Machine Learning with R: Linear Regression

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DASH: Data Analysis Support Hub Workshop Series
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Register for upcoming DASH events:

February 24: Introduction to Python – Vivek Jadon

February 27: Multivariable Analysis with R – Humayun Kabir

March 22: Machine Learning with R: Logistic Regression– Humayun Kabir

March 28: Intermediate Python Programming – Seyed Amirreza Mousavi

April 30: Survival Analysis with R – Humayun Kabir

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- Analyzing data with software including SPSS, Python, R, SAS, ArcGIS, MATLAB, and Excel
- Choosing which software package to use, including free and open-source software
- Troubleshooting problems related to file formats, data retrieval, and download
- Selecting methodology and type of data analysis to use in a thesis project

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Machine Learning with R: Linear Regression

Objective

LEARNING THE BASICS OF LINEAR REGRESSION

MACHINE LEARNING WITH R

Covariance

$$\operatorname{cov}(x,y) = \frac{\sum_{i=1}^{n}(x_i - \bar{X})(y_i - \bar{Y})}{n-1}$$

Source: Dr. Dipak Kumar Mitra, North South University

Interpreting Covariance

$cov(X,Y) > 0 \longrightarrow$ X and Y are positively correlated

$cov(X,Y) < 0 \longrightarrow$ X and Y are inversely correlated

$cov(X,Y) = 0 \longrightarrow$ X and Y are independent

Source: Dr. Dipak Kumar Mitra, North South University

Correlation coefficient (standardized)

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

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

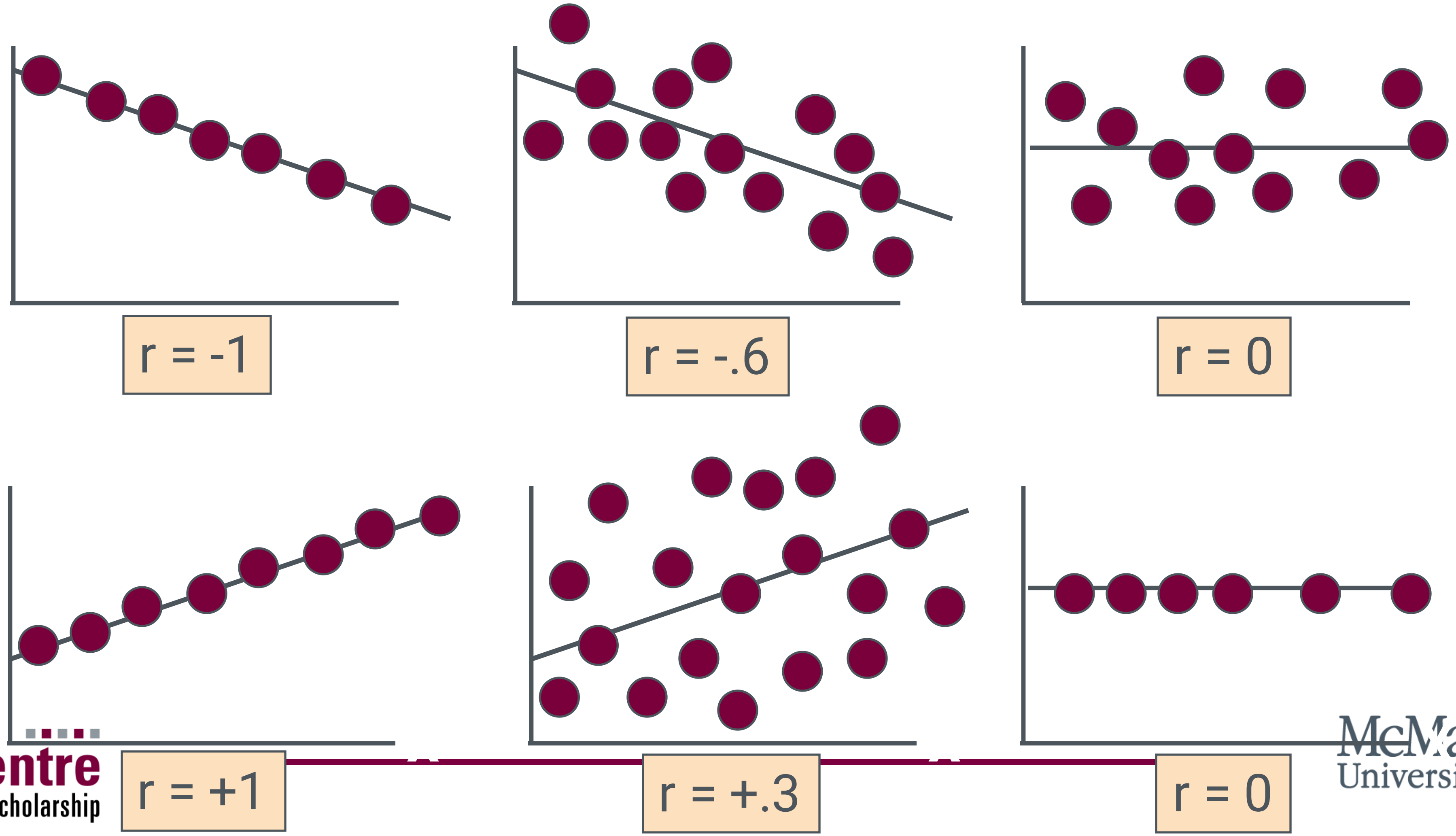
Source: Dr. Dipak Kumar Mitra, North South University

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

Source: Dr. Dipak Kumar Mitra, North South University

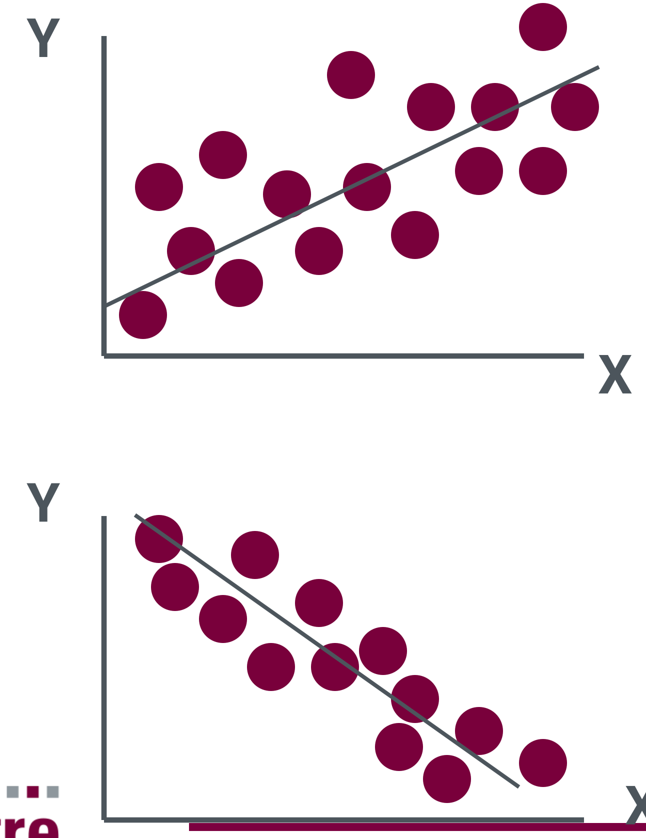
Scatter Plots of Data with Various Correlation Coefficients



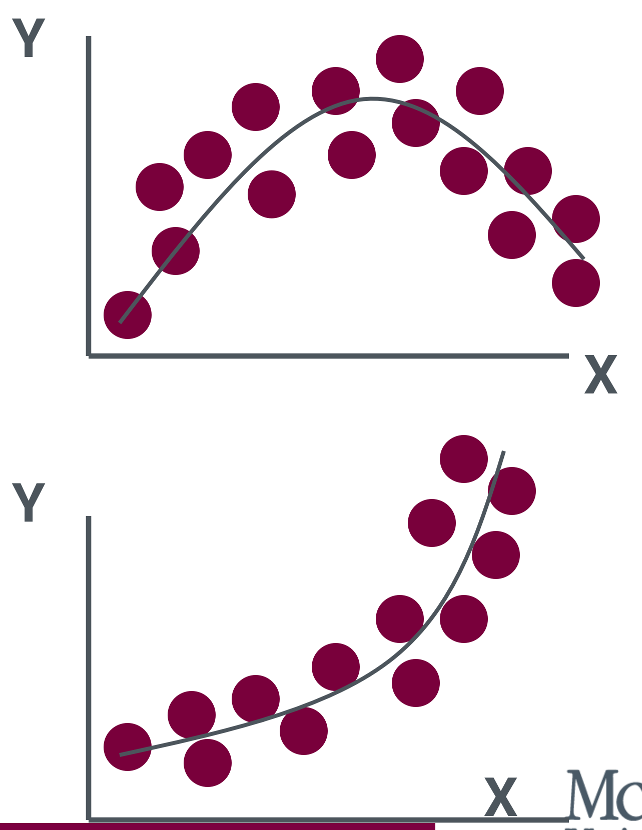
Source: Dr. Dipak Kumar Mitra, North South University

