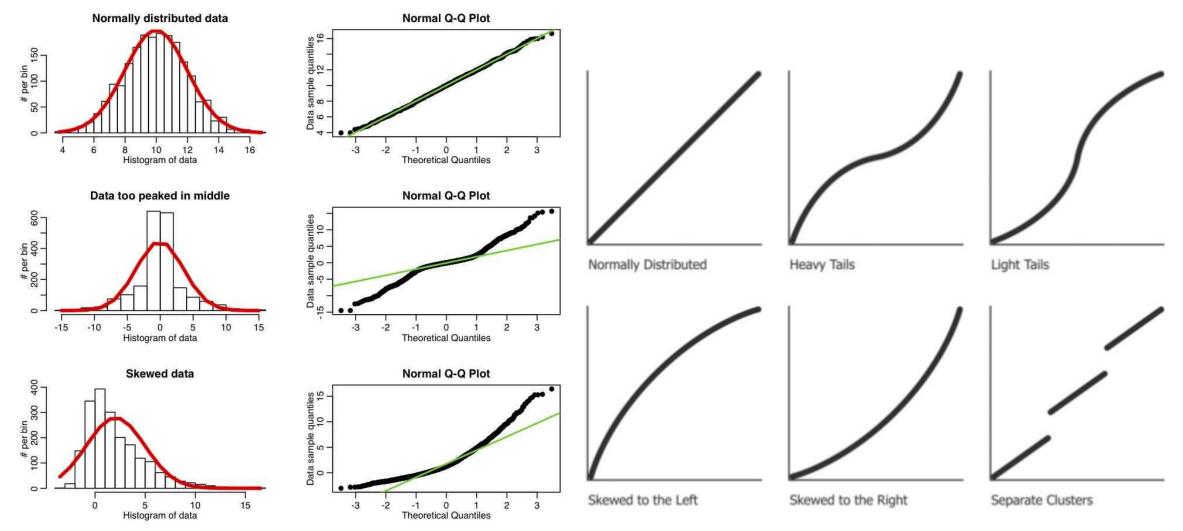
- Residual distribution is normal?
 - Plot & check
- Q-Q plot
 - Used to validate distributional assumptions of a data set.
 - Normality → z-scores of the residuals should be equal to the expected z-scores at corresponding quantiles.



http://sherrytowers.com/wp-content/uploads/2013/08/qqplot_examples.jpg



Noise (residuals) normally distributed? (cont'd)





Example

- In a real estate study, multiple variables were explored to determine the price of a house.
 - # of bedrooms
 - # of bathrooms
 - Age of the house
 - # of square feet of living space
 - Total # of square feet of space
 - # of garages
- Predict the price of the house by total square feet and age of the house.

$$\hat{y} = 57.35 + 0.0177 Area - 0.666 Age$$

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%
Intercept	57.35074586	10.00715186	5.73097587	1.31298E-05	36.47619286	78.22529885
Area (sq ft) (x1)	0.017718036	0.00314562	5.632605205	1.63535E-05	0.011156388	0.024279685
Age of House (years) (x2)	-0.666347946	0.227996703	-2.922620973	0.008417613	-1.141940734	-0.190755157



Inferential statistic: Caution!

- p-value for a regression coefficient
 - Probability of obtaining a t-statistic very far from 0 by chance
 - Expected number of coefficient for which this will happen by chance?
 - What if number of dimensions =10? 100? 1000?
 - p-value=0.05, number of dimensions = 100 → 5 predictor variables may show up as "significant" by chance!
- F-statistic for k-dimensional multiple regression model
 - Tests that at least one of the regression coefficients is different from 0. (Null hypothesis: All coefficients 0)

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

•
$$F = \frac{ESS/k}{TSS/(n-k-1)} = \frac{(TSS-RSS)/k}{TSS/(n-k-1)}$$

- F-test: Comparing "the variance explained by the model" to "the variance not explained by the model"
- When there is no relationship between the dependent variables and the predictors F is close to 1
- If F is large, there is a relationship



(Multi)-collinearity

More isn't always better



(Multi)-collinearity

- Violation of "independence" among predictor variables
 - Predictor variables are correlated
 - Which coefficient should be higher in the model?

