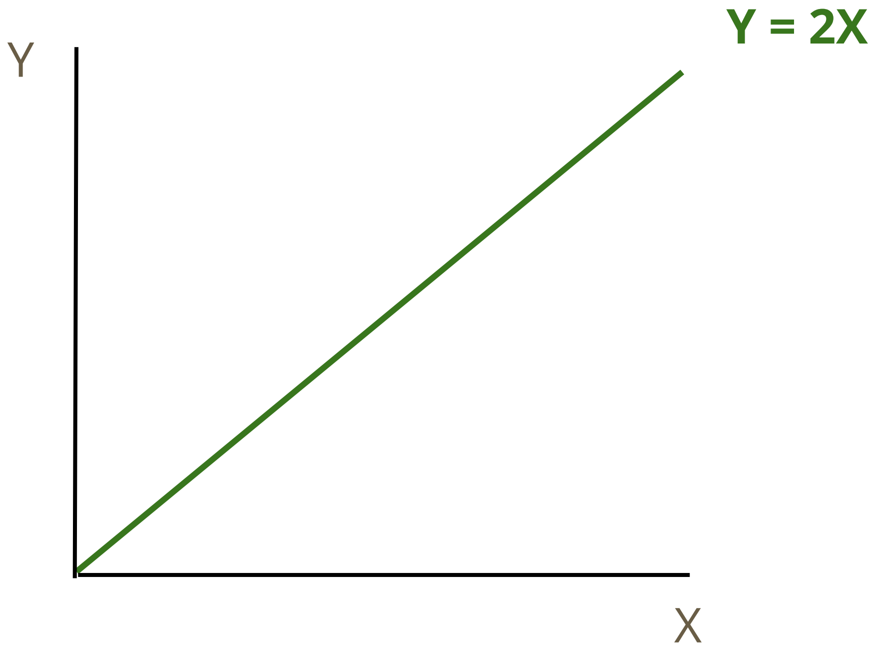
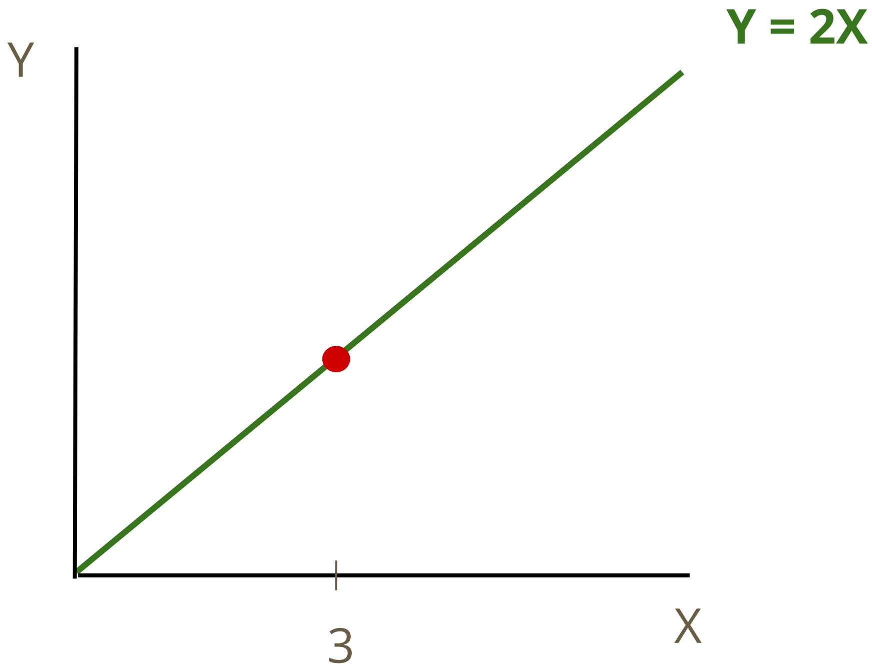
Linear Model Evaluation

Boston University CS 506 - Lance Galletti

Linear Function

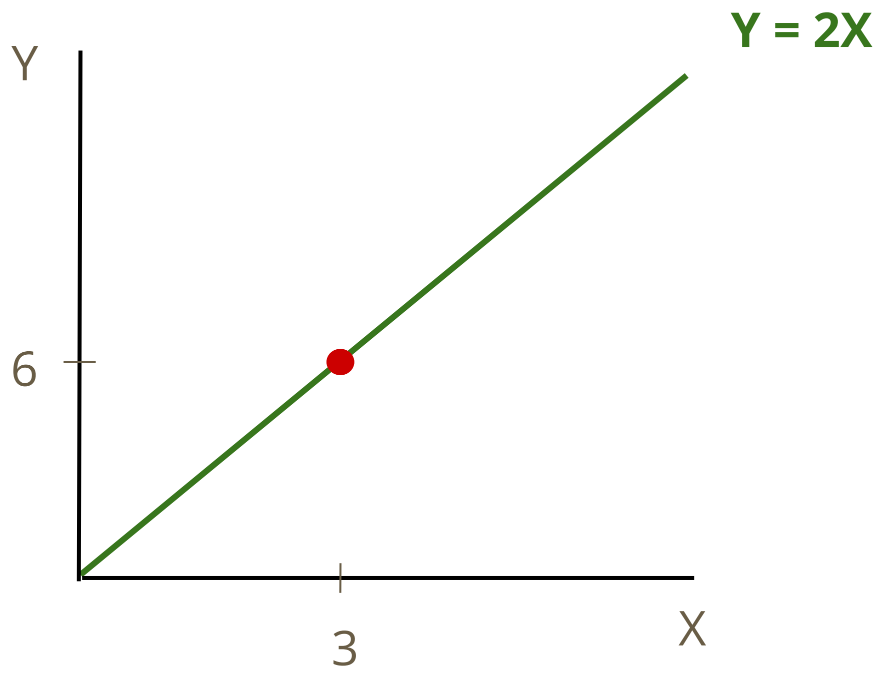


Linear Function

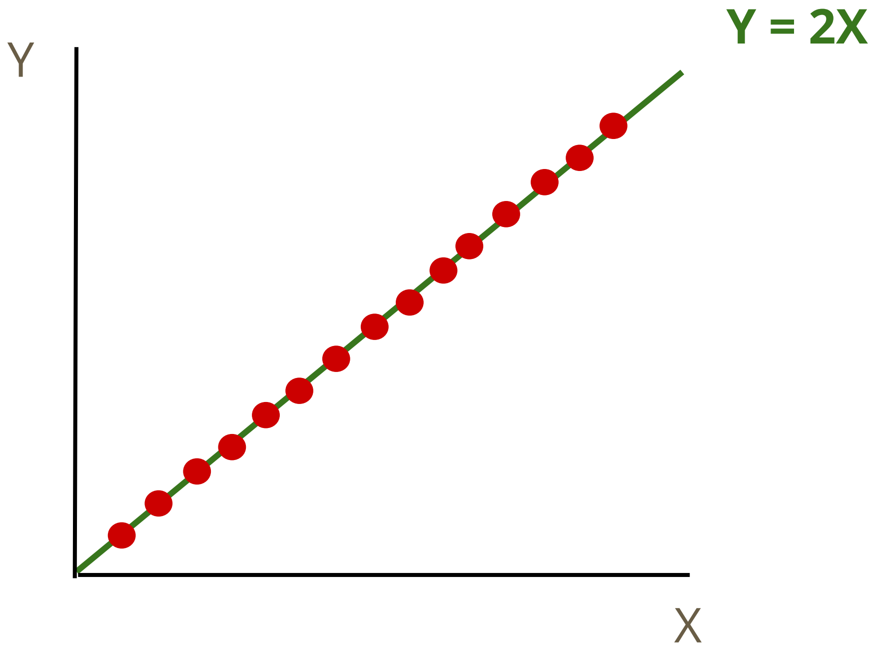


Linear Function

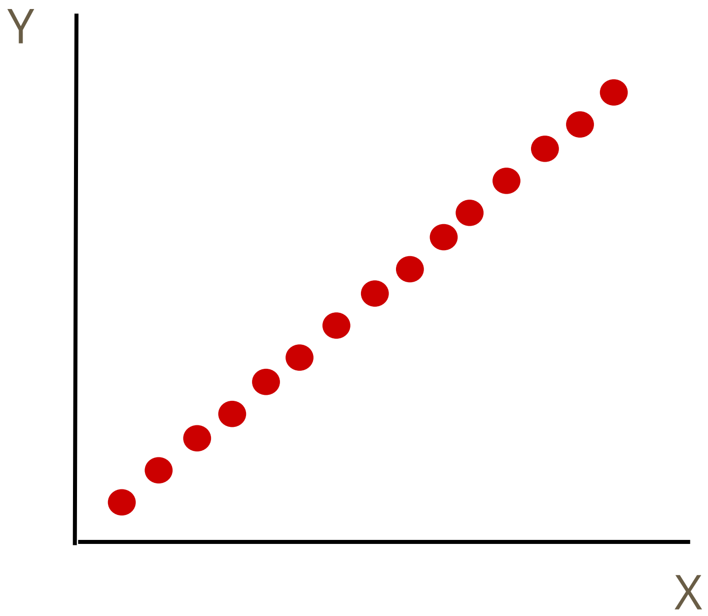
I know for sure what value of Y I’m gonna get



Linear Function



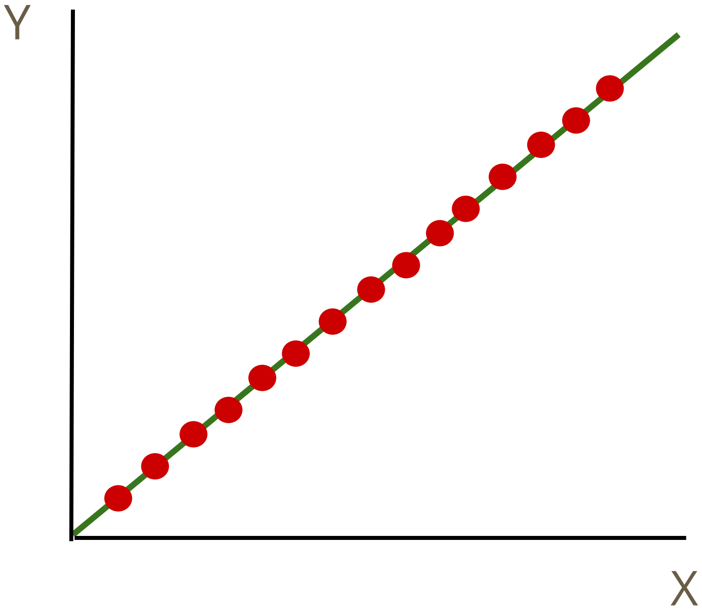
Ideally



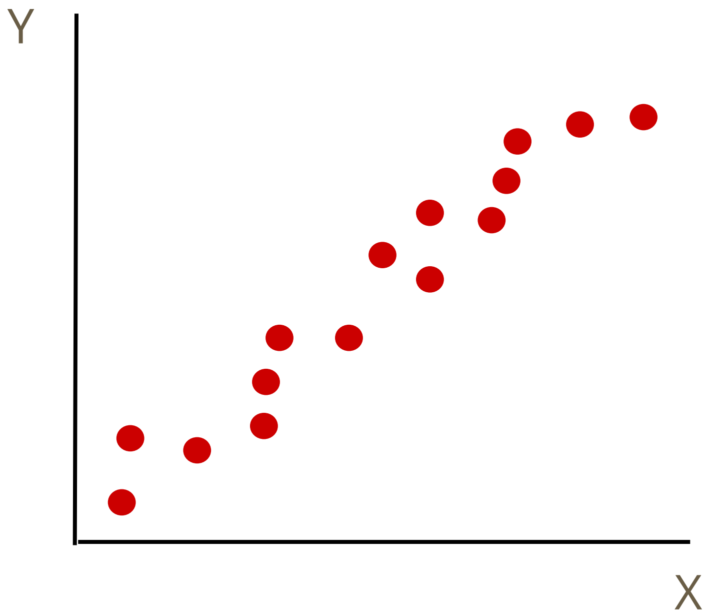
Ideally

Guess the relationship
(**a** and **b**) from the data

Y = aX + b



Practically



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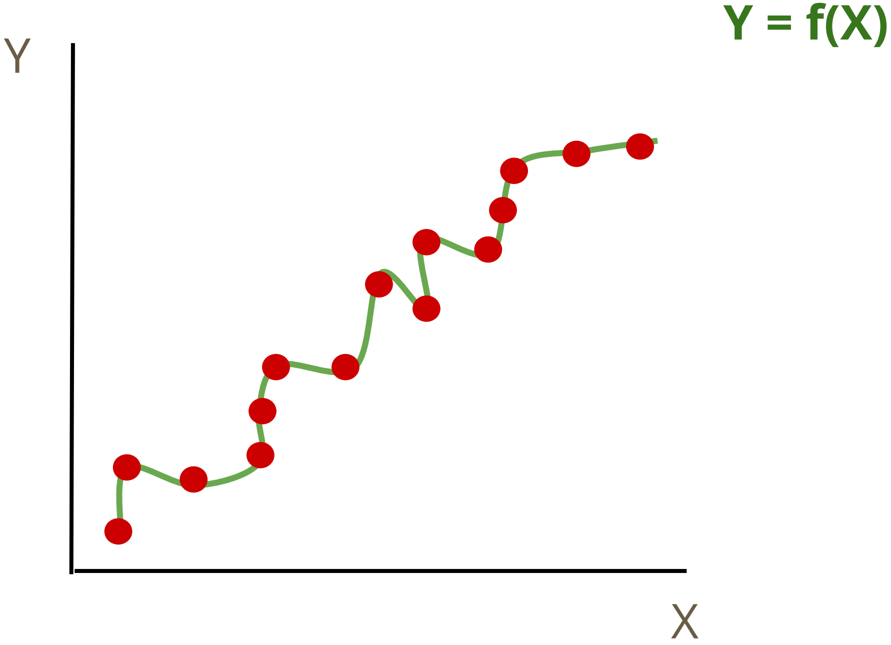
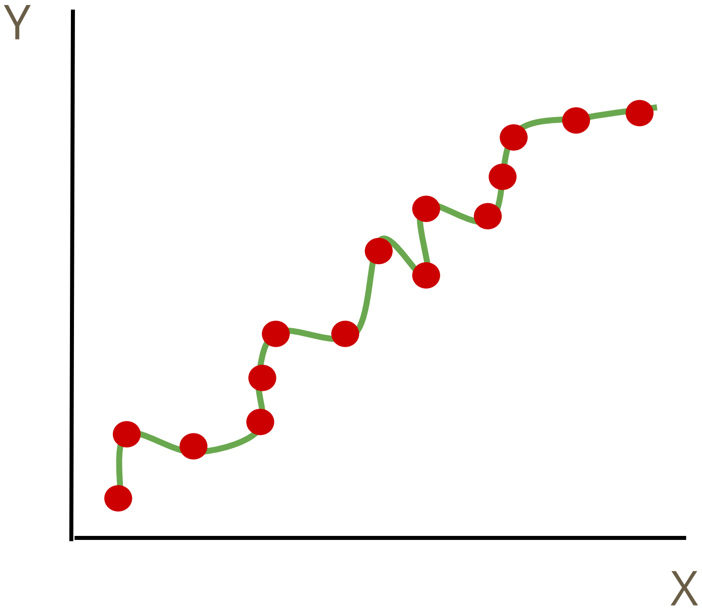