Linear Correlation

Linear relationships



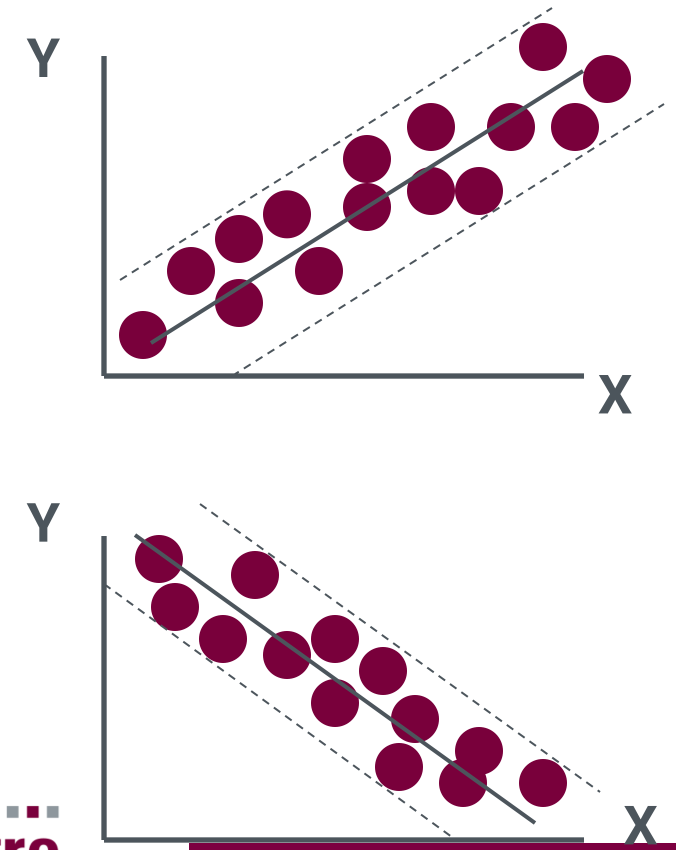
Curvilinear relationships



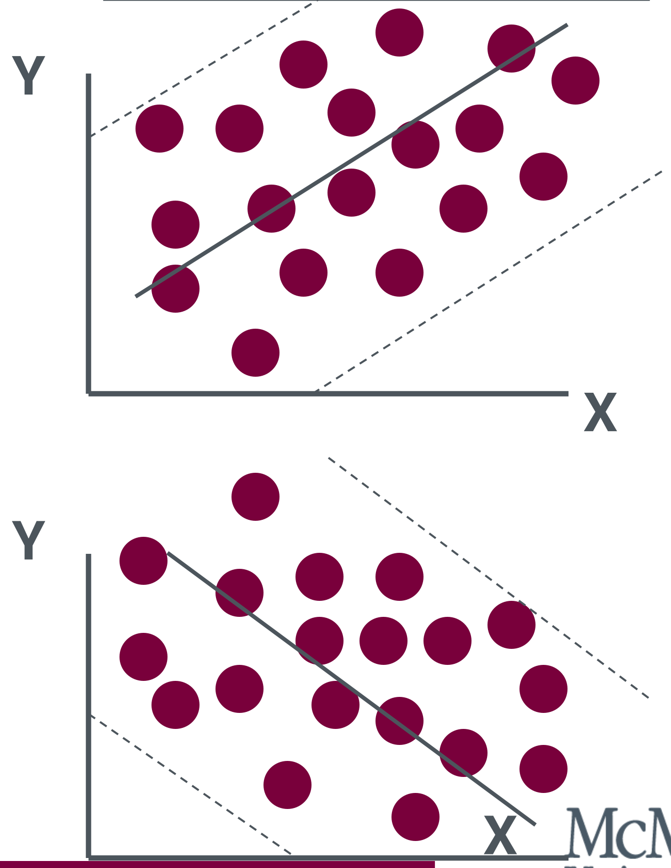
Source: Dr. Dipak Kumar Mitra, North South University

Linear Correlation

Strong relationships

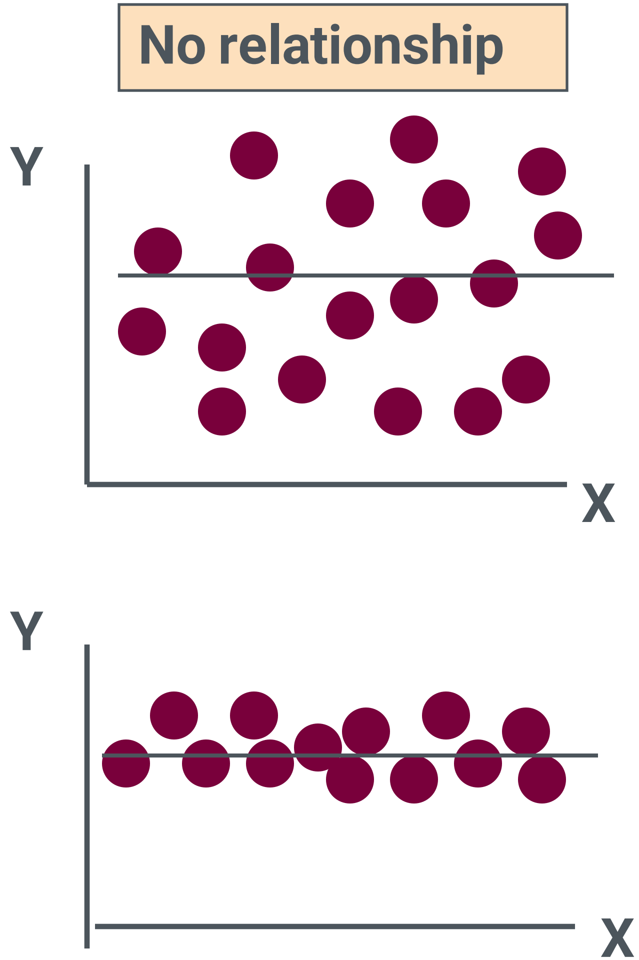


Weak relationships



Source: Dr. Dipak Kumar Mitra, North South University

Linear Correlation



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Source: Dr. Dipak Kumar Mitra, North South University

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Calculating by hand…

$$\hat{r} = \frac{\mathrm{cov}\,ariance(x,y)}{\sqrt{\mathrm{var}\ x}\sqrt{\mathrm{var}\ y}} = \frac{\dfrac{\sum_{i=1}^{n}(x_i-\bar{x})(y_i-\bar{y})}{n-1}}{\sqrt{\dfrac{\sum_{i=1}^{n}(x_i-\bar{x})^2}{n-1}}\sqrt{\dfrac{\sum_{i=1}^{n}(y_i-\bar{y})^2}{n-1}}}$$

Source: Dr. Dipak Kumar Mitra, North South University

Simpler calculation formula…

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

$$\frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2}\sqrt{\sum_{i=1}^{n}(y_i - \bar{y})^2}} = \frac{SS_{xy}}{\sqrt{SS_x SS_y}}$$

Numerator of covariance

$$\hat{r} = \frac{SS_{xy}}{\sqrt{SS_x SS_y}}$$

Numerators of variance

Standard error of the correlation coefficient:

$$SE(\hat{r}) = \sqrt{\frac{1 - r^2}{n - 2}}$$

The sample correlation coefficient follows a t-distribution with n-2 degrees of freedom (since you have to estimate the standard error).

*note, like a proportion, the variance of the correlation coefficient depends on the correlation coefficient itself→substitute in estimated r

Linear regression

- 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*

Source: Dr. Dipak Kumar Mitra, North South University

Prediction

- If you know something about X, this knowledge helps you predict something about Y
- Sound familiar?…sound like conditional probabilities?