	Energy consumpti on	Nuclear	Coal	Dry gas	Fuel rate
Energy consumpti on	1				
Nuclear	0.856	1			
Coal	0.791	0.952	1		
Dry gas	0.057	-0.404	-0.448	1	
Fuel rate	0.791	0.972	0.968	-0.423	1

Impact

- Impacts the interpretability of the model (not necessarily predictive power)
- A variable which is in fact important may end with a lower coefficient (correlated variable gets a higher coefficient)
- A regression coefficient which should be +ve ends up –ve (correlated variable gets a high +ve coefficient)
- Removing one independent variable drastically changes the coefficient of others
- For example, fuel rate and coal production are highly correlated (0.968).
 - $\hat{y} = 44.869 + 0.7838 (fuel rate)$
 - $\hat{y} = 45.072 + 0.0157(coal)$
 - \hat{y} =45.806+0.0277(coal)-0.3934($fuel\ rate$)



(Multi)-collinearity

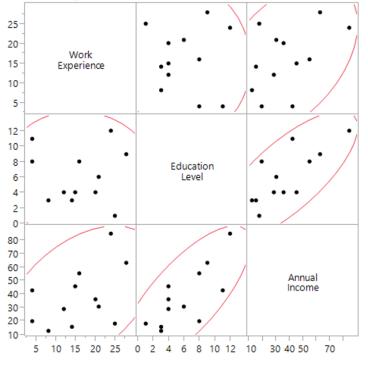
- What next?
 - Check for correlation among predictor variables.
 - Ideally before building the model
 - Drop correlated predictor variables
 - Feature transformation: PCA, PLS

- Inferential Statistics Explanation
 - Challenge: Which coefficient should be higher in the model?
 - Reduces the accuracy of the estimates of the model coefficients
 - **>** Sampling distribution variance increases
 - Standard Errors of the coefficients increases
 - + t-statistic decreases
 - **→** p-value increases

Multivariate FCorrelations

	Work Experience	Education Level	Annual In
Work Experience	1.0000	-0.0423	0.4628
Education Level	-0.0423	1.0000	0.7551
Annual Income	0.4628	0.7551	1.0000

Scatterplot Matrix





http://circabook.com/multicollinearity-in-regression-models-penn-state-eberly-

Example

- A drug precursor molecule is extracted from a type of nut, which is commonly contaminated by a fungal toxin that is difficult to remove during the purification process. The suspected predictors of the amount of fungus are:
 - Rainfall (cm/week)
 - Noon temperature (oC)
 - Sunshine (h/day)
 - Wind speed (km/h)
 - The fungal toxin concentration is measured in $\mu g/100$ g.

> correlation

```
Toxin
                              Rain
                                      NoonTemp
                                                  Sunshine
                                                              WindSpeed
          1.000000000
                      0.868734134 -0.07319548 -0.05169949
                                                          -0.270555628
Toxin
          0.86873413
                     1.0000000000
                                   0.11691043
                                               0.16841144 -0.002180167
Rain
                                              0.50082303 -0.368972511
NoonTemp
         -0.07319548 0.116910426
                                   1.00000000
Sunshine
         -0.05169949 0.168411437
                                   0.50082303
                                               1.000000000
                                                           -0.018439486
WindSpeed -0.27055563 -0.002180167 -0.36897251 -0.01843949
                                                           1.0000000000
```

Call:

lm(formula = ToxinConc\$Toxin ~ ToxinConc\$Rain + ToxinConc\$NoonTemp +
 ToxinConc\$Sunshine + ToxinConc\$WindSpeed, data = ToxinConc\$

Residuals:

```
1 2 3 4 5 6 7 8
-1.8818 2.0498 -0.6314 0.4787 -0.5805 1.2508 -0.1921 -0.1813
9 10
-1.1552 0.8429
```