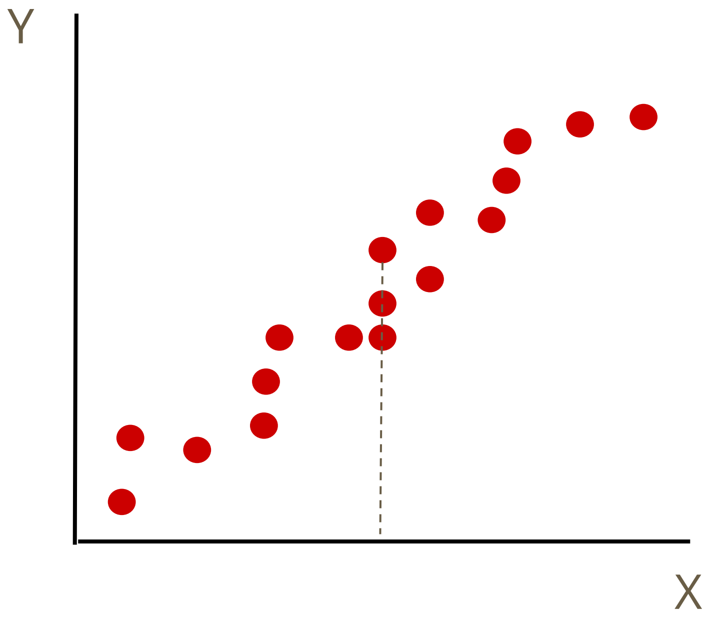
Practically



$Y = f(X)$

f can be anything: too complex a problem to solve…

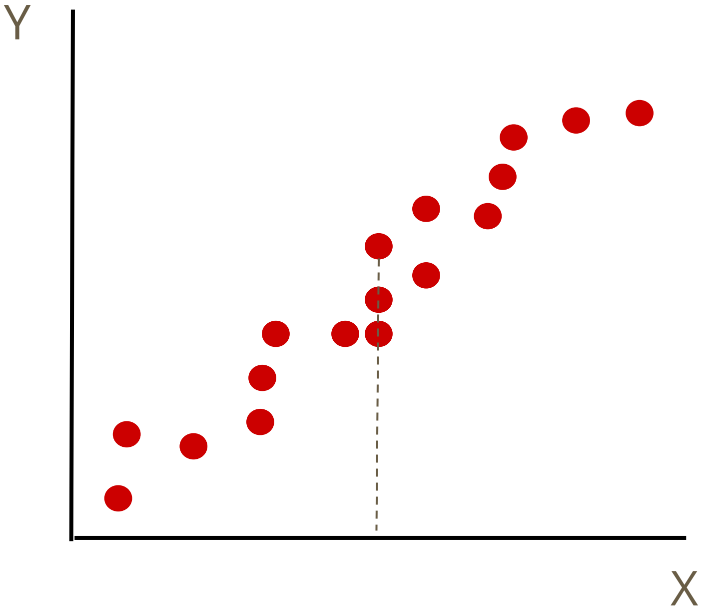
Practically



Y = f(X)

f can not even be a math function

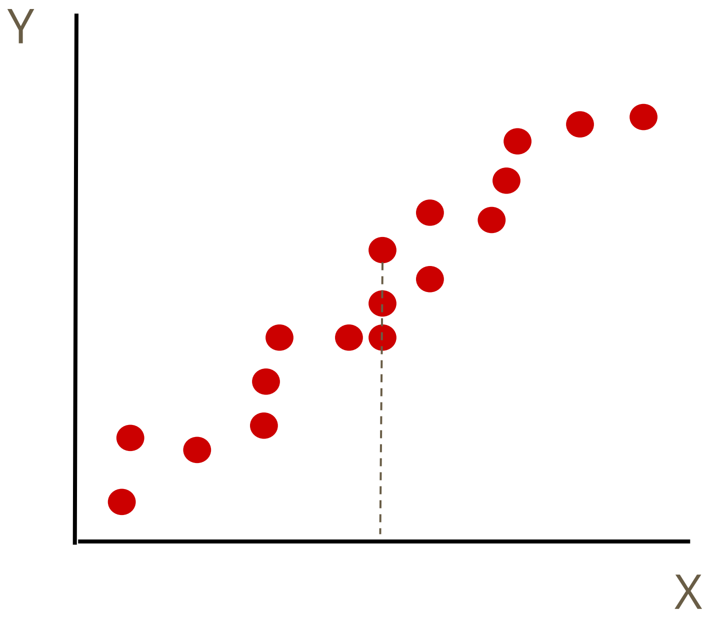
Practically



Y = random

For a given **x** we could get many **y** values

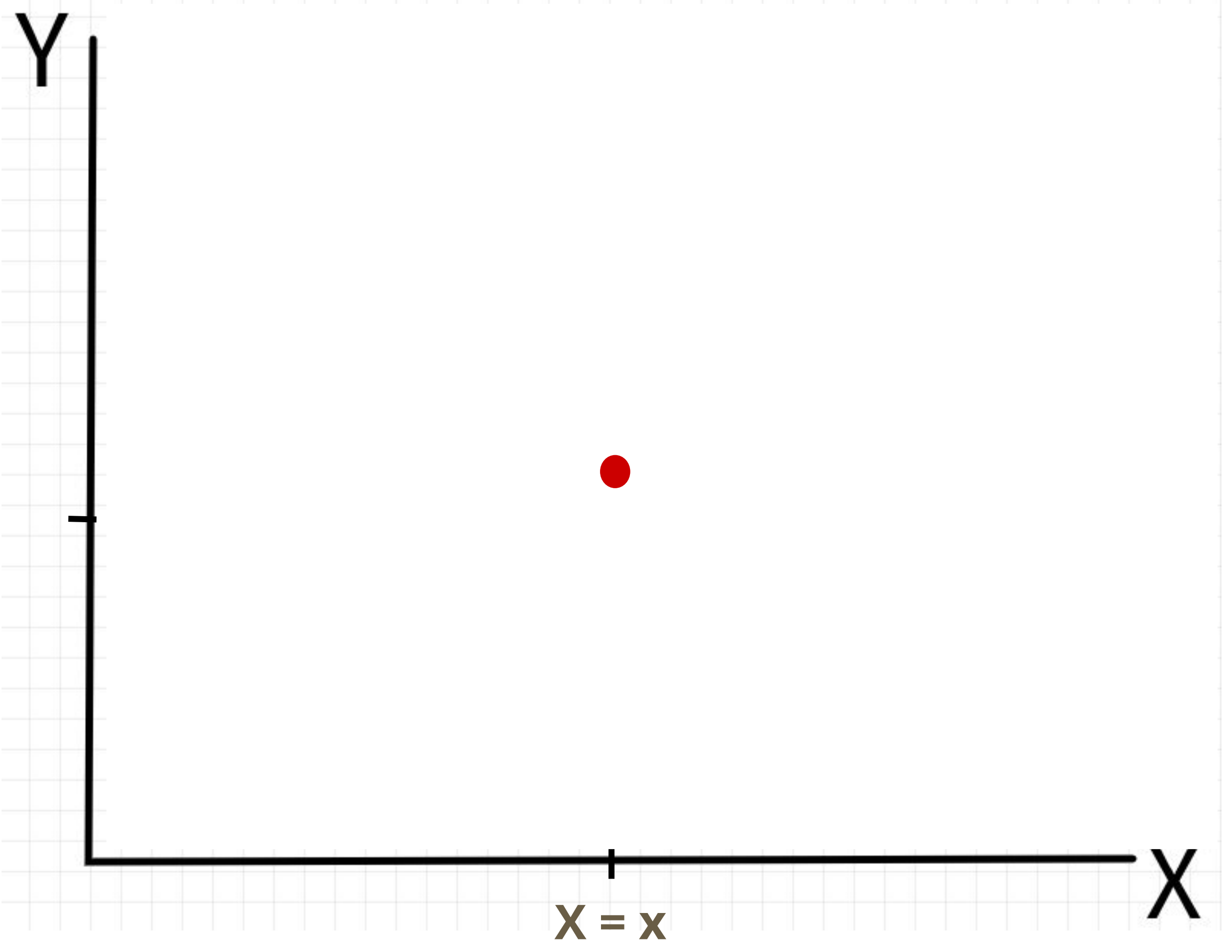
Practically



E[Y] = f(X)

So let’s capture the function that describes **E[y]** (i.e. the expected value that y should have for a given x)

Assumptions



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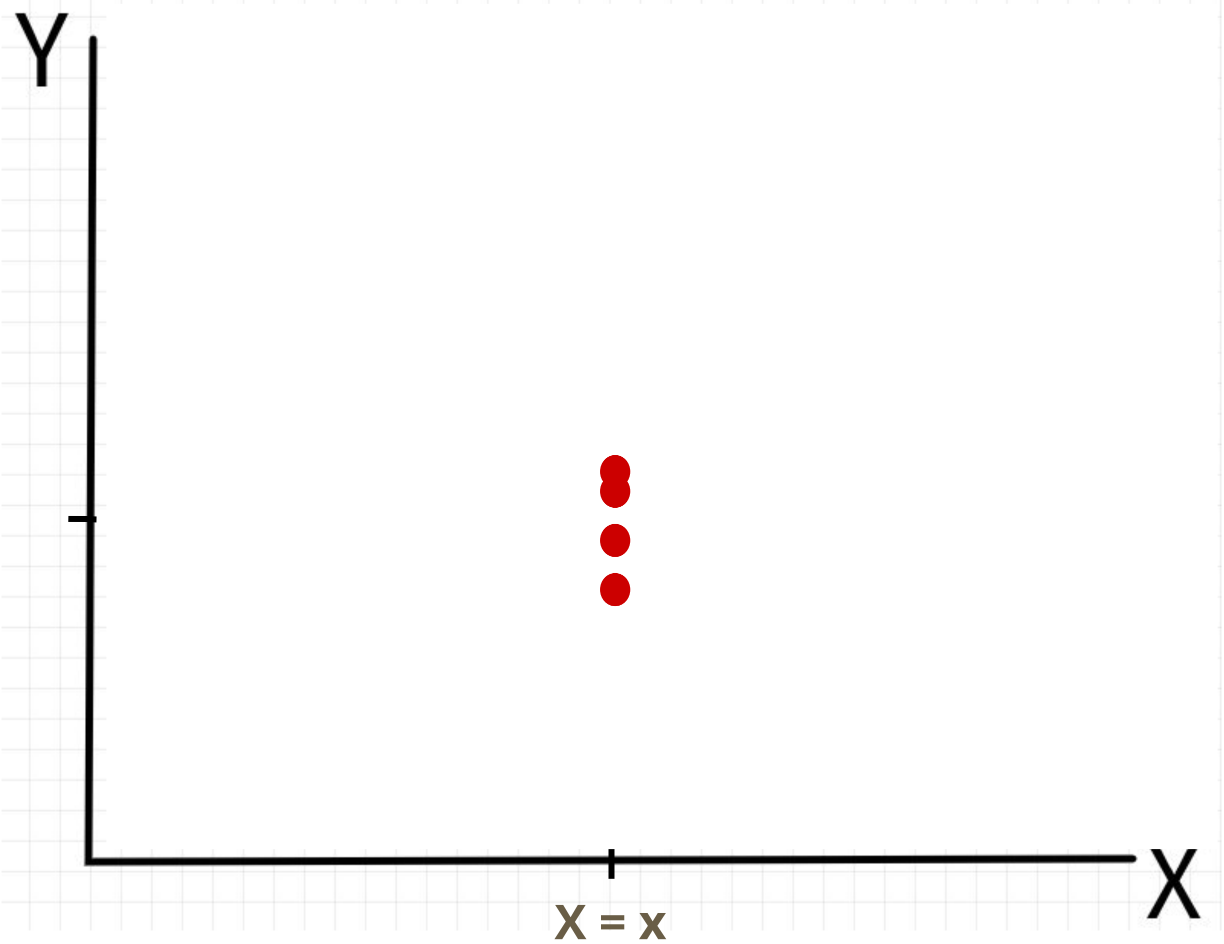

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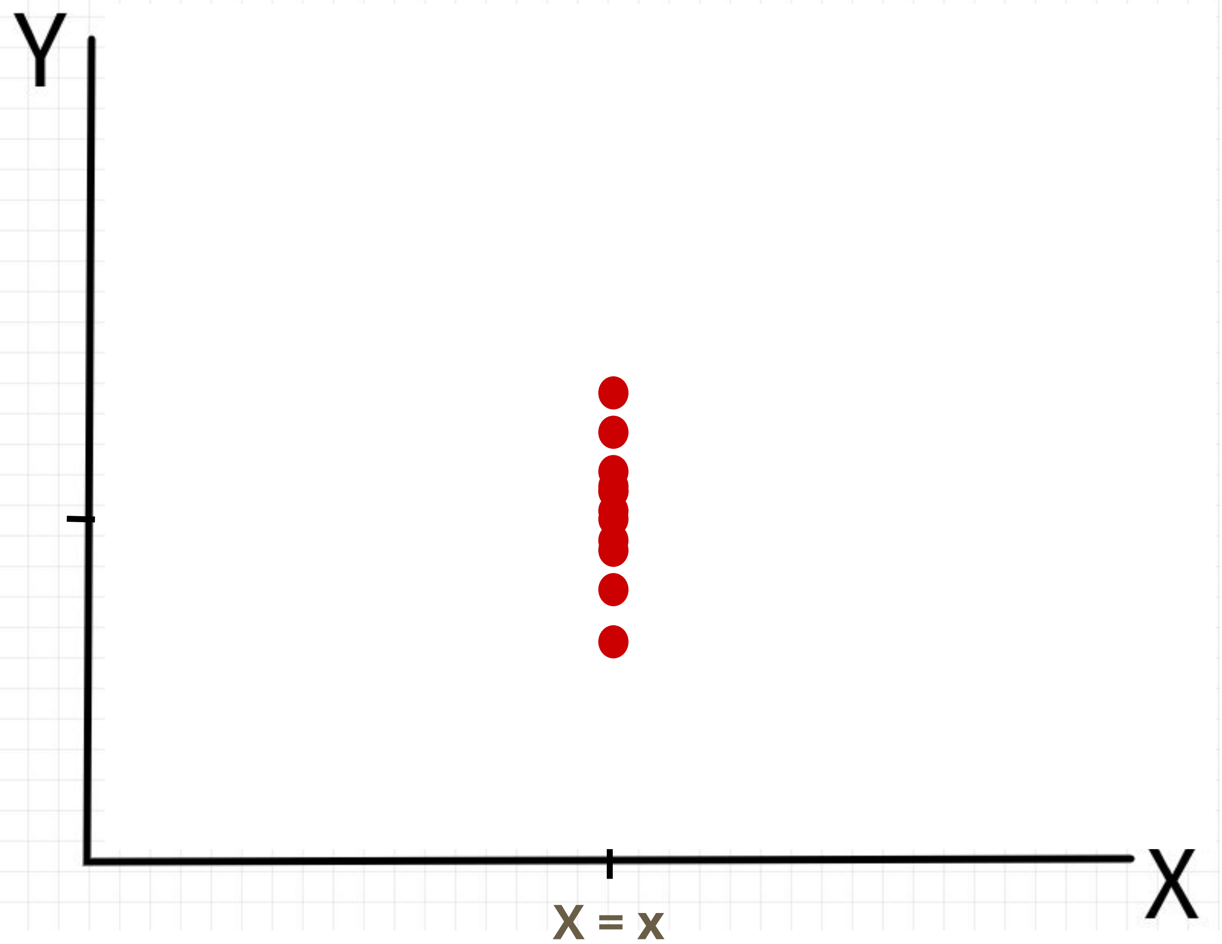