Source: Dr. Dipak Kumar Mitra, North South University

What’s Slope?

A slope of 2 means that every 1-unit change in X yields a 2-unit change in Y.

Source: Dr. Dipak Kumar Mitra, North South University

Regression equation…

Expected value of y at a given level of *x*=

$$E(y_i / x_i) = \alpha + \beta x_i$$

Predicted value for an individual…

$$y_i = \underbrace{\alpha + \beta * x_i}_{\text{Fixed – exactly on the line}} + \boxed{\text{random error}_i}$$

Follows a normal distribution

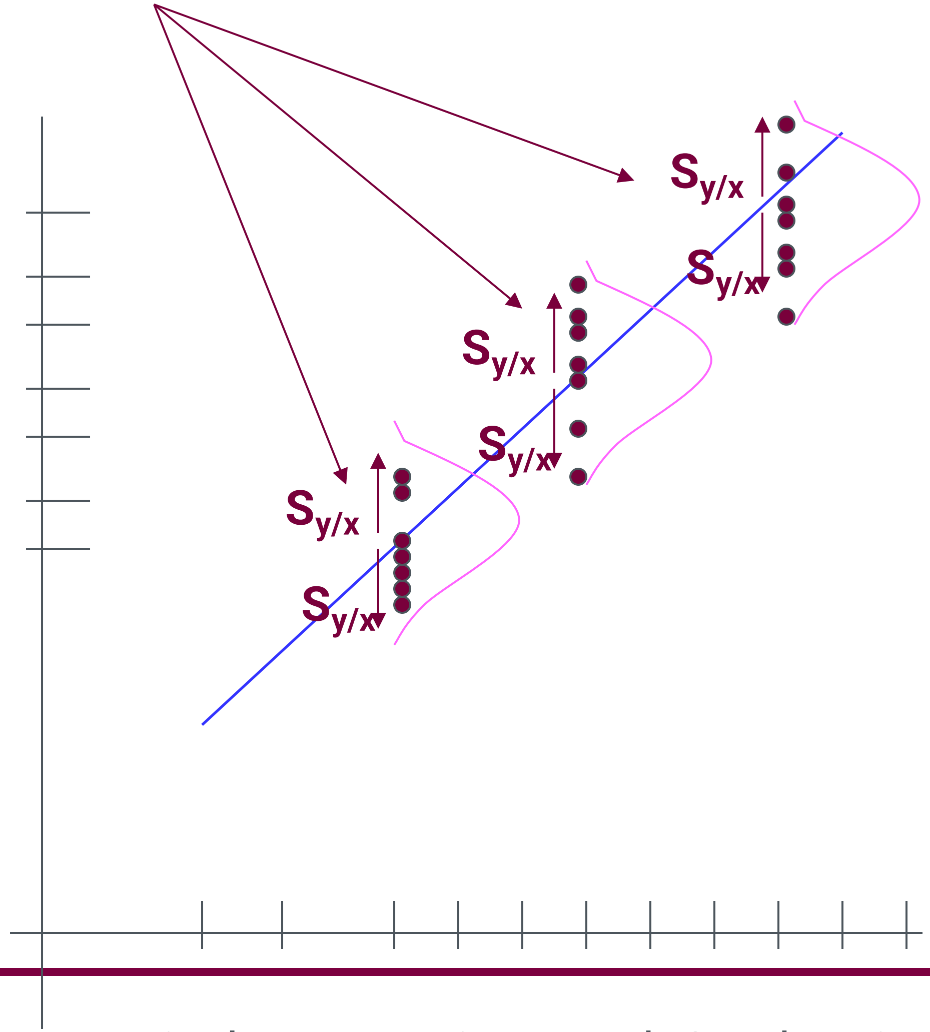
Source: Dr. Dipak Kumar Mitra, North South University

Assumptions (or the fine print)

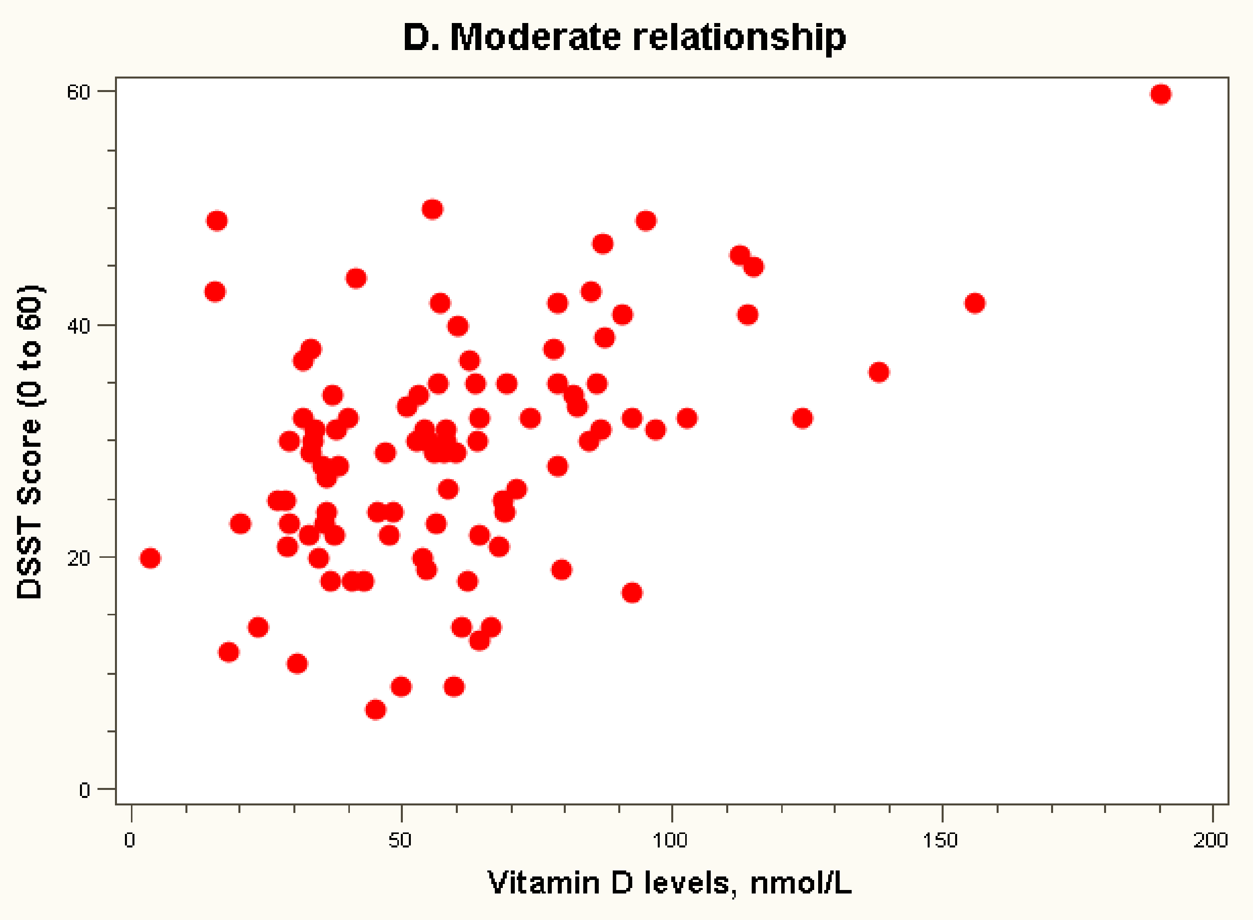
- Linear regression assumes that…
  1. Linearity: True mean of y is a linear function of x
  2. Y is distributed normally at each value of X
  3. The variance of Y at every value of X is constant (homogeneity of variances) (in next slide)
  4. The observations are independent