Coefficients:

```
Estimate Std. Error t value Pr(>|t|)
(Intercept)
                    31,6084
                                7.1051
                                                0.00671 **
ToxinConc$Rain
                     7.0676
                                1.0031
                                         7.046 0.00089 ***
ToxinConc$NoonTemp
                    -0.4201
                                0.2413
                                       -1.741 0.14215
ToxinConc$Sunshine
                    -0.2375
                                0.5086
                                       -0.467 0.66018
ToxinConc$WindSpeed
                    -0.7936
                                0.2977
                                       -2.666 0.04458 *
Signif. codes: 0
                 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Residual standard error: 1.574 on 5 degrees of freedom
Multiple R-squared: 0.9186. Adjusted R-squared: 0.8535
F-statistic: 14.11 on 4 and 5 DF, p-value: 0.006232
```



Example (cont'd)

- Remove one of the correlated variables
- Rebuild model
- Business Implication
 - Toxin concentrations increase with increasing rainfall and decrease in drier climates characterized Coefficients: by higher temperatures and wind speeds.
 - The business can take a decision to rent farms in drier climates if the cost benefits of saved nuts versus higher rents are high.

Call:

lm(formula = ToxinConc\$Toxin ~ ToxinConc\$Rain + ToxinConc\$NoonTemp + ToxinConc\$WindSpeed, data = ToxinConc)

Residuals:

Min 10 Median Max -1.6394 -0.9308 0.1394 0.6545 2.0909

```
Estimate Std. Error t value Pr(>|t|)
(Intercept)
                   31.5651
                              6.6253
                                       4.764 0.00311 **
ToxinConc$Rain
                                     7.551 0.00028 ***
                    7.0108
                              0.9285
ToxinConc$NoonTemp -0.4790
                              0.1919 -2.495 0.04682 *
                              0.2718 -3.023 0.02331 *
ToxinConc$WindSpeed -0.8218
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Residual standard error: 1.468 on 6 degrees of freedom Multiple R-squared: 0.915, Adjusted R-squared: 0.8726 F-statistic: 21.54 on 3 and 6 DF, p-value: 0.001298



Multicollinearity

- Testing for pair-wise correlation not enough
 - A predictor variable may be correlated with two other variables taken together
- Variance Inflation Factor (VIF)
 - Intuition: Regress each predictor variable w.r.t. other predictors.

$$VIF(\hat{\beta}_j) = \frac{1}{1 - R_{X_j|X_{-j}}^2}$$

- Predict an independent variable by the other independent variables.
- The independent variable being predicted becomes the dependent variable in this analysis.
- A "large" VIF (>> 10) indicates multicollinearity.
- Stepwise regression prevents this problem to a great extent.



Checking for multi-collinearity in R