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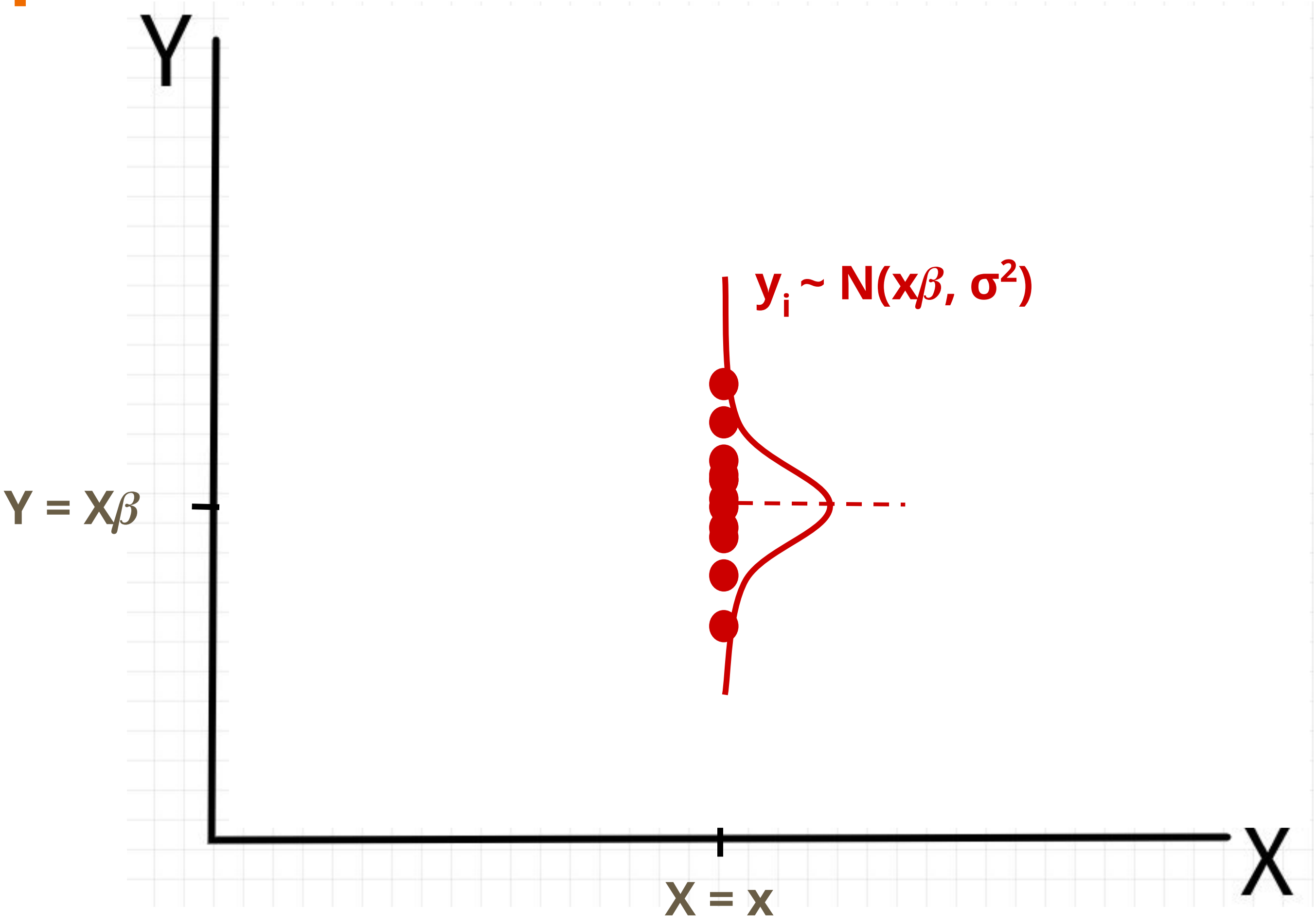

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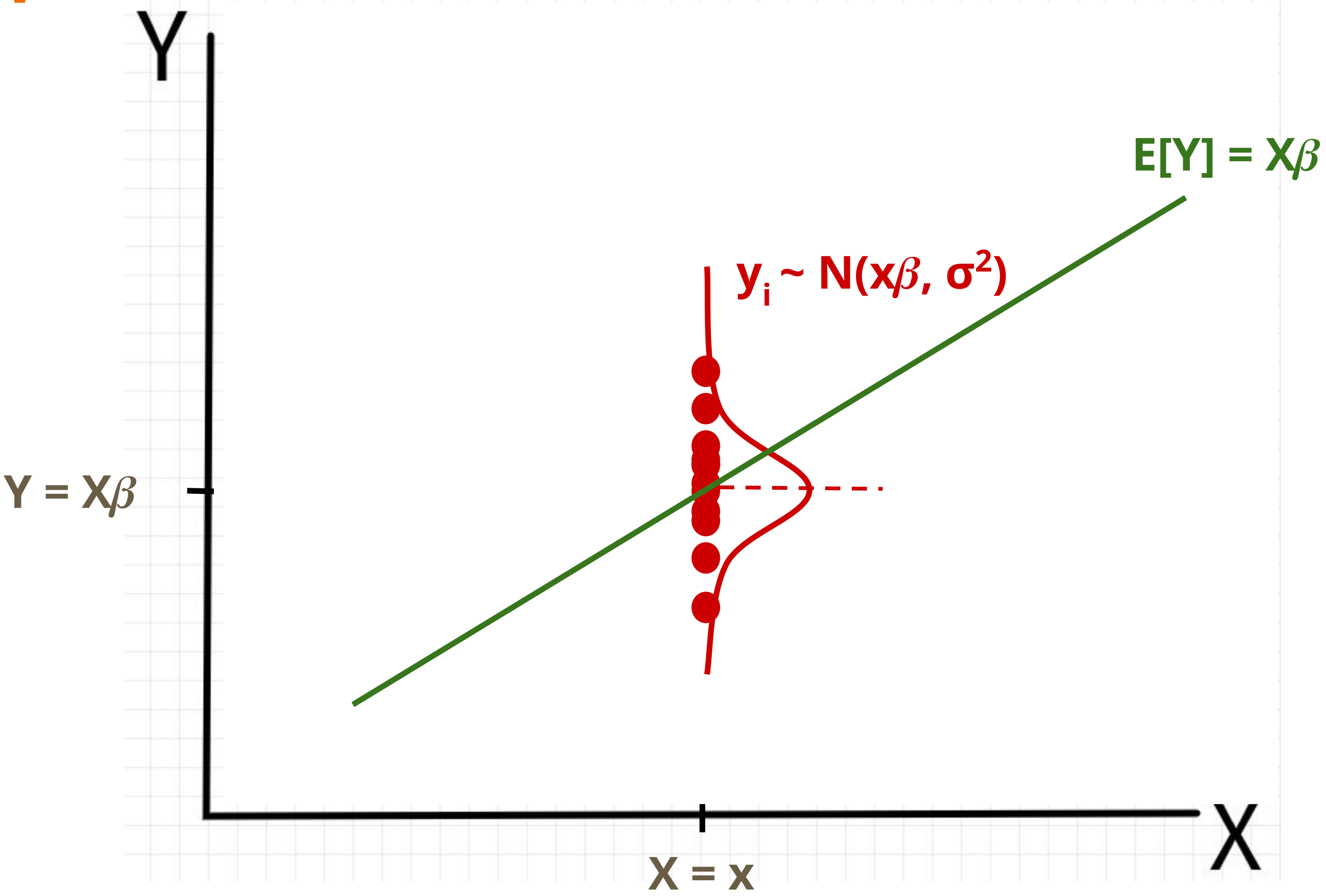

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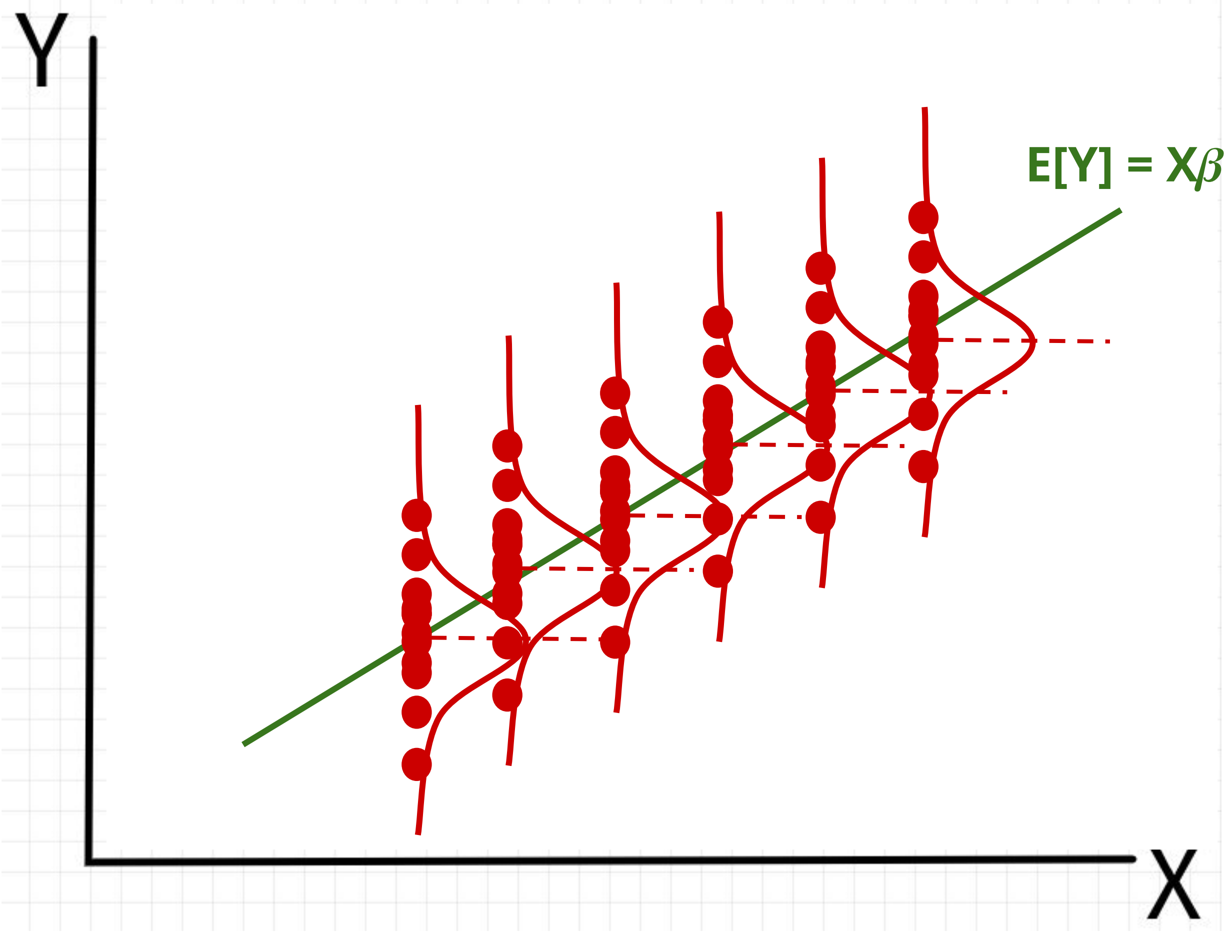

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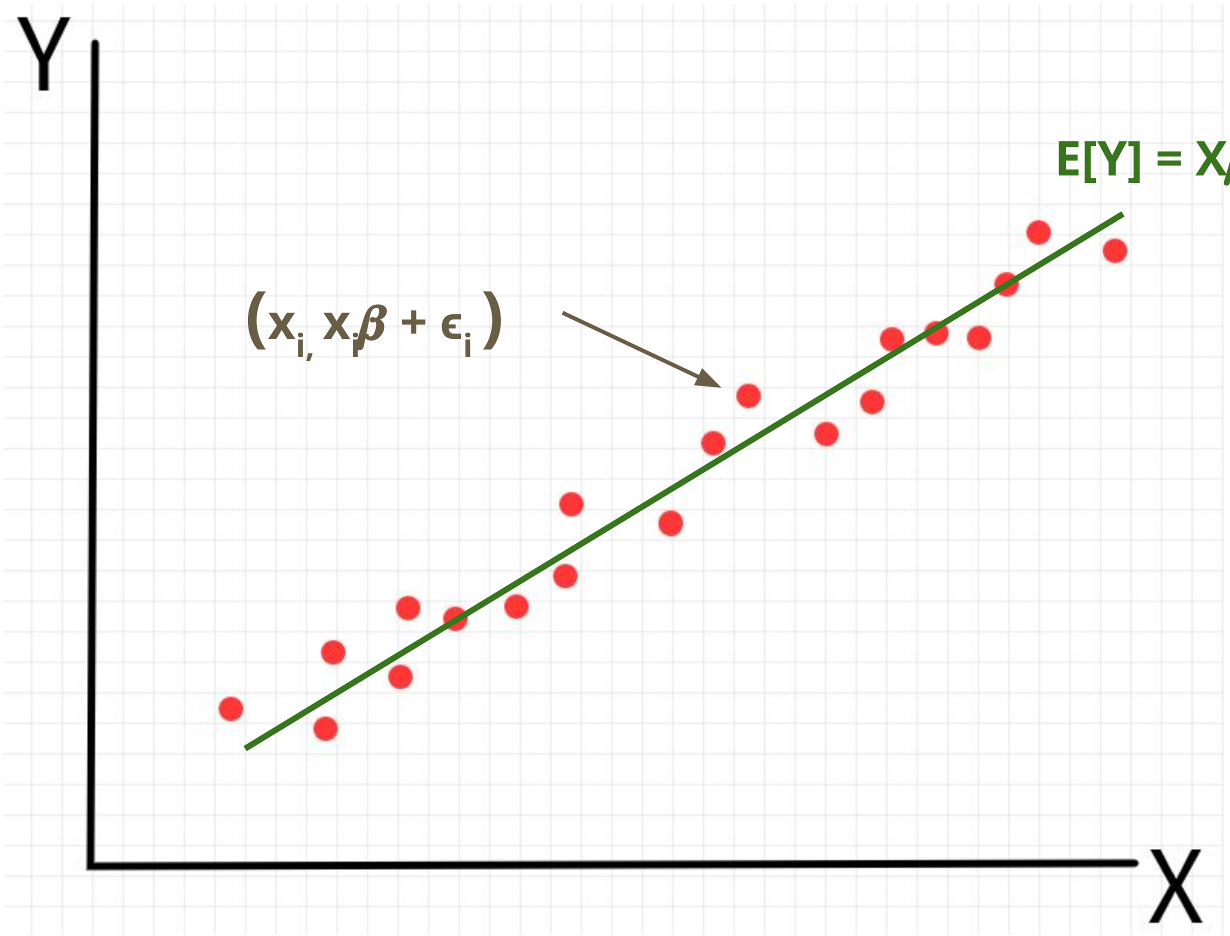

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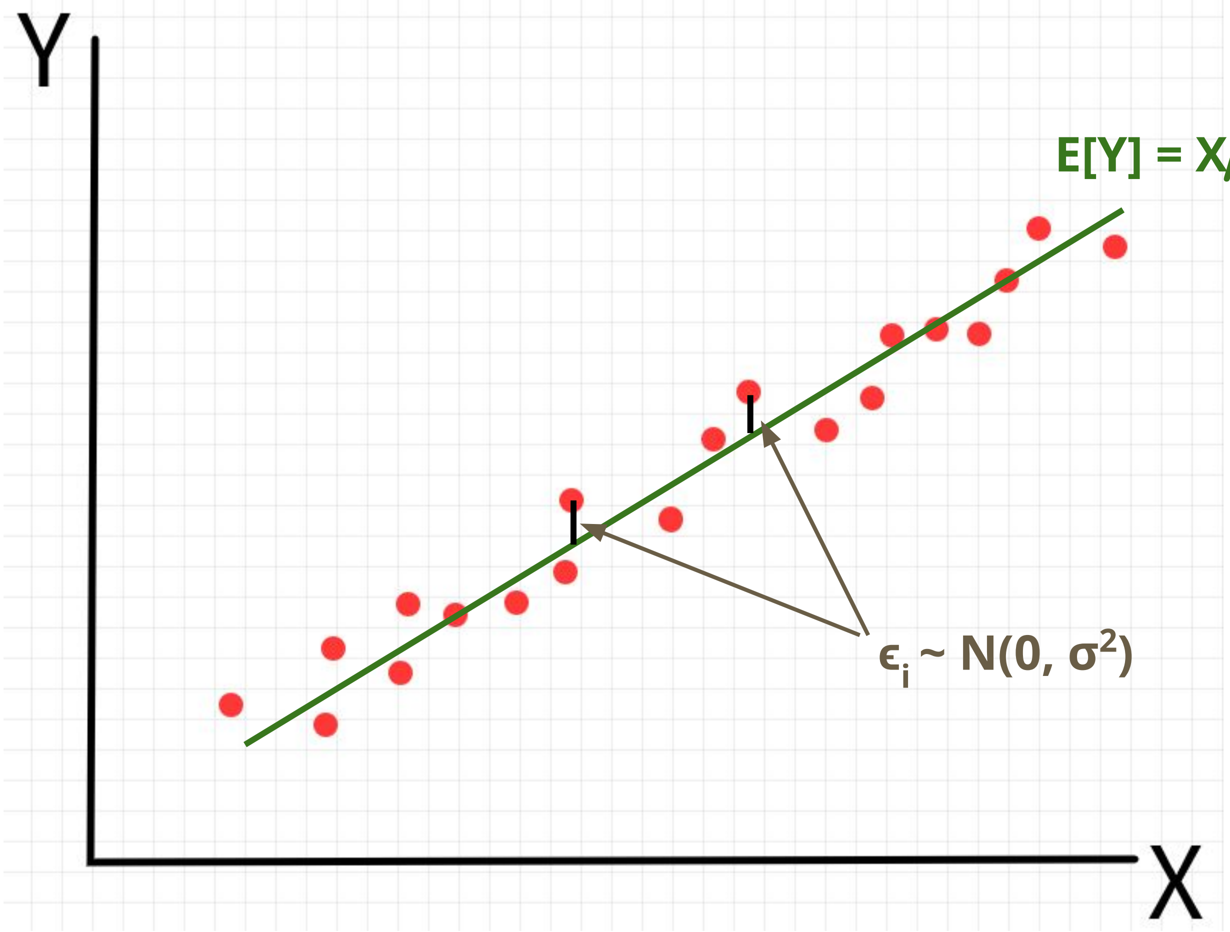