Source: Dr. Dipak Kumar Mitra, North South University

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

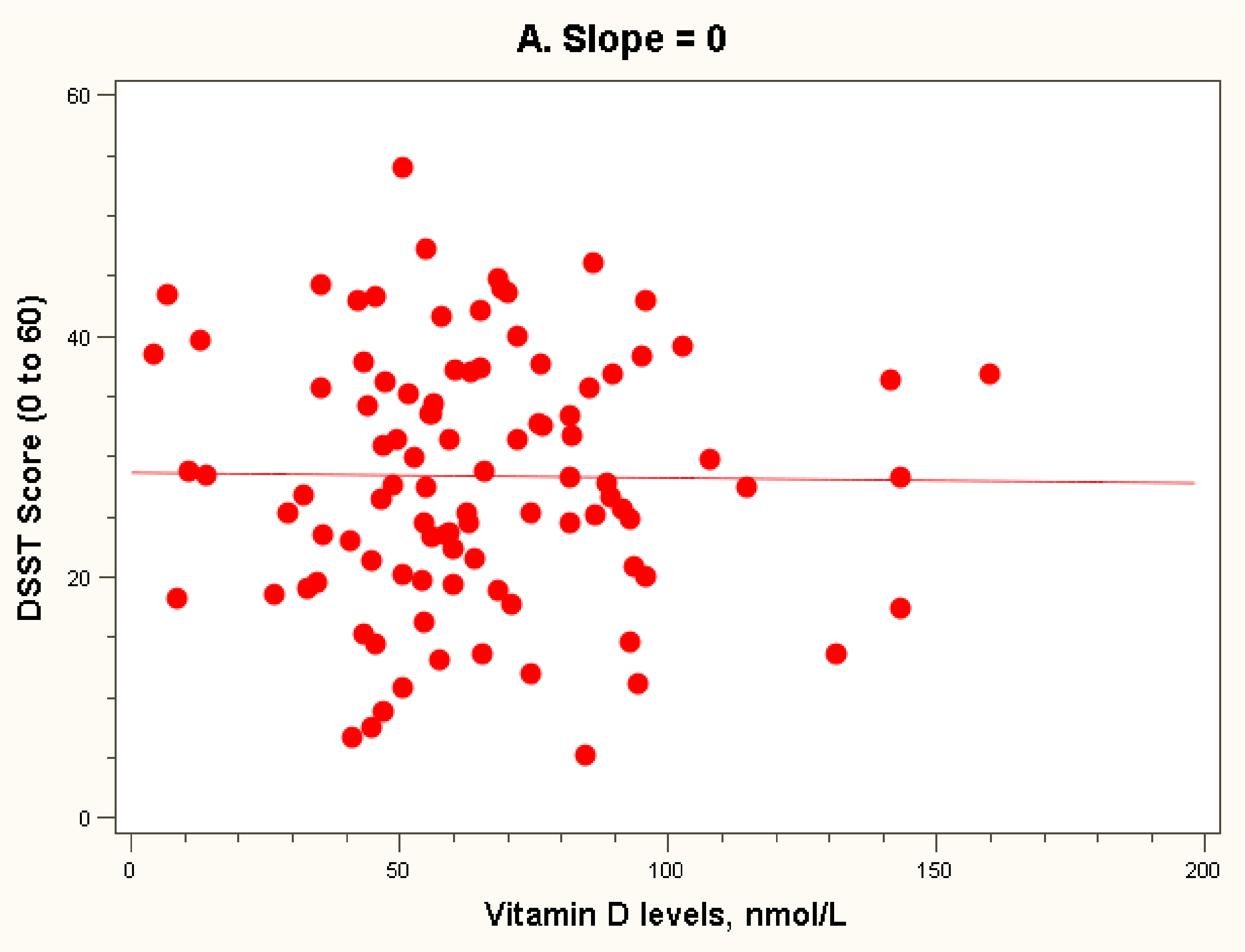


Moderate relationship



Source: Dr. Dipak Kumar Mitra, North South University

The “Best fit” line

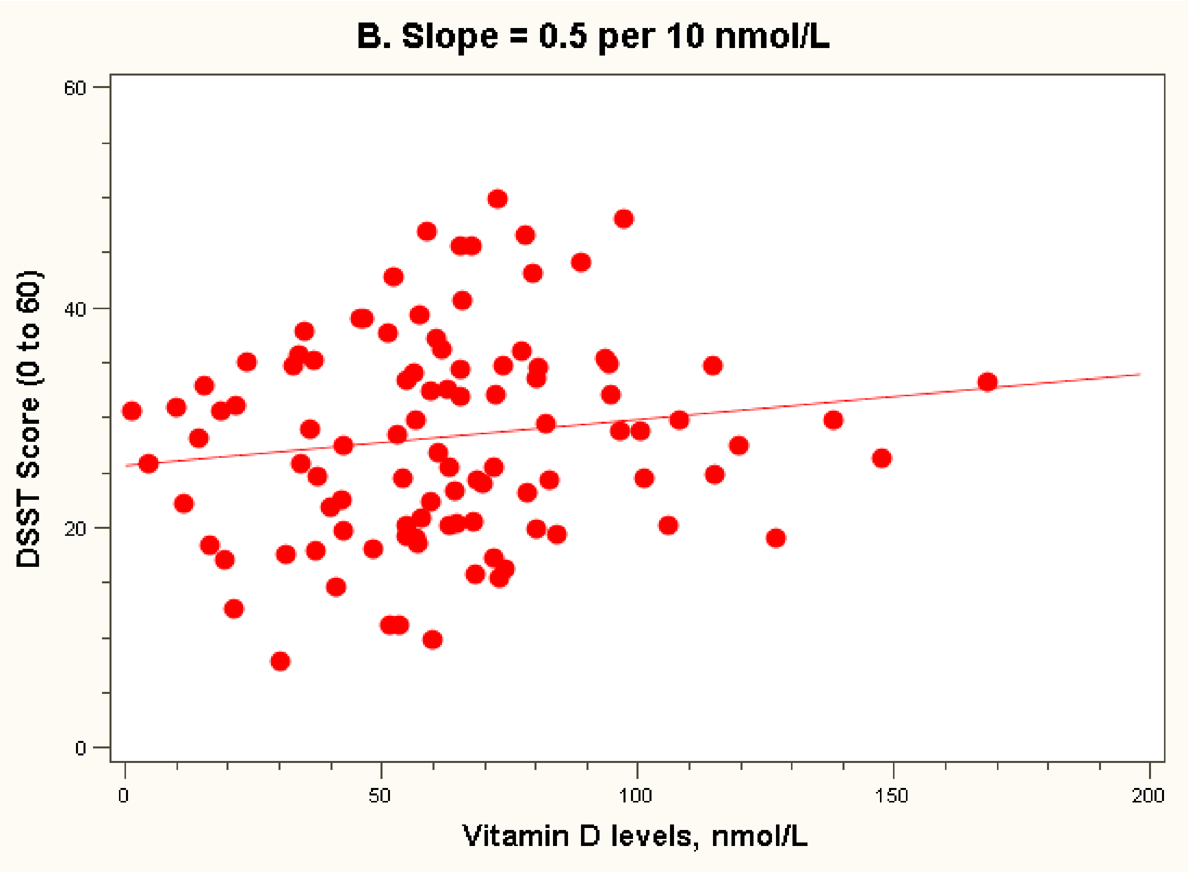


Regression equation:

$E(Y_i) = 28 + 0 * \text{vit } D_i$ (in 10 nmol/L)