```
Call:
lm(formula = model0, data = regData)
Residuals:
     Min
                   Median
                                        Max
-0.25843 -0.11727 -0.00533 0.07364 0.49503
Coefficients:
               Estimate Std. Error t value Pr(>|t|)
(Intercept)
               10.85028
                           3.07946
                                     3.523 0.00182 **
log(Miles)
                0.42533
                           0.22528
                                     1.888 0.07170 .
log(Speed)
                -0.75004
                           0.73563 -1.020 0.31853
log(Hours)
                -0.45601
                           0.18423 -2.475 0.02111 *
log(Population)
                0.02401
                           0.04341
                                   0.553 0.58559
LoadFactor
                -5.82500
                           0.49084 -11.867 2.76e-11 ***
log(Capacity)
               -1.80998
                           0.14851 -12.187 1.62e-11 ***
log(AdjAsset)
                0.11555
                           0.07611 1.518 0.14259
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' '1
Residual standard error: 0.1747 on 23 degrees of freedom
Multiple R-squared: 0.9898, Adjusted R-squared: 0.9868
F-statistic: 320.3 on 7 and 23 DF, p-value: < 2.2e-16
> vif(fit)
     log(Miles)
                    log(Speed)
                                    log(Hours) log(Population)
                                                                    LoadFactor
                                                                                 log(Capacity)
                                                                                                log(AdjAsset)
                                                                                     6.951357
     15.437923
                     14.227428
                                      2.600507
                                                      3.761584
                                                                      4.586951
                                                                                                    18.006015
```

http://subhasis4analytics.blogspot.in/2014/09/linear-regression-analysis-with-r-and.html



Feature (Model) Selection

Feature engineering



Feature Selection

- Best subset selection
 - Brute force: Try all possible combinations from the available set of predictors
 - Number of models to try 2^p
 - Computational load?
- Forward subset selection
 - p simple linear regression models; Select the best one.
 - Greedy approach: May not find THE best model but often good enough
- Backward subset selection
 - Start will all variables in.
 - Remove insignificant variables one-by-one
- Hybrid subset selection
 - Grown & prune



Forward (Hybrid) subset selection

- Starts a model with a single predictor and then adds or deletes predictors one step at a time.
- Step 1
 - Simple regression model for each of the independent variables one at a time.
 - Model with largest absolute value of t selected and the corresponding independent variable considered the best single predictor, denoted x1.
 - If no variable produces a significant t, the search stops with no model.
- Step 2
 - All possible two-predictor regression models with x1 as one variable.
 - Model with largest absolute t value in conjunction with x1 and one of the other k-1 variables denoted x2.
 - Occasionally, if x1 becomes insignificant, it is dropped and search continued with x2.
 - If no other variables are significant, procedure stops.