Evaluating Our Regression Model

Some Notation:

$\mathbf{y_i}$ is the "true" value from our data set (i.e. $\mathbf{x_i}\boldsymbol{\beta} + \boldsymbol{\epsilon_i}$)

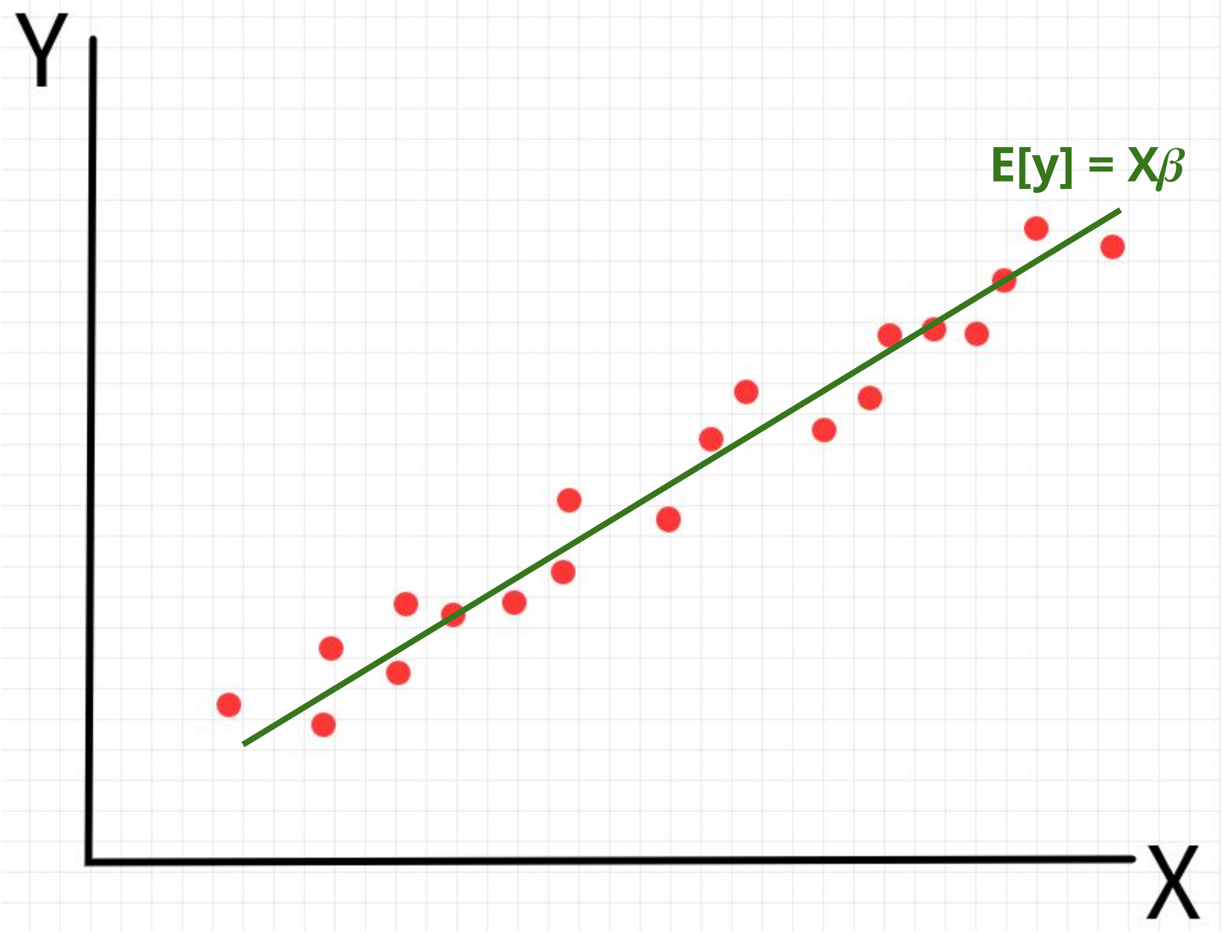
$\mathbf{\hat{y}_i}$ is the estimate of y_i from our model (i.e. $\mathbf{x_i}\boldsymbol{\beta}_{\mathbf{LS}}$)

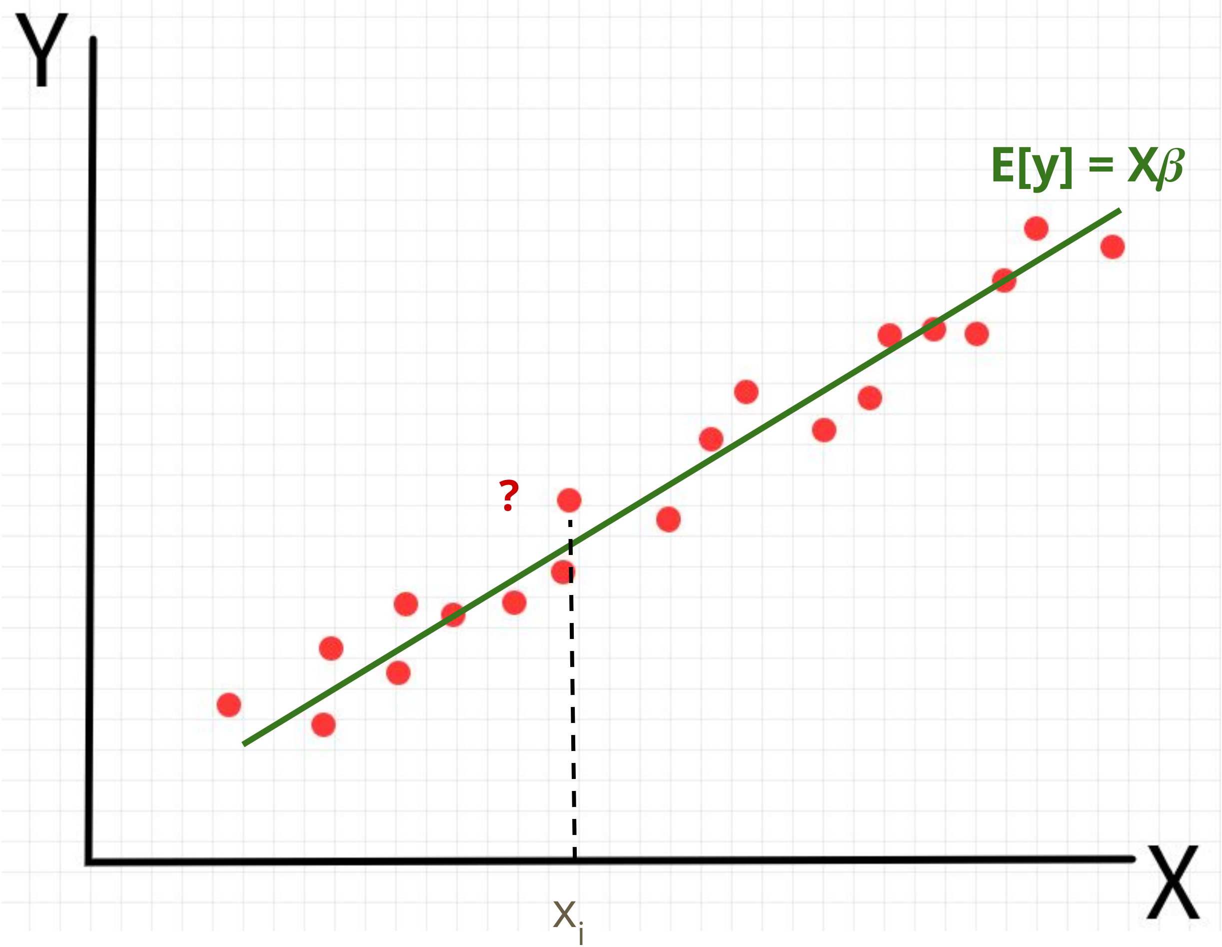
$\mathbf{\bar{y}}$ is the sample mean all $\mathbf{y_i}$

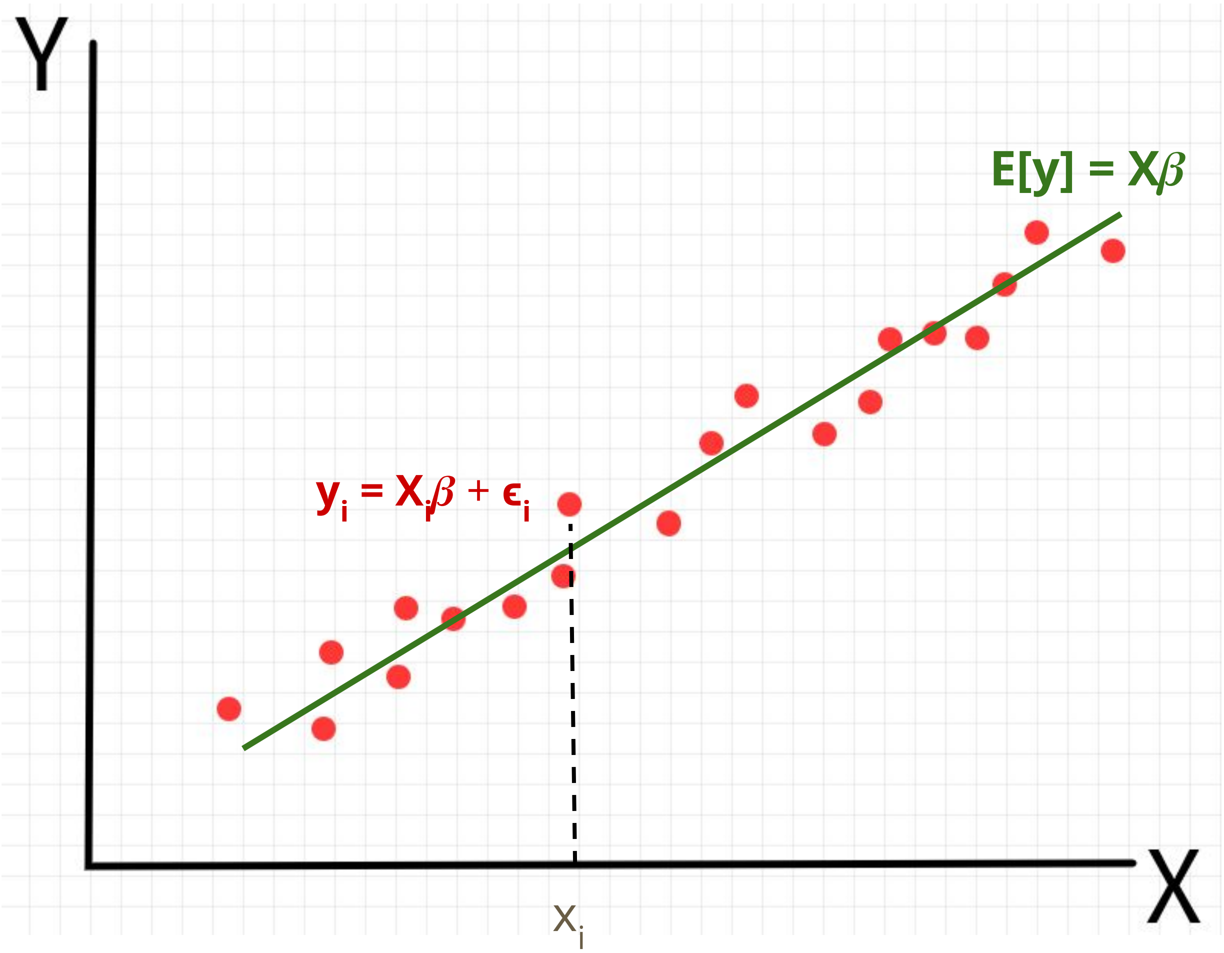
$\mathbf{y_i} - \mathbf{\hat{y}_i}$ are the estimates of $\boldsymbol{\epsilon_i}$ and are referred to as residuals