Source: Dr. Dipak Kumar Mitra, North South University

The "Best fit" line



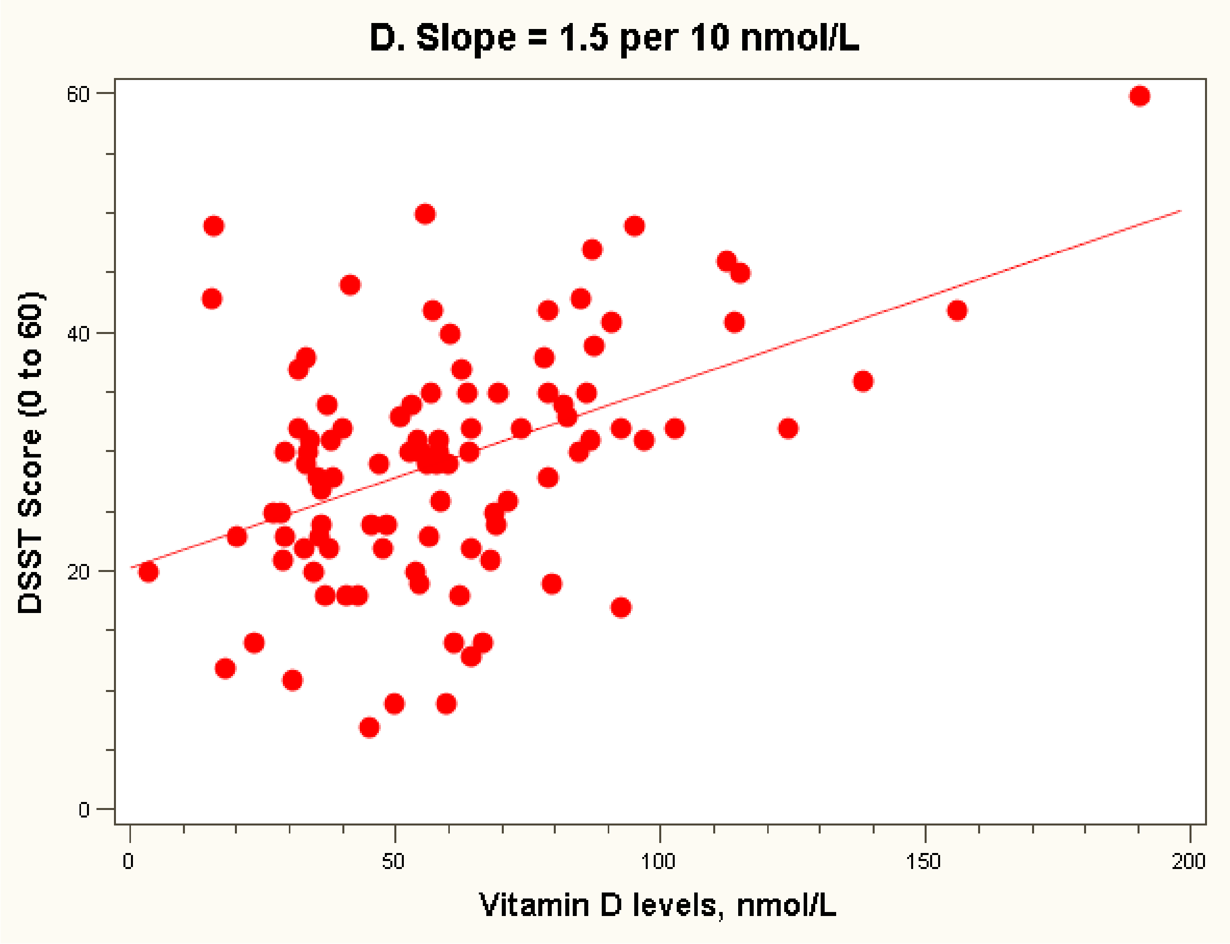
Note how the line is a little deceptive; it draws your eye, making the relationship appear stronger than it really is!

Regression equation:

$E(Y_i) = 26 + 0.5*\text{vitD}_i$ (in 10 nmol/L)

Source: Dr. Dipak Kumar Mitra, North South University

The "Best fit" line



Regression equation:

$E(Y_i) = 20 + 1.5*vit D_i$ (in 10 nmol/L)

Note: all the lines go through the point (63, 28)!

Statistical Concepts

- Based on ıtimate the model

$$\hat{\beta}_1 = \frac{\sum(x_i - \bar{x})(y_i - \bar{y})}{\sum(x_i - \bar{x})^2}$$

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

- Since $\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X$ and $\hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{X}$
- We can re-write the equation like $\hat{Y} = \bar{Y} + \hat{\beta}_1 (X - \bar{X})$
- So the regression line goes through the point $(\bar{X}, \bar{Y})$

Source: Dr. Shofiqul Islam, McMaster University

Correlation and Regression Slope

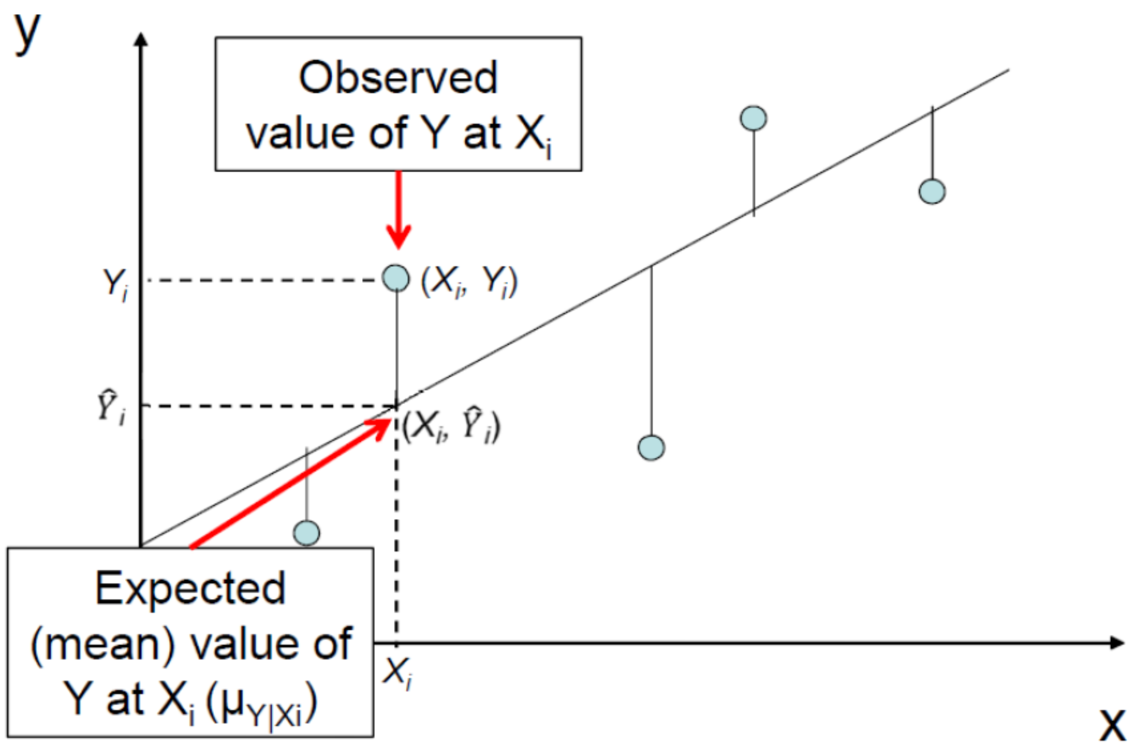
- Relationship between Pearson product-moment correlation and the slope of the simple linear regression line?
- Pearson's correlation coefficient measures the amount of linear association between Y and X
  - Non-directional –one 'is associated' with the other

$$r = \frac{Cov(x,y)}{\sqrt{Var(x)Var(y)}}$$

- The slope of the simple linear regression line tells how much a change in X impacts a change in Y
  - Directional –one 'predicts' the other