 - The above process continues with the 3rd variable added to the above 2 selected and so on.



Example: Feature (Model) selection

- Suppose a model to predict the world crude oil production (barrels per day) is to be developed and the predictors used are:
 - US energy consumption (BTUs)
 - Gross US nuclear electricity generation (kWh)
 - US coal production (short-tons)
 - Total US dry gas (natural gas) production (cubic feet)
 - Fuel rate of US-owned automobiles (miles per gallon)
- What does your intuition say about how each of these variables would affect the oil production?
- Search procedures help choose the more attractive model.
 - If 3 variables can explain the variation nearly as well as 5 variables, the simpler model is better.
 - All variables used in all combinations → search among 31 models
 - Tedious, Time-Consuming, Inefficient, Overwhelming.
 - Use Forward subset selection



Example (cont'd)

Dependent Variable	Independent Variable	t Ratio	<i>p</i> -value	R ²
Oil production	Energy consumption	11.77	1.86e-11	85.2%
Oil production	Nuclear	4.43	0.000176	45.0
Oil production	Coal	3.91	0.000662	38.9
Oil production	Dry gas	1.08	0.292870	4.6
Oil production	Fuel rate	3.54	0.00169	34.2

$$y = 13.075 + 0.580x_1$$

$$y = 7.14 + 0.772x_1 - 0.517x_2$$

Dependent Variable, y	Independent Variable, x_1	Independent Variable, x ₂	t Ratio of x ₂	<i>p</i> -value	R ²
Oil production	Energy consumption	Nuclear	-3.60	0.00152	90.6%
Oil production	Energy consumption	Coal	-2.44	0.0227	88.3
Oil production	Energy consumption	Dry gas	2.23	0.0357	87.9
Oil production	Energy consumption	Fuel rate	-3.75	0.00106	90.8



Example (cont'd)

Dependent Variable, y	Independent Variable, x_1	Independent Variable, x ₂	Independent Variable, x ₃	t Ratio of x ₃	<i>p</i> -value
Oil production	Energy consumption	Fuel rate	Nuclear	-0.43	0.672
Oil production	Energy consumption	Fuel rate	Coal	1.71	0.102
Oil production	Energy consumption	Fuel rate	Dry gas	-0.46	0.650

• No t ratio is significant at $\alpha=0.05$. No new variables are added to the model.



Categorical Predictor Variables



Dealing with categorical variables

- Type of r.v. (Till now: Assume all numeric)
 - If dependent r.v. categorical: Logistic regression
 - If independent r.v. categorical: One hot encoding
- Categorical Predictor variables
 - Gender, geographic region, occupation, marital status, level of education, economic class, buying/renting a home, etc.
- Replace with Indicator (Dummy) random variables
 - If a survey question asks about the region of country your office is located in, with North, South, East and West as the options, the **recoding** can be done as follows:
 - If there are *n* categories, *n-1* dummy variables need to be inserted into the regression analysis.

Region	North	West	South
North	1	0	0
East	0	0	0
South	0	0	1
West	0	1	0



Example

• Consider the issue of gender discrimination in the salary earnings of workers in some industries. If there is discrimination, how much is one gender earning more than the other?

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%
Intercept	1.732060612	0.235584356	7.352189	8.83E-06	1.218766395	2.245354829
Age (10 years)	0.111220164	0.072083424	1.542937	0.148796	-0.045836124	0.268276453
Gender (1=Male, 0=Female)	0.458684065	0.053458498	8.58019	1.82E-06	0.342208003	0.575160126

• Interpret as two equations.



LR with categorical variables & ANOVA

- Consider a LR with
 - Dependent variable : Numeric
 - Predictor variables: Categorical