Let’s label the diagram

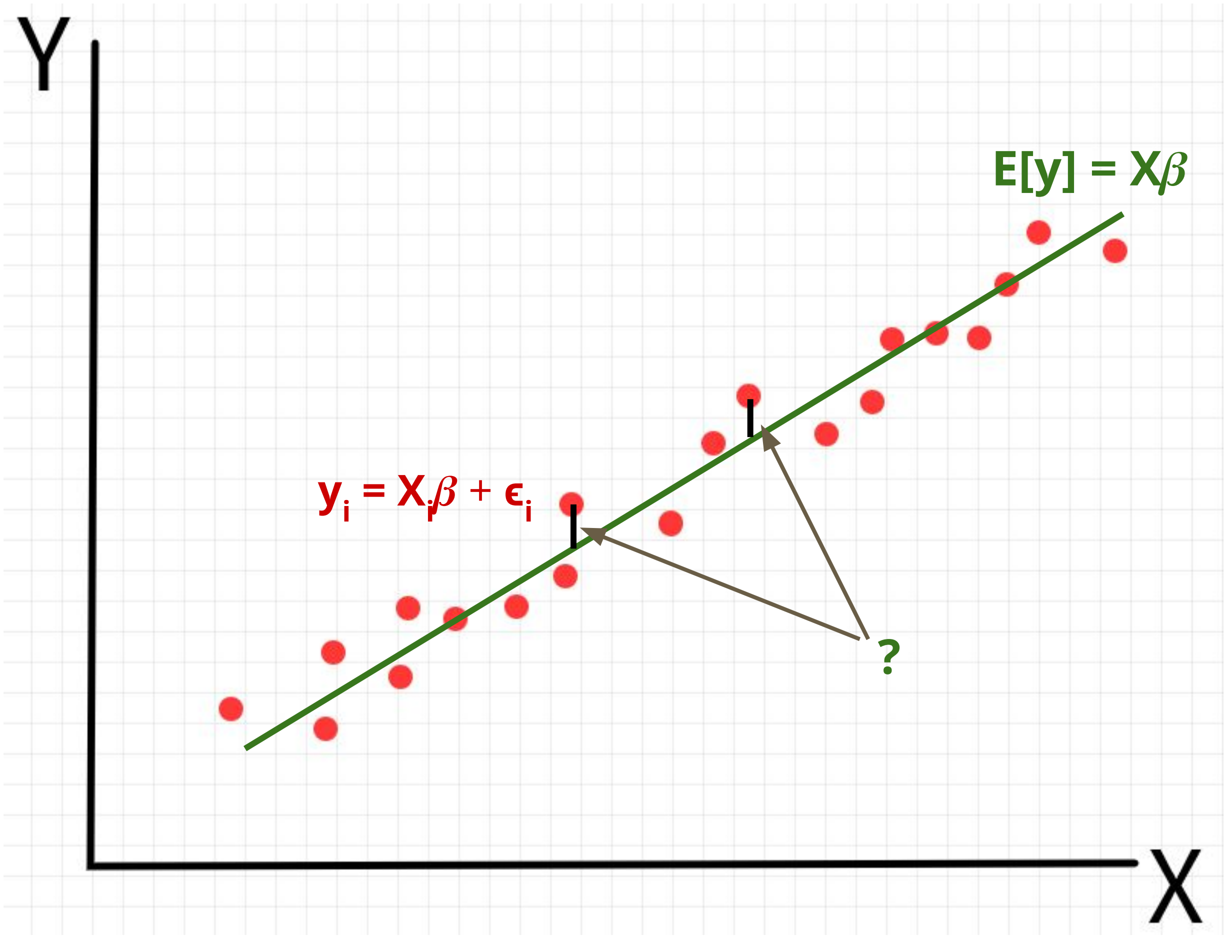

Y
?
X

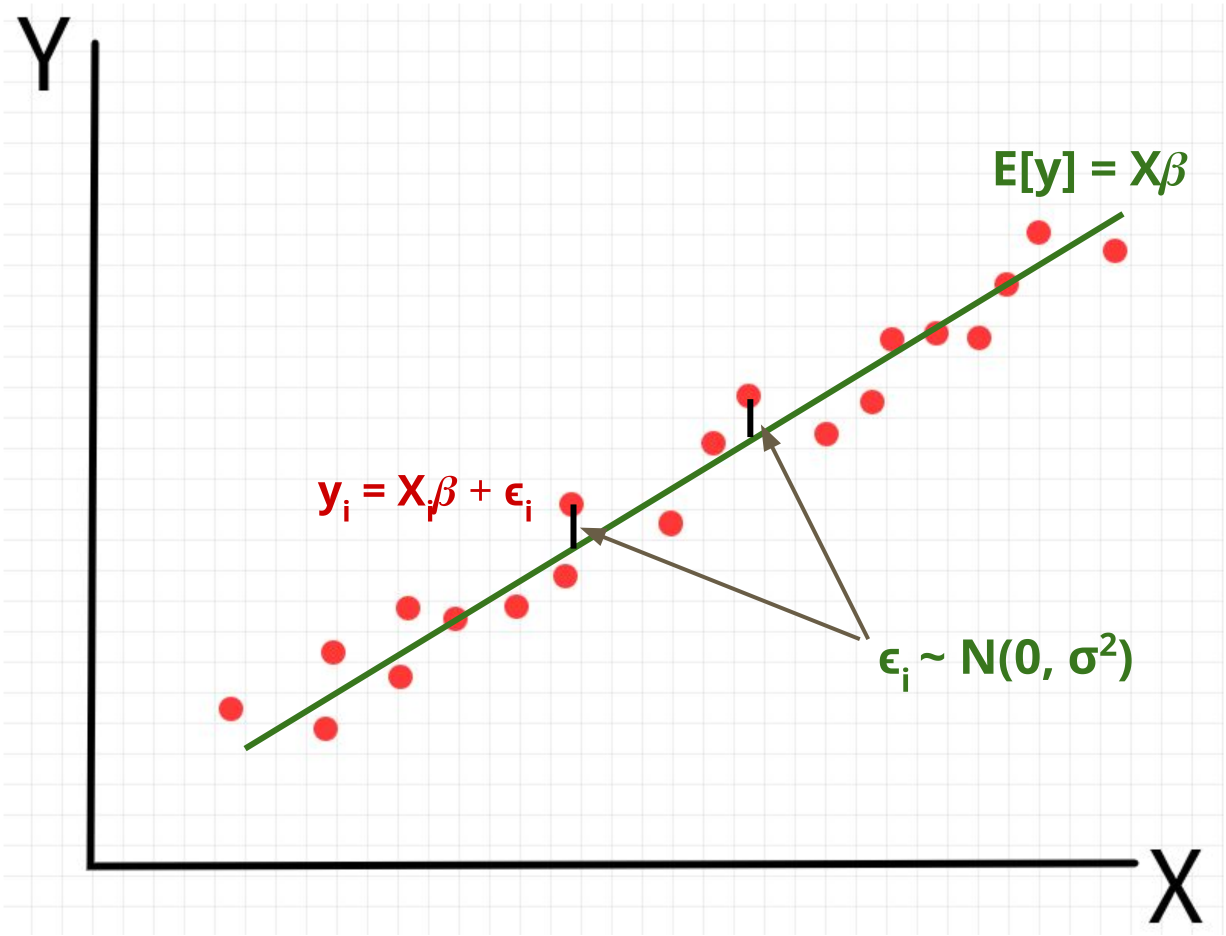

Y
E[y] = Xβ
X

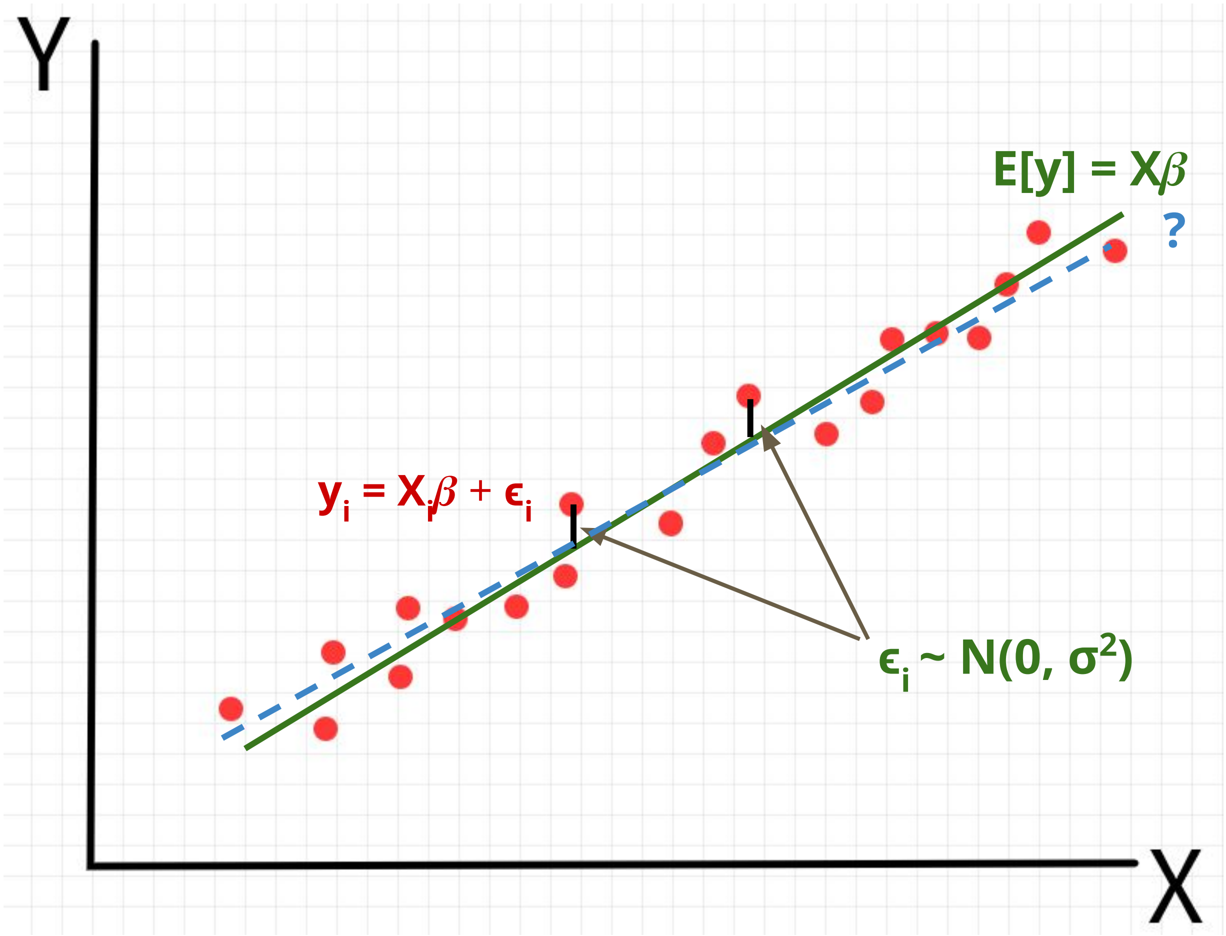

Y
E[y] = Xβ
?
X
x_i



Y
E[y] = Xβ
yi = Xiβ + ϵi
X
xi


Y
E[y] = Xβ
y_i = X_iβ + ϵ_i
?
X


Y
X
E[y] = Xβ
yi = Xiβ + ϵi
ϵi ~ N(0, σ2)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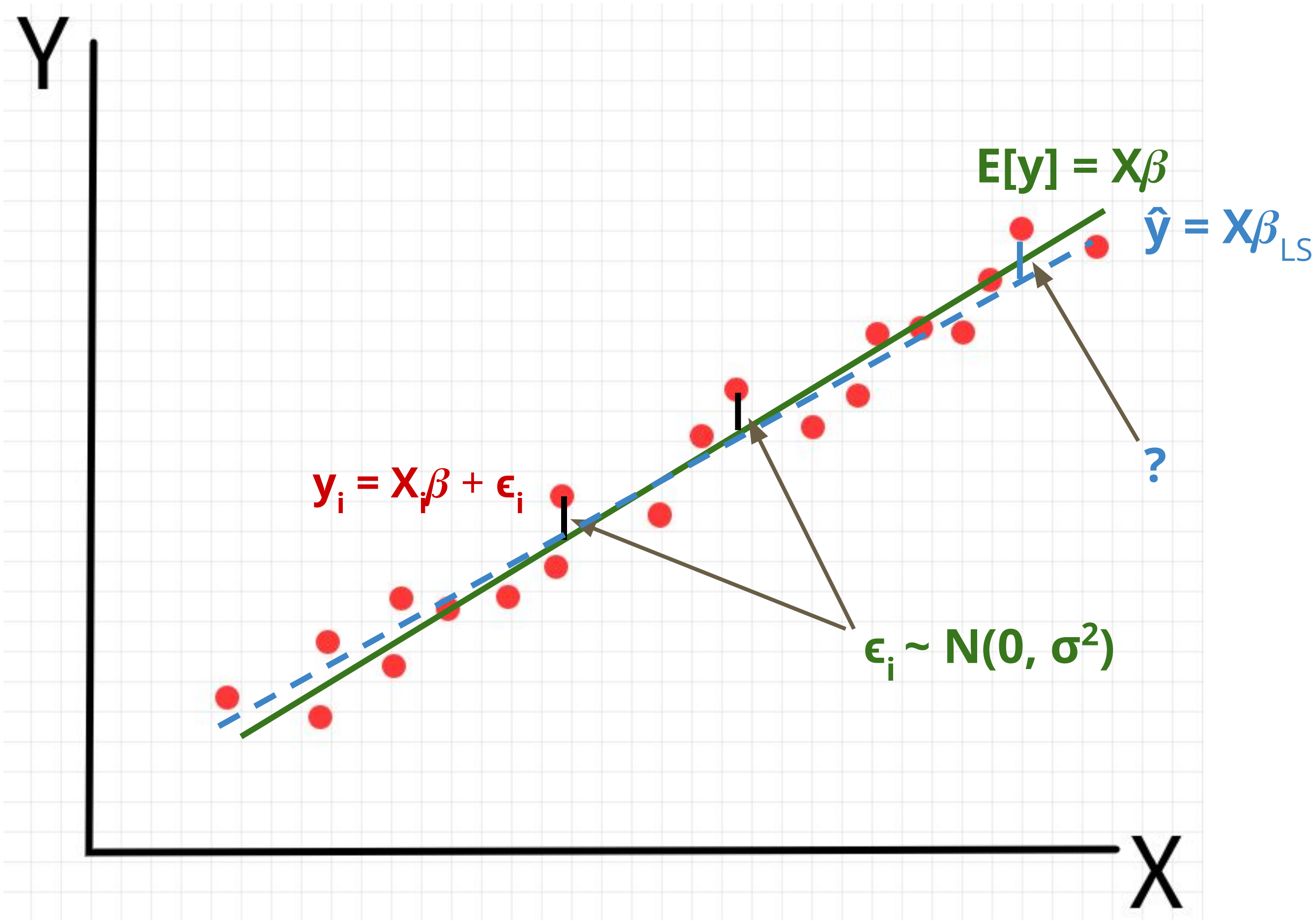
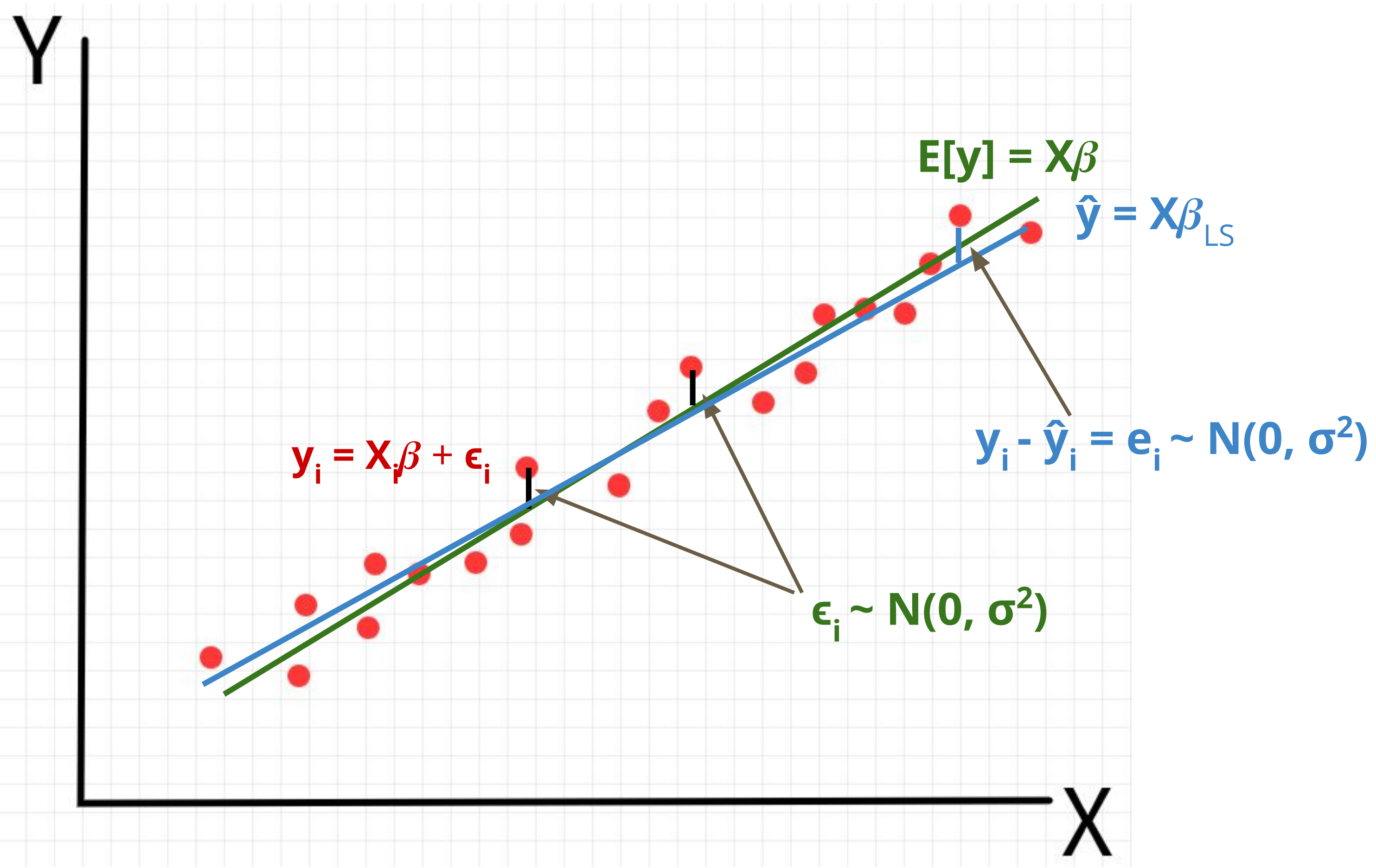
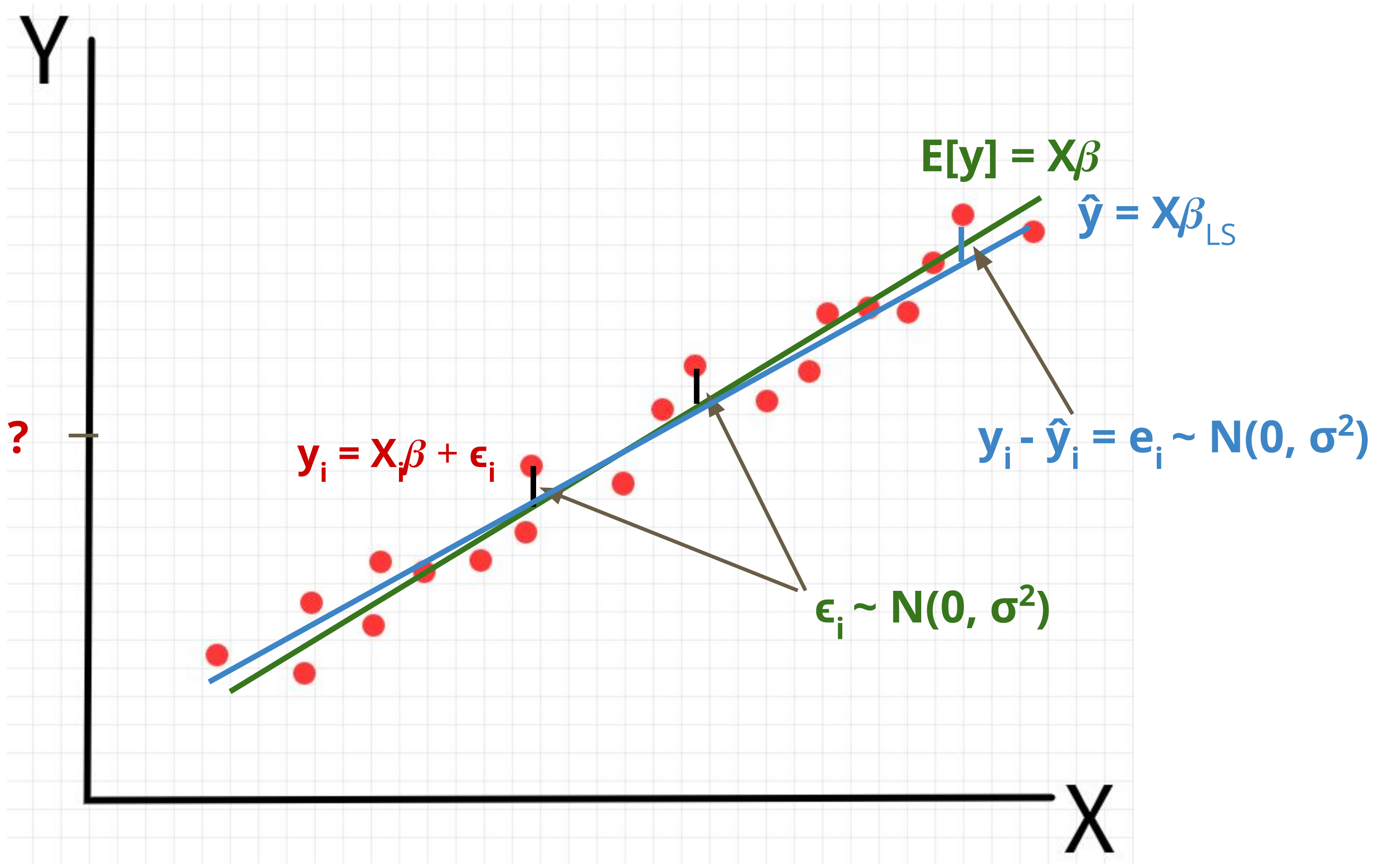
X