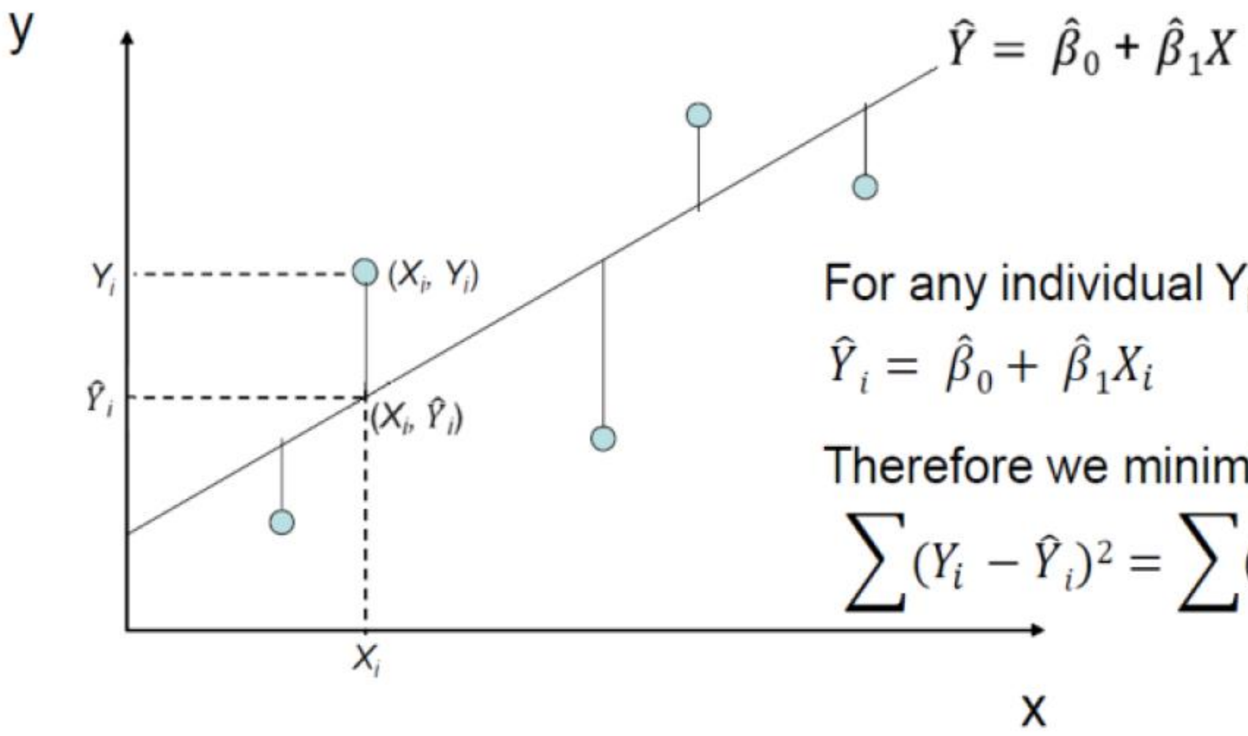
$$\hat{\beta}_1 = r\frac{S_Y}{S_X}$$

Geometry



Source: Dr. Shofiqul Islam, McMaster University

Geometry of Least Square



For any individual Y_i,

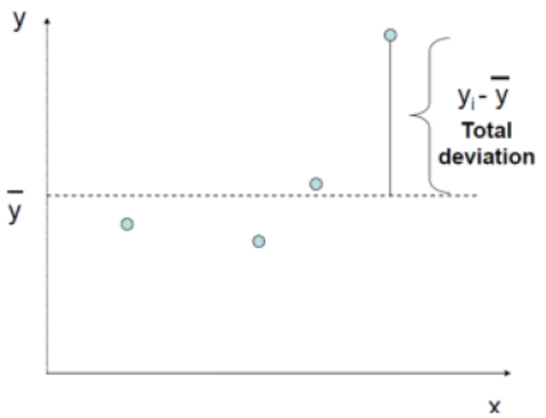
$$\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 X_i$$

Therefore we minimize:

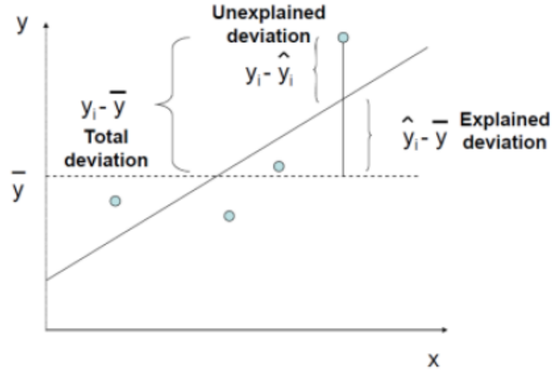
$$\sum (Y_i - \hat{Y}_i)^2 = \sum (Y_i - (\hat{\beta}_0 + \hat{\beta}_1 X_i))^2$$

Source: Dr. Shofiqul Islam, McMaster University

Variance decomposition



$$Var\ Y = \frac{\Sigma(y_i - \bar{y})^2}{n-1}$$

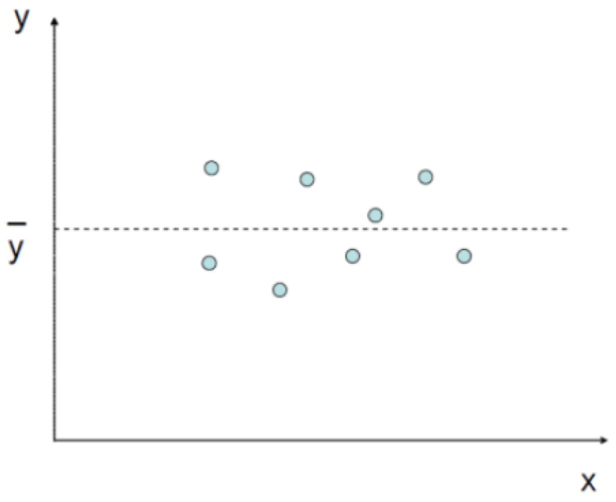


$$\Sigma(y_i - \bar{y})^2 = \Sigma(y_i - \hat{y}_i)^2 + \Sigma(\hat{y}_i - \bar{y})^2$$

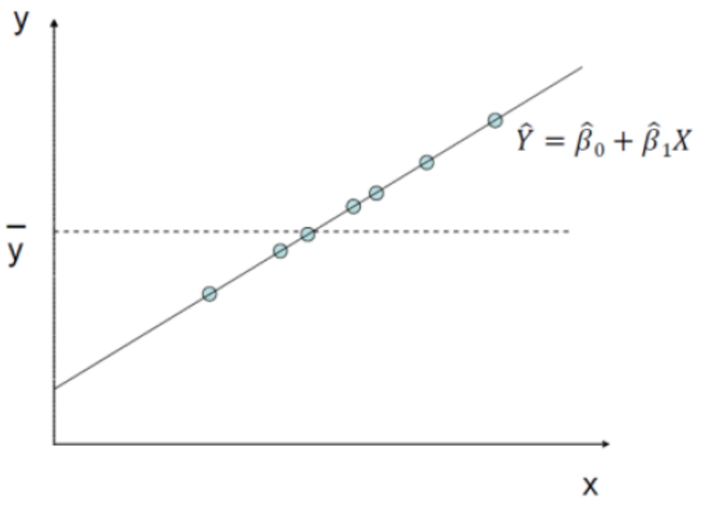
Total SS Residual SS Regression SS

Source: Dr. Shofiqul Islam, McMaster University

Extreme Results



$$SS_{Total} \cong SS_{Error}$$



$$SS_{Total} \cong SS_{Reg}$$

Source: Dr. Shofiqul Islam, McMaster University

ANOVA Table

of predictors (x variables)=1

	Sum of Squares SS	Degrees of Freedom df	Mean Square MS	F Value F
Regression	SS_{reg}	p	SS_{reg}/p	MS_{reg}/MS_{err}
Residual	SS_{err}	n-p-1	SS_{err} /(n-p-1)	
Total	SS_{tot}	n-1		

# of observations - # of parameters estimated

# of observation - 1

Where:

$SS_{reg} = \sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2$

$SS_{err} = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$

$SS_{tot} = \sum_{i=1}^{n}(y_i - \bar{y})^2$

$E(Ms_{err}) = \sigma^2$

$E(MS_{reg}) = \sigma^2 + \beta_1^2 \sum(X_i - \bar{X})^2$

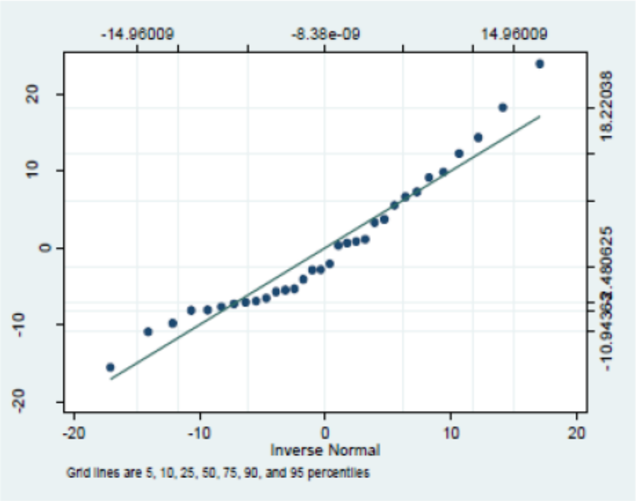
If H_o is true, i.e., $\beta_1 = 0$, then MS_{reg} is also an estimate of σ^2

Source: Dr. Shofiqul Islam, McMaster University

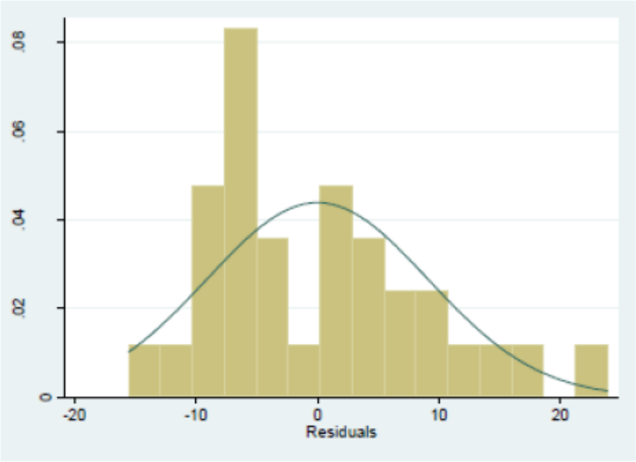
Assessing 'goodness of fit' assumptions

Normality – of residuals or of Y?