- If the model is a good fit:
 - \rightarrow categorization from the input X is a good way to explain the output.
 - \rightarrow there is some significant difference between the groups which impacts the mean value of the dependent variable
- If the model is a good fit (F-statistic is large enough)
 - F-test, comparing "the variance explained by the model" to "the variance not explained by the model".
 - This is exactly how one-way ANOVA works!
 - ANOVA is often expressed in terms of comparing variance within groups to variance between groups.
- Thus, ANOVA assumed
 - Identical variance between groups: the variance from the group mean for each group is the regression residual.
 - ANOVA is particularly sensitive to this assumption: if the data are heteroscedastic (i.e., the groups have different variances), ANOVA-based tests will often fail.



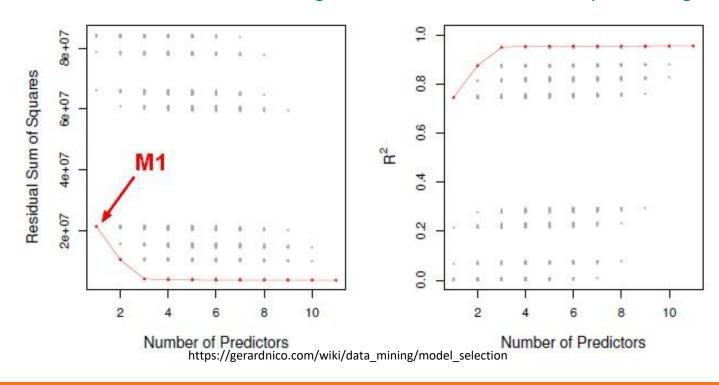
Model Comparison

Apples & Oranges



Model Comparison : Challenge

- Comparing two models with the same number of predictor variables
 - Higher R² better
- Comparing two models with different number of predictor variables
 - Apples & Oranges
 - More predictor variables → More "flexibility" in the model
 - However, sometimes these variables are insignificant and add no real value, yet inflating the R2 value.





Model Comparison : Challenge

- Comparing two models with different number of predictor variables
 - Apples & Oranges
 - More predictor variables → More "flexibility" in the model
 - Potential of overfitting
- Generalization Error (BIG Idea)
 - Sample vs. Population
- Two considerations in model building:
 - Explaining most variation in dependent variable
 - Keeping the model simple AND economical
 - Quite often, the above two considerations are in conflict of each other.

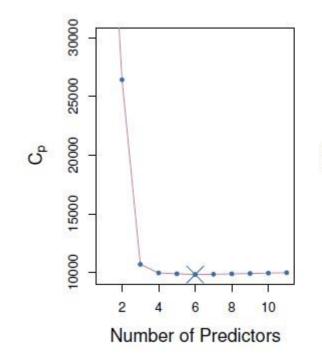


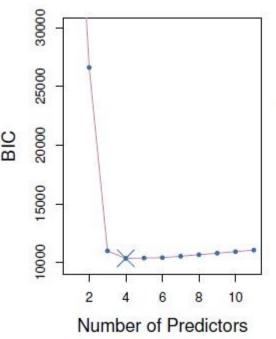
Model Comparison : Statistics

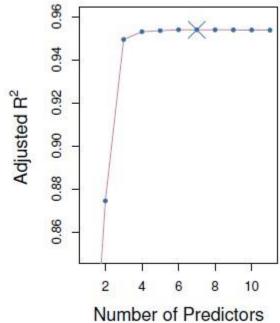
- Key Idea
 - Penalize models for using more parameters (predictor variables)

• Adjusted
$$R^2 = 1 - \frac{\frac{RSS}{(n-d-1)}}{\frac{TSS}{n-1}}$$

- Cp, AIC, BIC
- Aim to estimate the performance of the model learnt from sample on the population (train-test)







 $C_p = \frac{1}{n}(RSS + 2d\hat{\sigma}^2)$ $AIC = \frac{1}{n\hat{\sigma}^2}(RSS + 2d\hat{\sigma}^2)$ $BIC = \frac{1}{n}(RSS + \log(n)d\hat{\sigma}^2)$



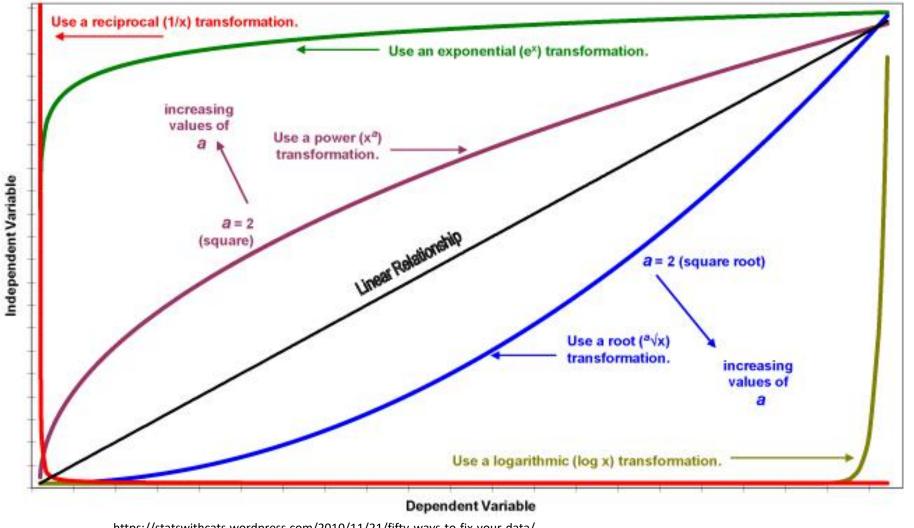
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Moving beyond Linearity

Feature engineering



Data Transformation cheat sheet





Other tricks in Multiple Linear Regression

- Interaction Terms
- Interaction can be examined as a separate independent variable in regression.
- For example, $y=\beta_0+\beta_1 x_1+\beta_2 x_2+\beta_3 x_1 x_2+\varepsilon$

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%
Intercept	50.85548009	3.790993168	13.41481713	1.38402E-08	42.59561554	59.11534464
Stock 2 (\$)	-0.118999968	0.19308237	-0.616317112	0.54919854	-0.539690313	0.301690376
Stock 3 (\$)	-0.07076195	0.198984841	-0.35561478	0.728301903	-0.504312675	0.362788775

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%
Intercept	12.04617703	9.312399791	1.29356313	0.222319528	-8.450276718	32.54263077
Stock 2 (\$)	0.878777607	0.26187309	3.355738482	0.006412092	0.302398821	1.455156393
Stock 3 (\$)	0.220492727	0.143521894	1.536300286	0.152714573	-0.095396832	0.536382286
Stock 2*Stock 3	-0.009984949	0.002314083	-4.314862356	0.00122514	-0.015078211	-0.00489169





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