Y
X
E[y] = Xβ
ŷ = Xβ_LS
y_i = X_iβ + ϵ_i
ϵ_i ~ N(0, σ²)
?


Y
E[y] = Xβ
ŷ = Xβ_LS
y_i - ŷ_i = e_i ~ N(0, σ²)
y_i = X_iβ + ϵ_i
ϵ_i ~ N(0, σ²)
X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X
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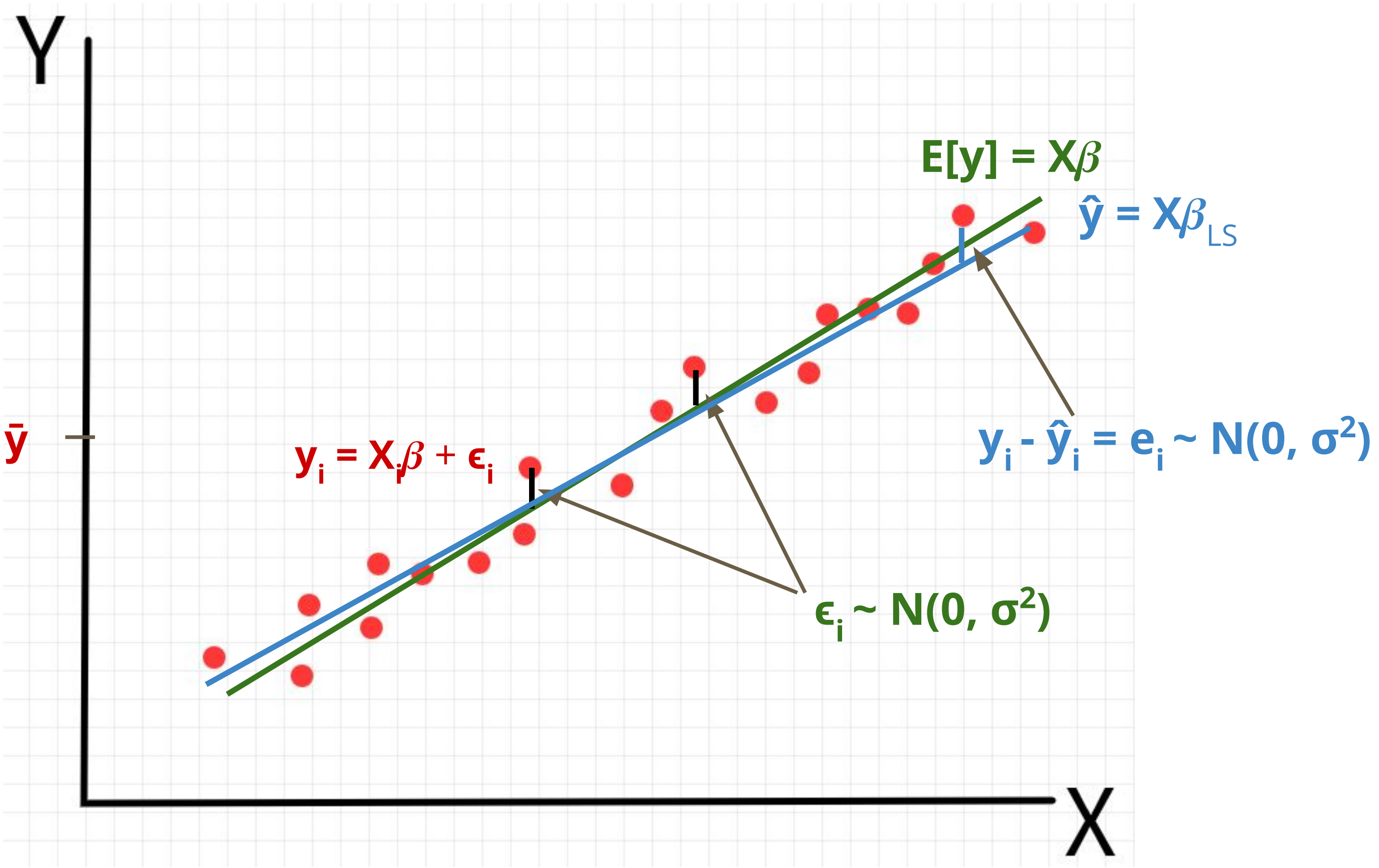

Y
X
E[y] = Xβ
ŷ = Xβ_LS
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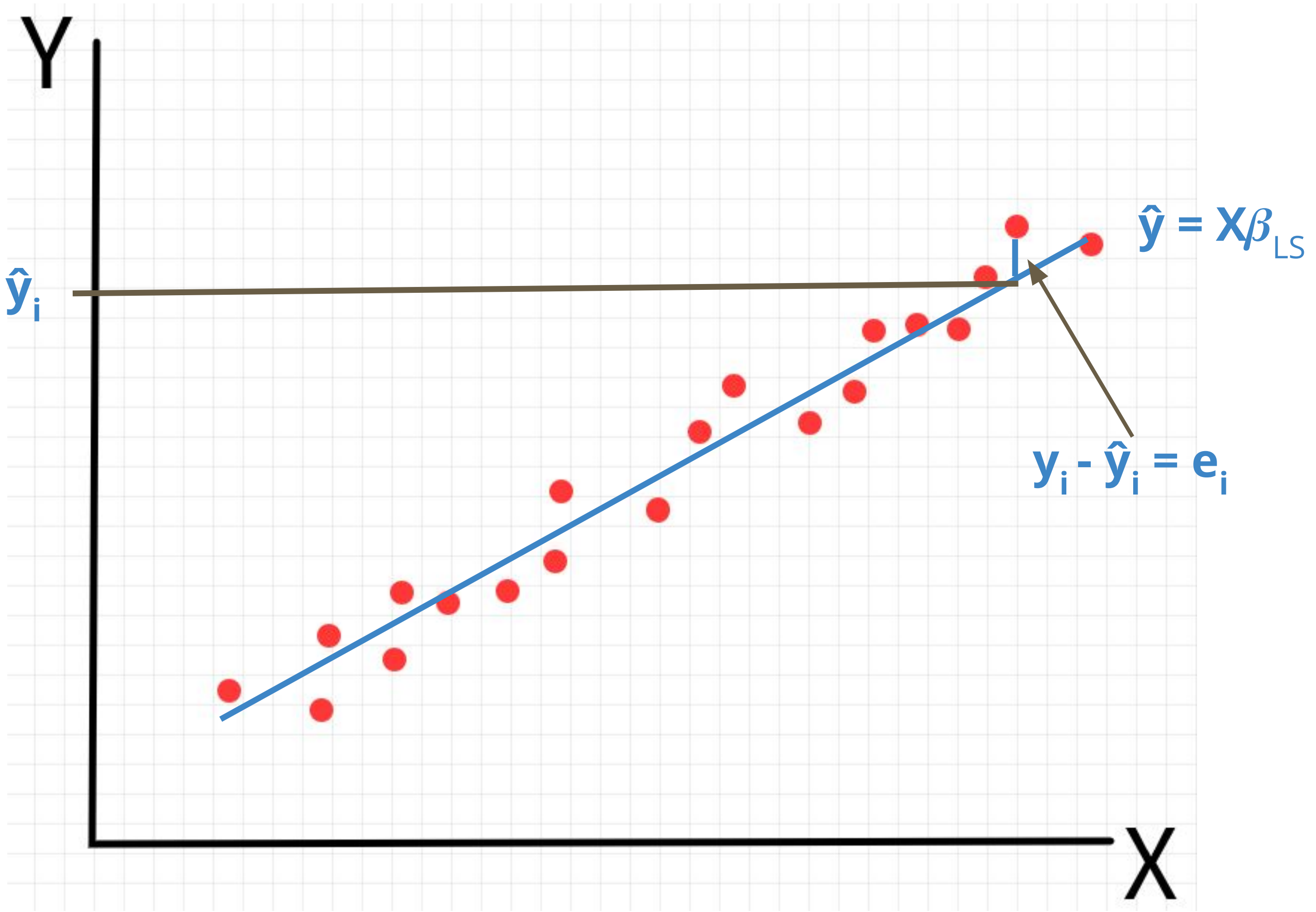
y_i = X_iβ + ϵ_i
y_i - ŷ_i = e_i ~ N(0, σ²)
ϵ_i ~ N(0, σ²)


Y
X
ŷ = Xβ_LS
ŷ_i
y_i - ŷ_i = e_i

How do we know a linear model is applicable?

Is it true that $\mathbf{y} = \mathbf{x}\boldsymbol{\beta} + \boldsymbol{\epsilon}$ where $\boldsymbol{\epsilon} \sim \mathbf{N(0, \sigma^2)}$?

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Lots of questions secretly hiding in here...

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Is it true that $\mathbf{y} = \mathbf{x}\boldsymbol{\beta} + \boldsymbol{\epsilon}$ where $\boldsymbol{\epsilon} \sim \mathbf{N(0, \sigma^2)}$?

Lots of questions secretly hiding in here...

1. Is the noise actually normally distributed?

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1. Is the noise actually normally distributed?
2. Is the variance of the noise actually constant?

How do we know a linear model is applicable?

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Lots of questions secretly hiding in here...

1. Is the noise actually normally distributed?
2. Is the variance of the noise actually constant?
3. Is the relationship actually linear (or does it just look that way by chance because of the noise)?

How do we know a linear model is applicable?

Is it true that $\mathbf{y} = \mathbf{x}\boldsymbol{\beta} + \boldsymbol{\epsilon}$ where $\boldsymbol{\epsilon} \sim \mathbf{N(0, \sigma^2)}$?

How do we check if we don't know what the true $\boldsymbol{\beta}$ is (and thus what $\boldsymbol{\epsilon}$ is)?

How do we know a linear model is applicable?

Is it true that $\mathbf{y} = \mathbf{x}\boldsymbol{\beta} + \boldsymbol{\epsilon}$ where $\boldsymbol{\epsilon} \sim \mathbf{N}(\mathbf{0}, \boldsymbol{\sigma}^{2})$?

If this is true then: $\mathbf{y_i - \hat{y}_i = e_i \sim N(0, variance)}$

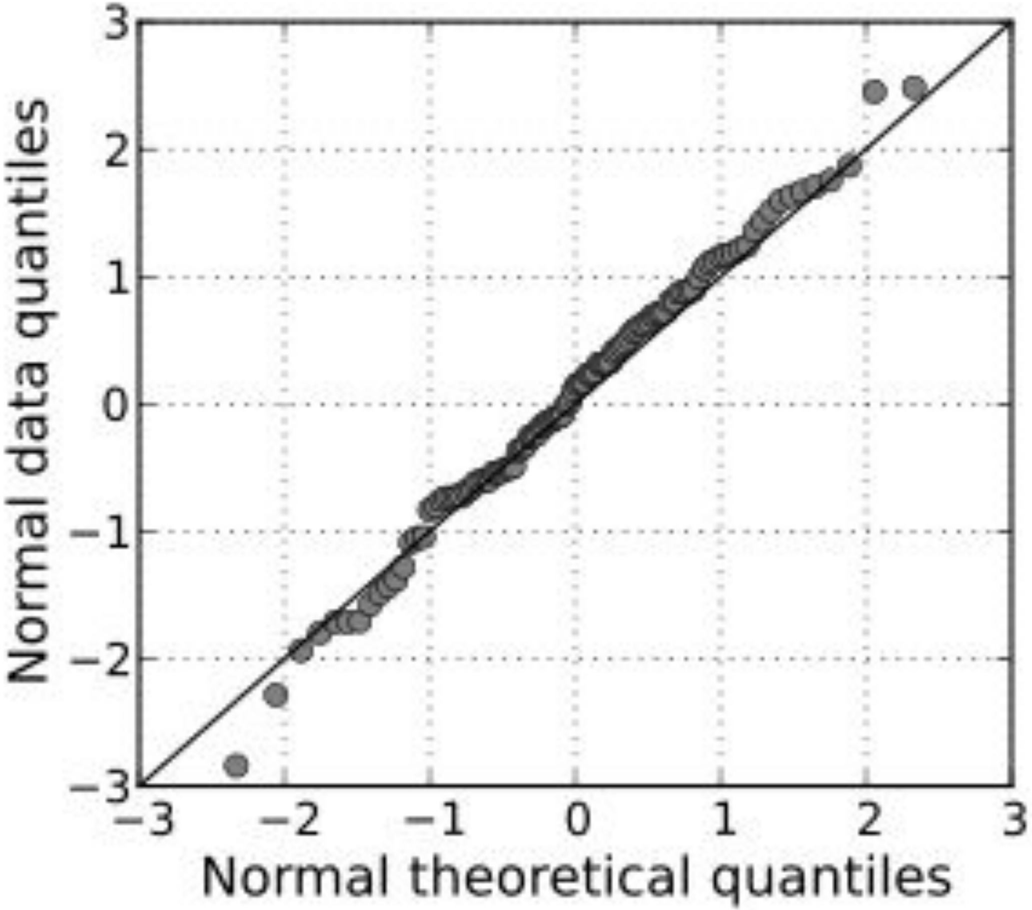
Checking the Normal assumption

Quantiles are the values for which a particular % of values are contained below it.

For example the 50% quantile of a N(0,1) distribution is 0 since 50% of samples would be contained below 0 were you to sample a large number of times.