- Q-Q plot, histogram
- Shapiro-Wilk test



. qnorm residuals, grid



. histogram residuals, normal bin(15)

Source: Dr. Shofiqul Islam, McMaster University

Multiple linear regression…

- What if age is a confounder here?
  - Older men have lower vitamin D
  - Older men have poorer cognition
- “Adjust” for age by putting age in the model:
  - DSST score = intercept + $slope_1$ *x* vitamin D + $slope_2$ *x* age

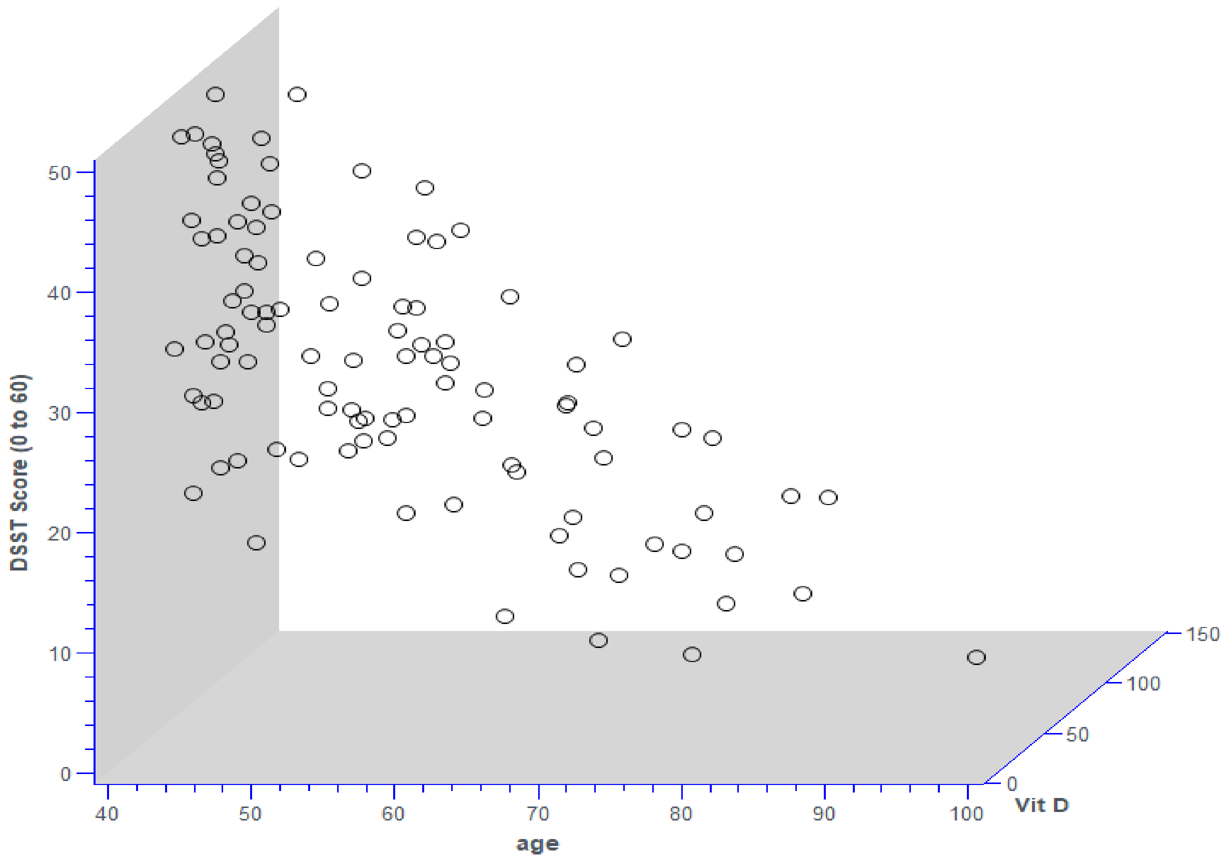
Multiple Linear Regression

- More than one predictor…

$$E(y) = \alpha + \beta_1 * X + \beta_2 * W + \beta_3 * Z \ldots$$

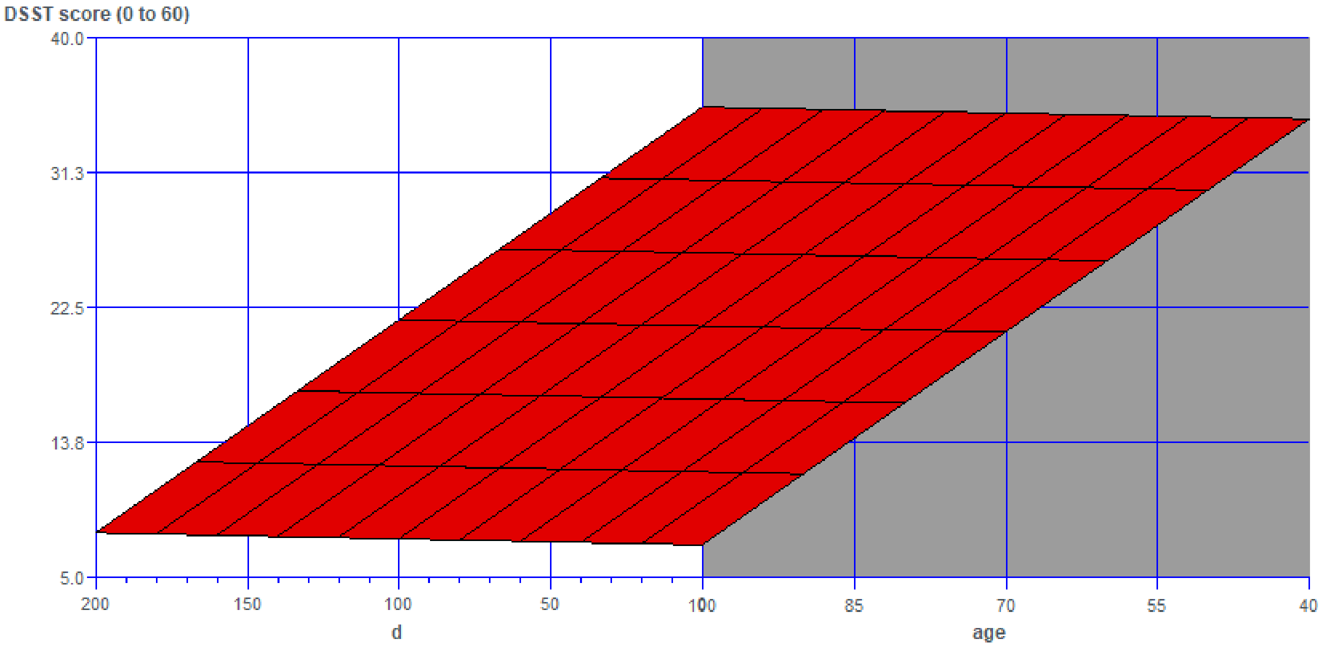
Each regression coefficient is the amount of change in the outcome variable that would be expected per one-unit change of the predictor, if all other variables in the model were held constant.

Different 3D view…



Source: Dr. Dipak Kumar Mitra, North South University

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.

Source: Dr. Dipak Kumar Mitra, North South University

Machine learning

Machine learning involves showing a large volume of data to a machine so that it can learn and make predictions, find patterns, or classify data.

Source: coursera.org

Types of machine learning

Basically, machine learning are three types.

Supervised

Unsupervised

Reinforcement learning.

Source: coursera.org

Supervised learning

*Machine learning **feeds historical input and output data** in machine learning algorithms, with processing in between each input/output pair that allows the algorithm to shift the model **to create outputs as closely aligned with the desired result as possible**.*

Common algorithms used during supervised learning include linear regression, neural networks, decision trees, and support vector machines.