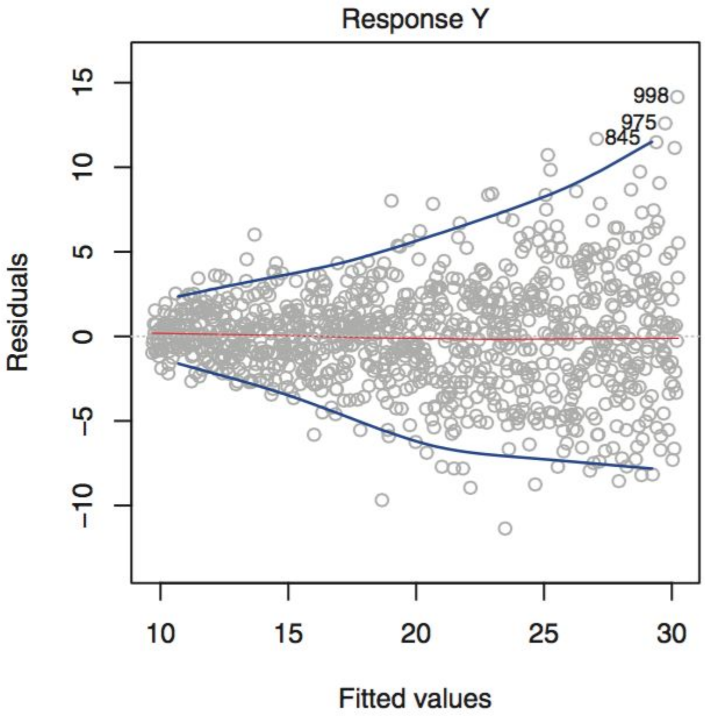
Forall quantiles q, if sample.q == known_distribution.q then they have the same distribution.

QQ plot



Normal data quantiles
Normal theoretical quantiles
3
2
1
0
−1
−2
−3
−3
−2
−1
0
1
2
3

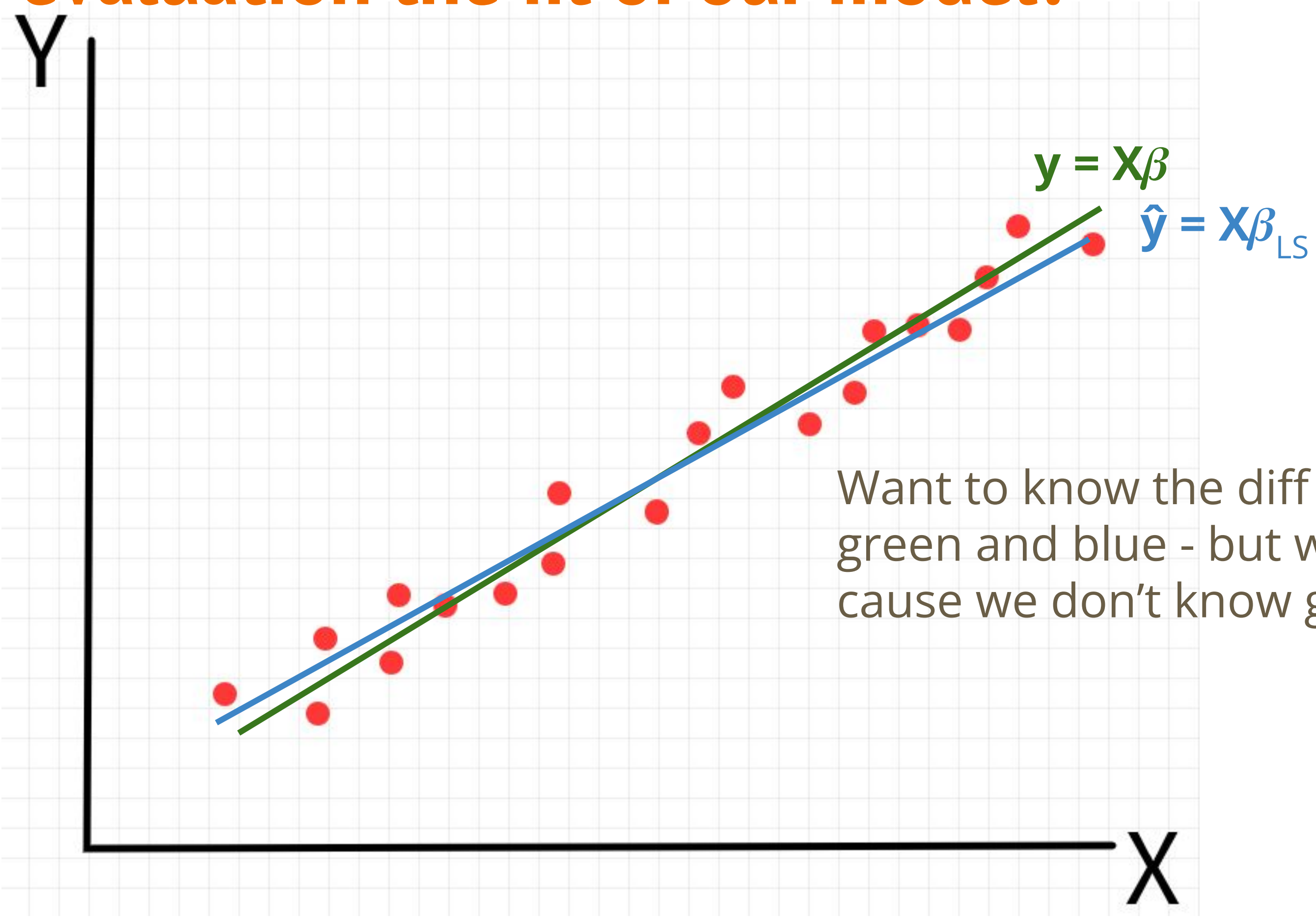
Checking the constant variance assumption



Checking the third assumption (relationship vs chance)

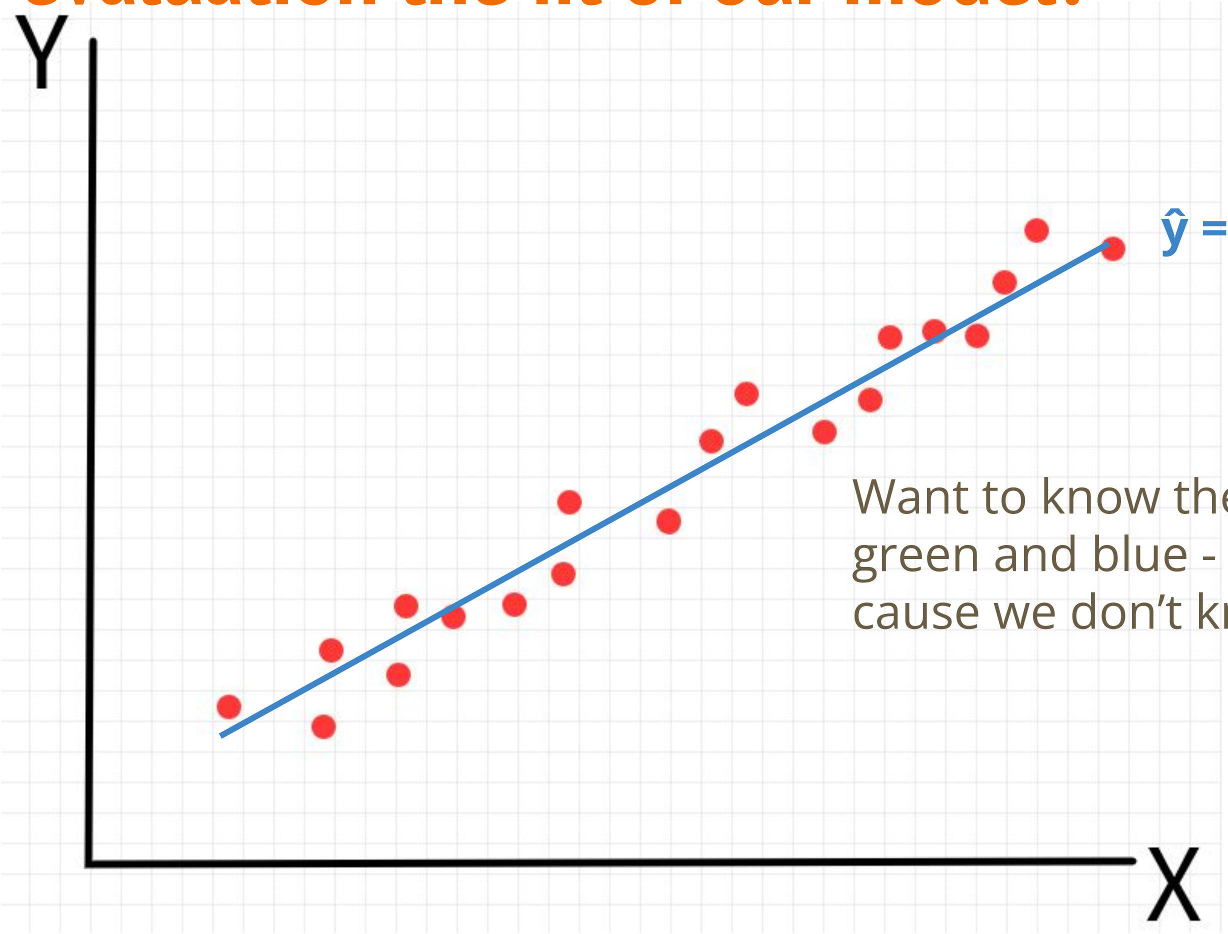
This one is a bit trickier and we need to take a long detour (i.e. an entire other lecture).

Metric for evaluation the fit of our model?



Want to know the diff between green and blue - but we can't cause we don't know green

Metric for evaluation the fit of our model?



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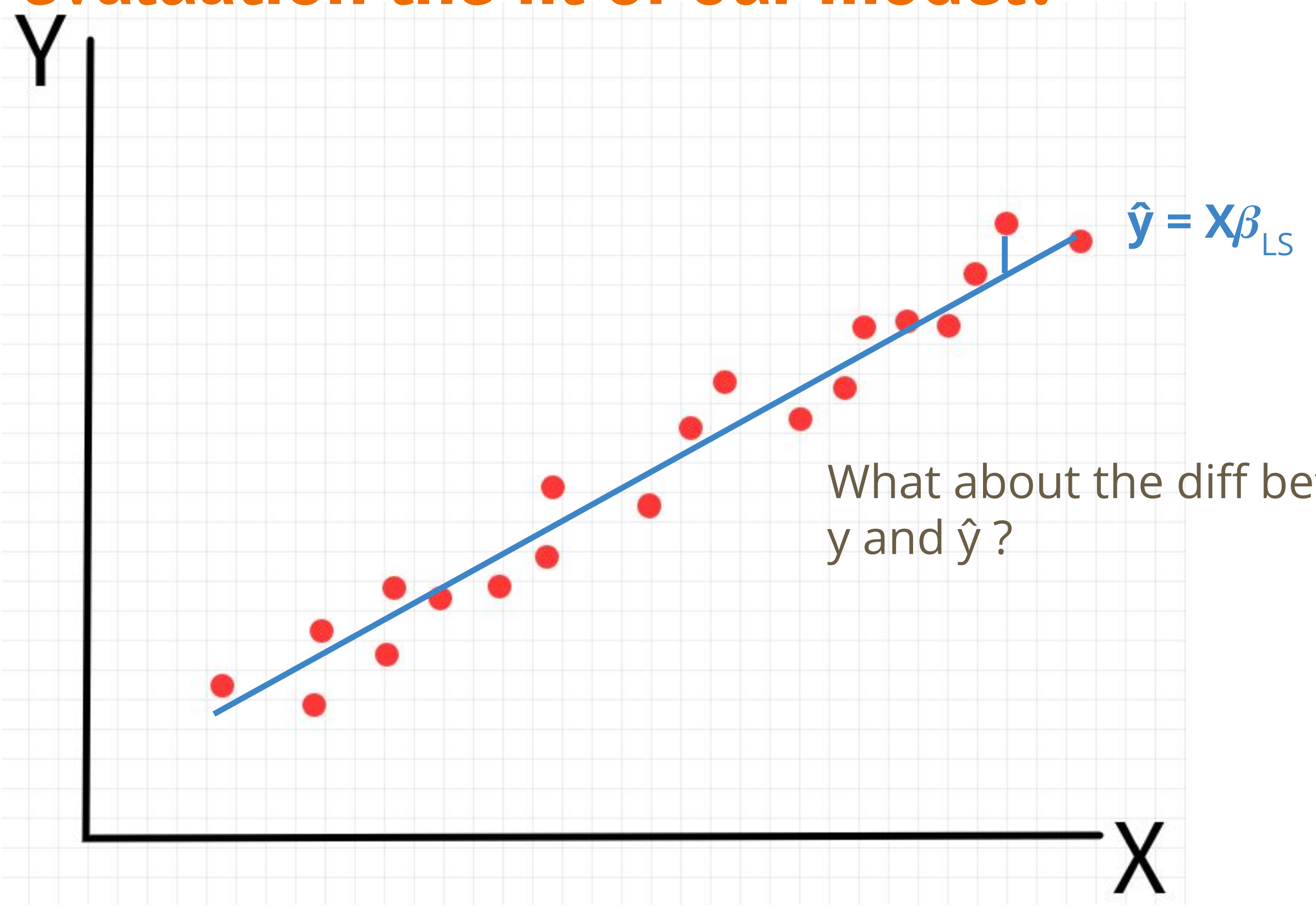
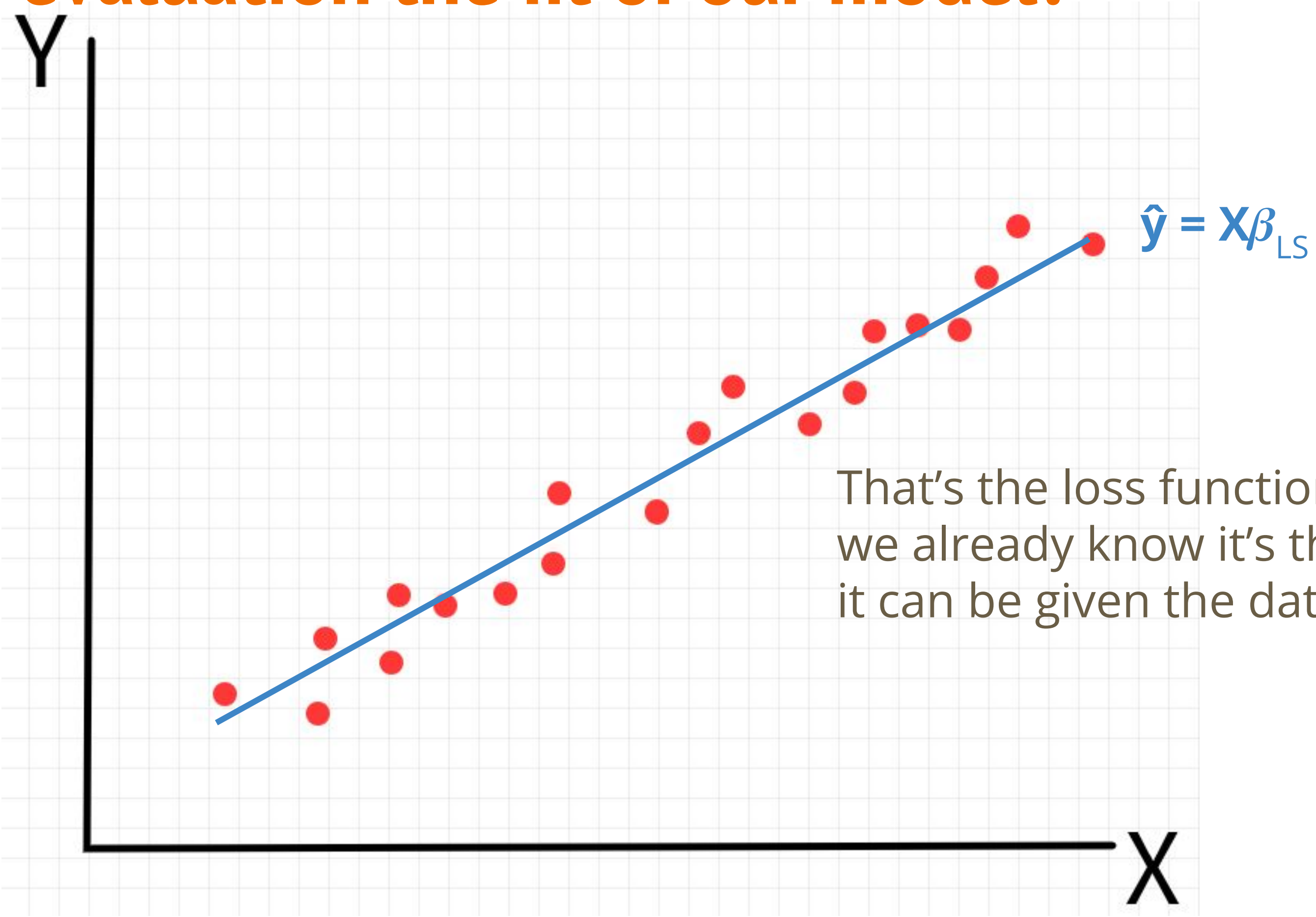


What about the diff between y and ŷ ?