Source: coursera.org

Unsupervised learning

*While supervised learning requires users to help the machine learn, unsupervised **learning algorithms don't use the same labeled training sets and data**. Instead, the machine looks for less obvious patterns in the data.*

*Unsupervised machine learning is very helpful when you need **to identify patterns** and use data to make decisions.*

Common algorithms used in unsupervised learning include k-means, hierarchical clustering, and Gaussian mixture models.

Source: coursera.org

Reinforcement learning

Reinforcement learning is the closest machine learning type to how humans learn.

*The algorithm used **learns by interacting with its environment and getting a positive or negative reward**.*

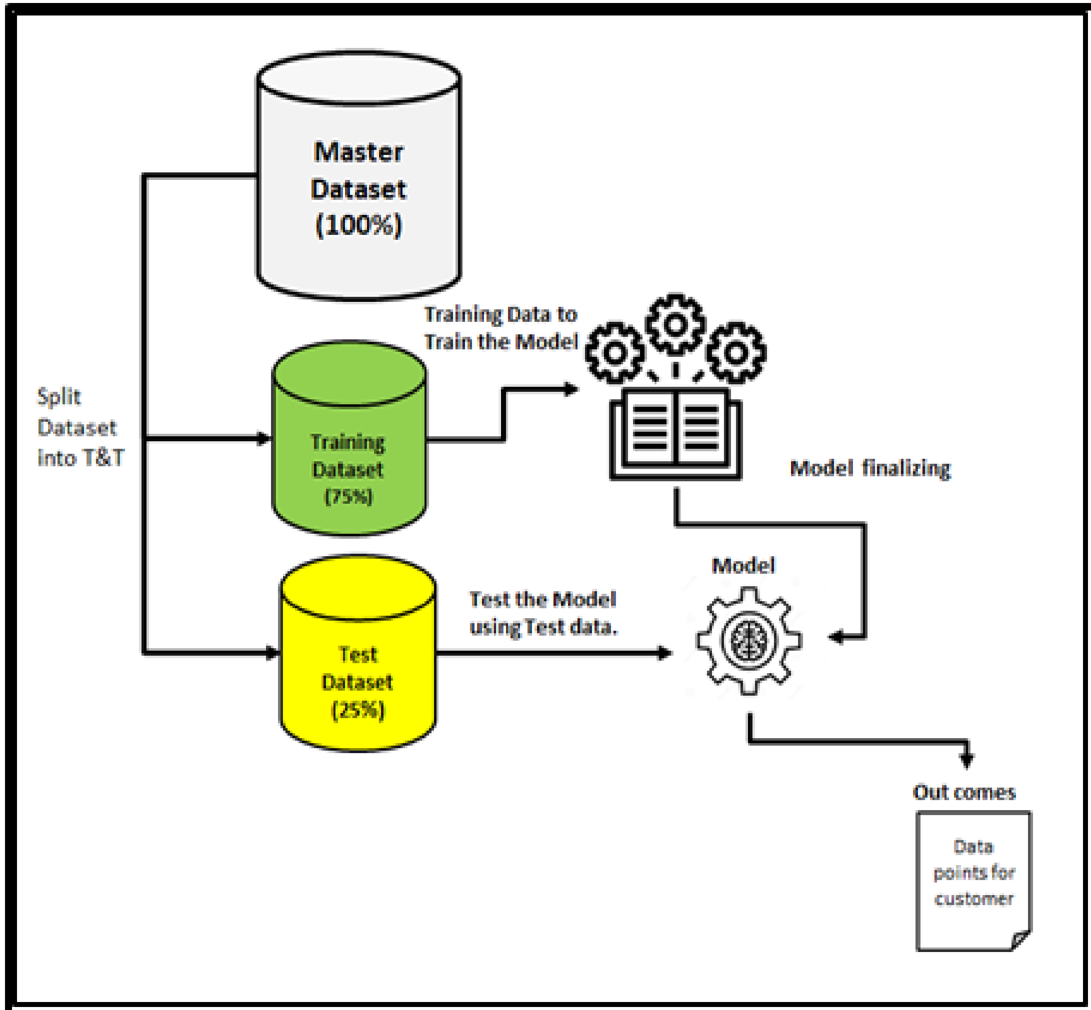
Common algorithms include temporal difference, deep adversarial networks, and Q-learning.

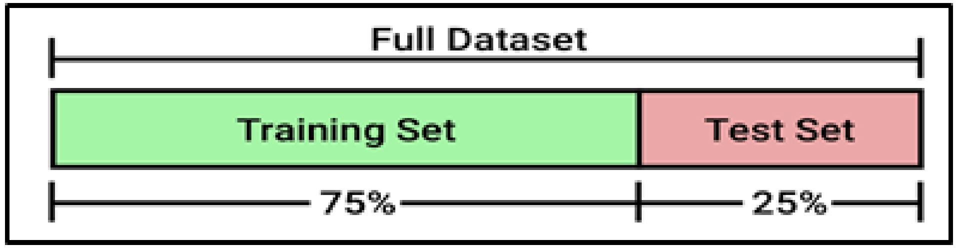
Source: coursera.org

Linear regression

- A supervised machine learning
- Learns from labeled data
- Make predictions on unseen data
- Goal of minimizing prediction errors

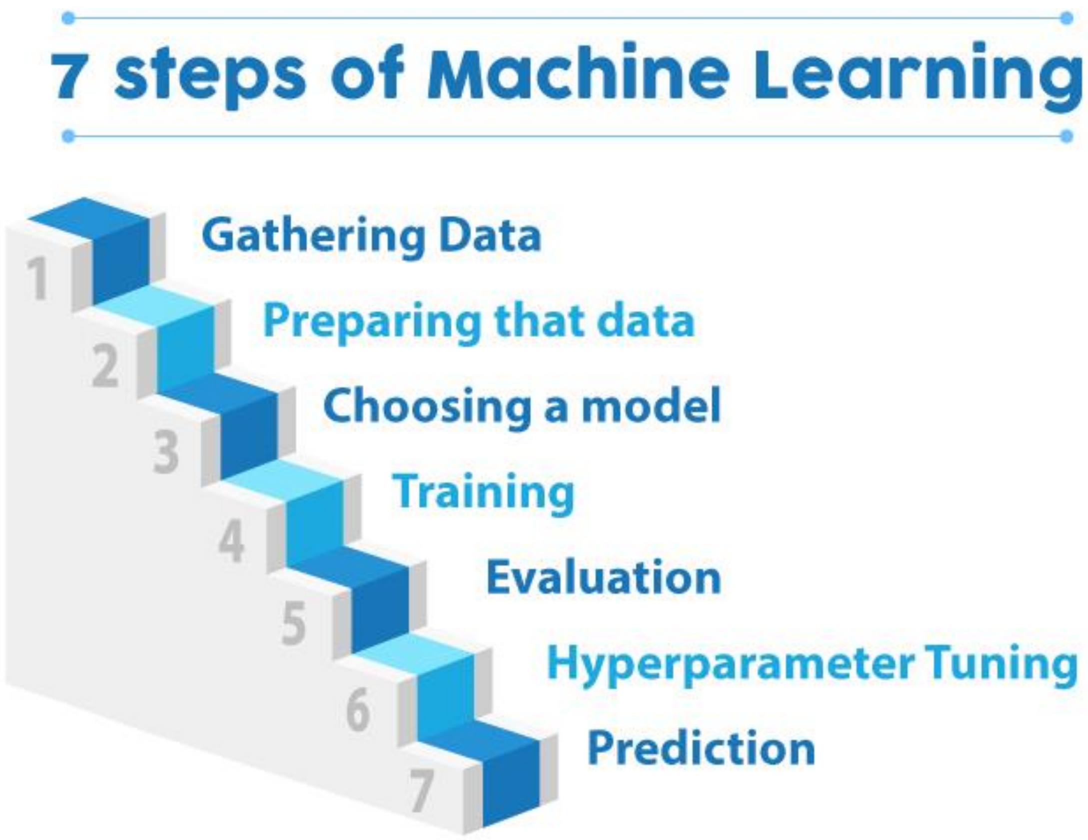
Steps of ML





https://www.analyticsvidhya.com/

Steps of ML including tuning



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Let move to the coding part

https://colab.research.google.com/drive/1PKxey0_YzdSrc_CcRPwh_Cd3JDglOi74#scrollTo=B_48FOMnQ5Yg