Metric for evaluation the fit of our model?



That's the loss function and we already know it's the best it can be given the data...

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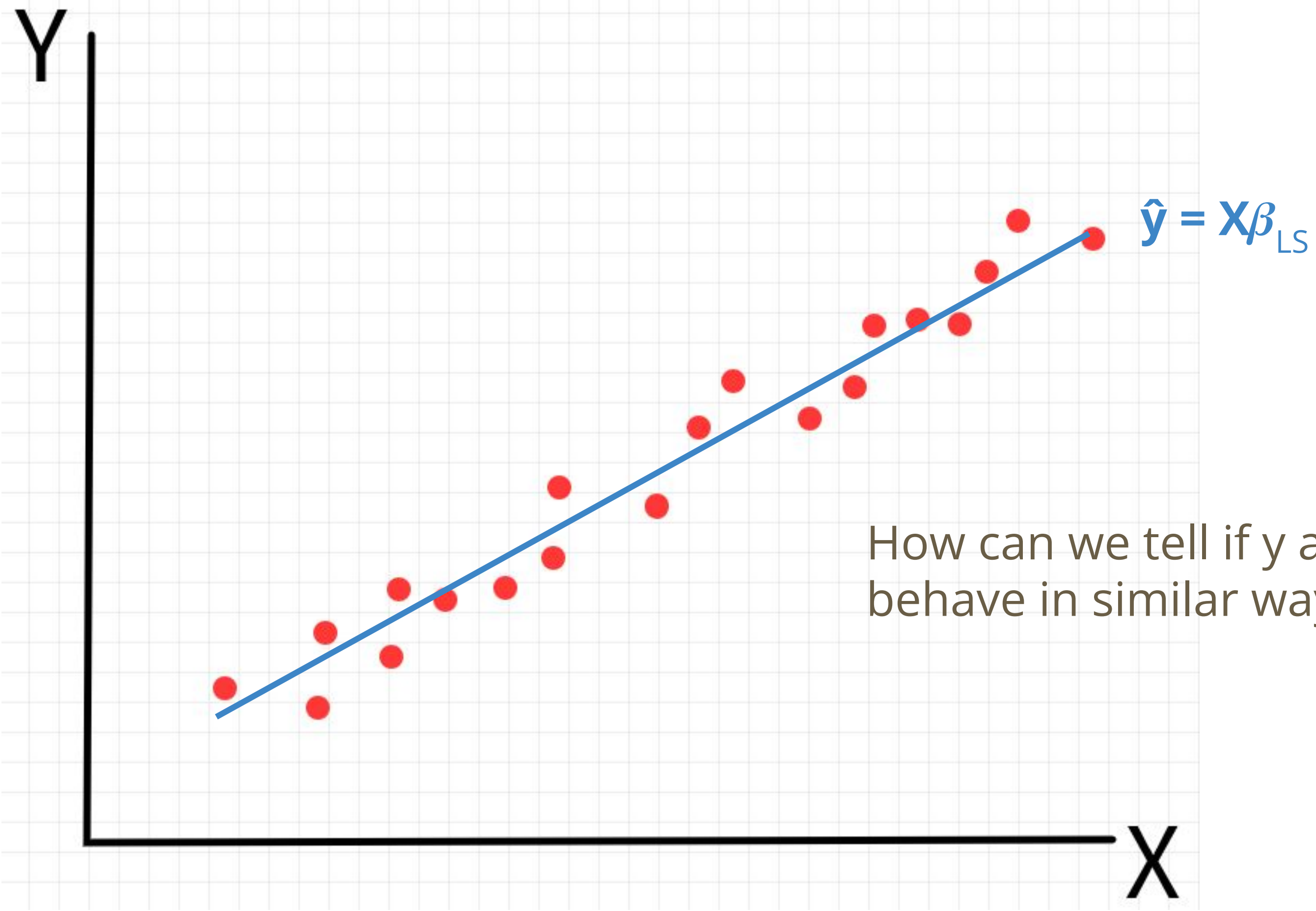
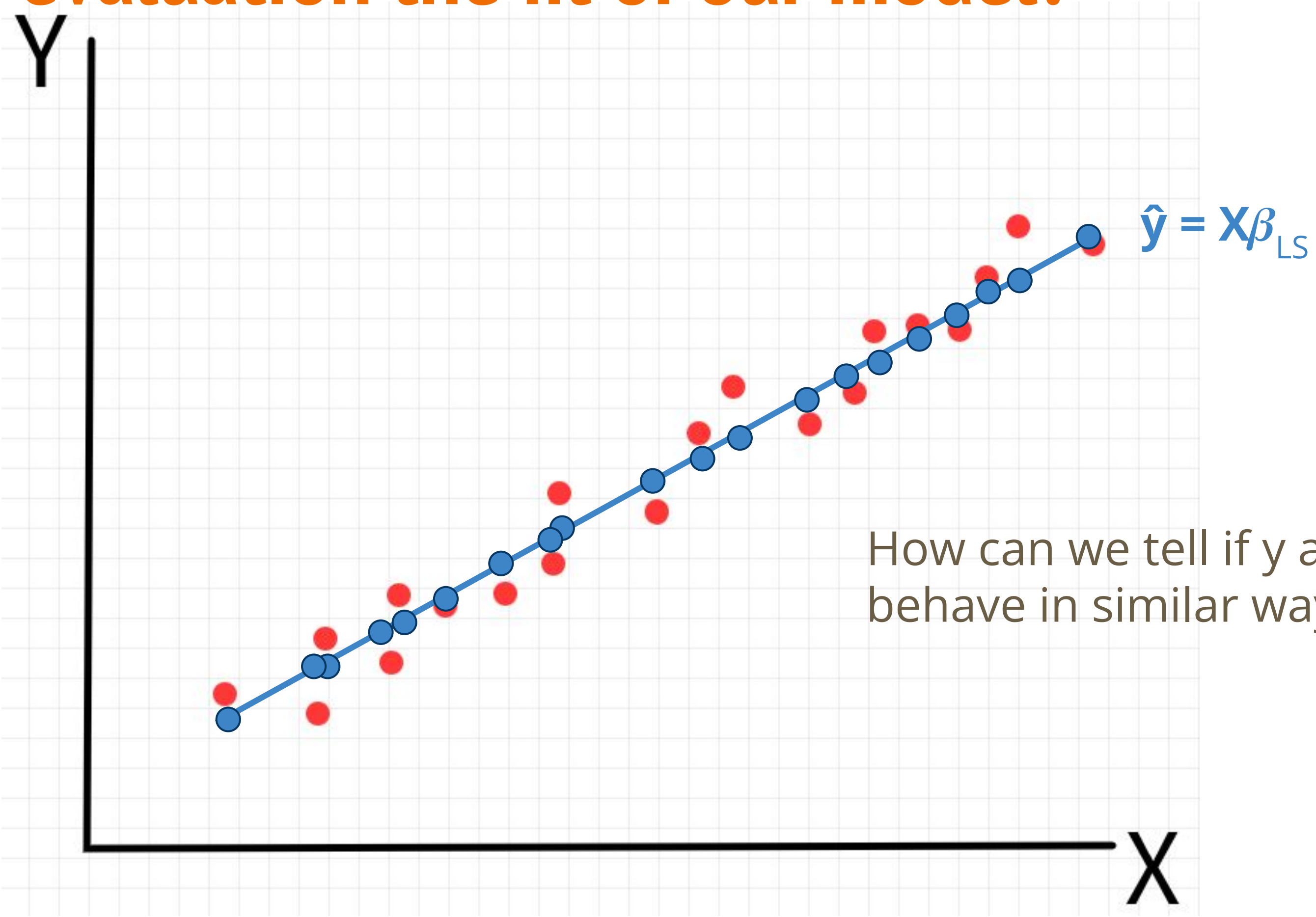


How can we tell if y and ŷ behave in similar ways?

Metric for evaluation the fit of our model?



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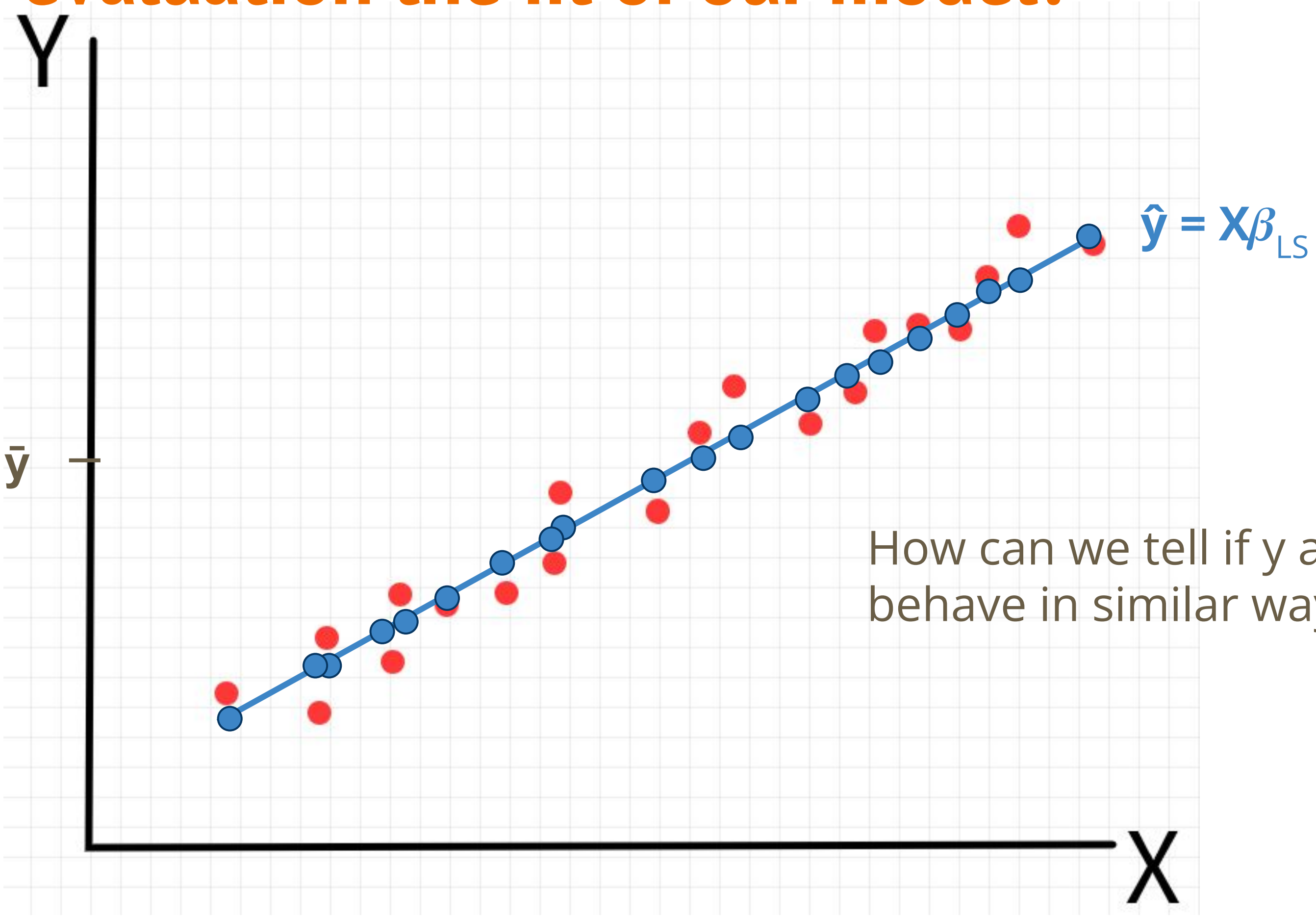

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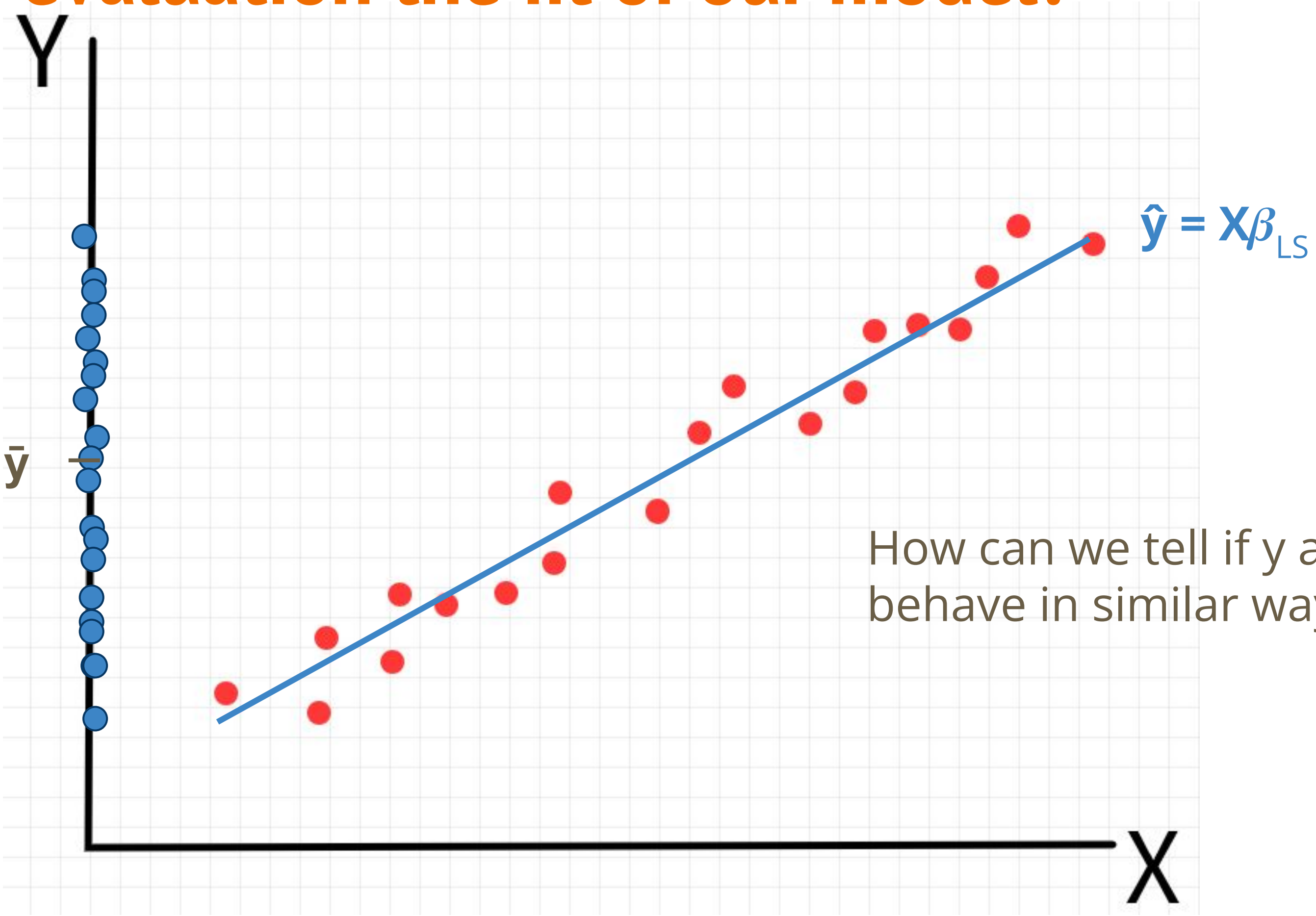

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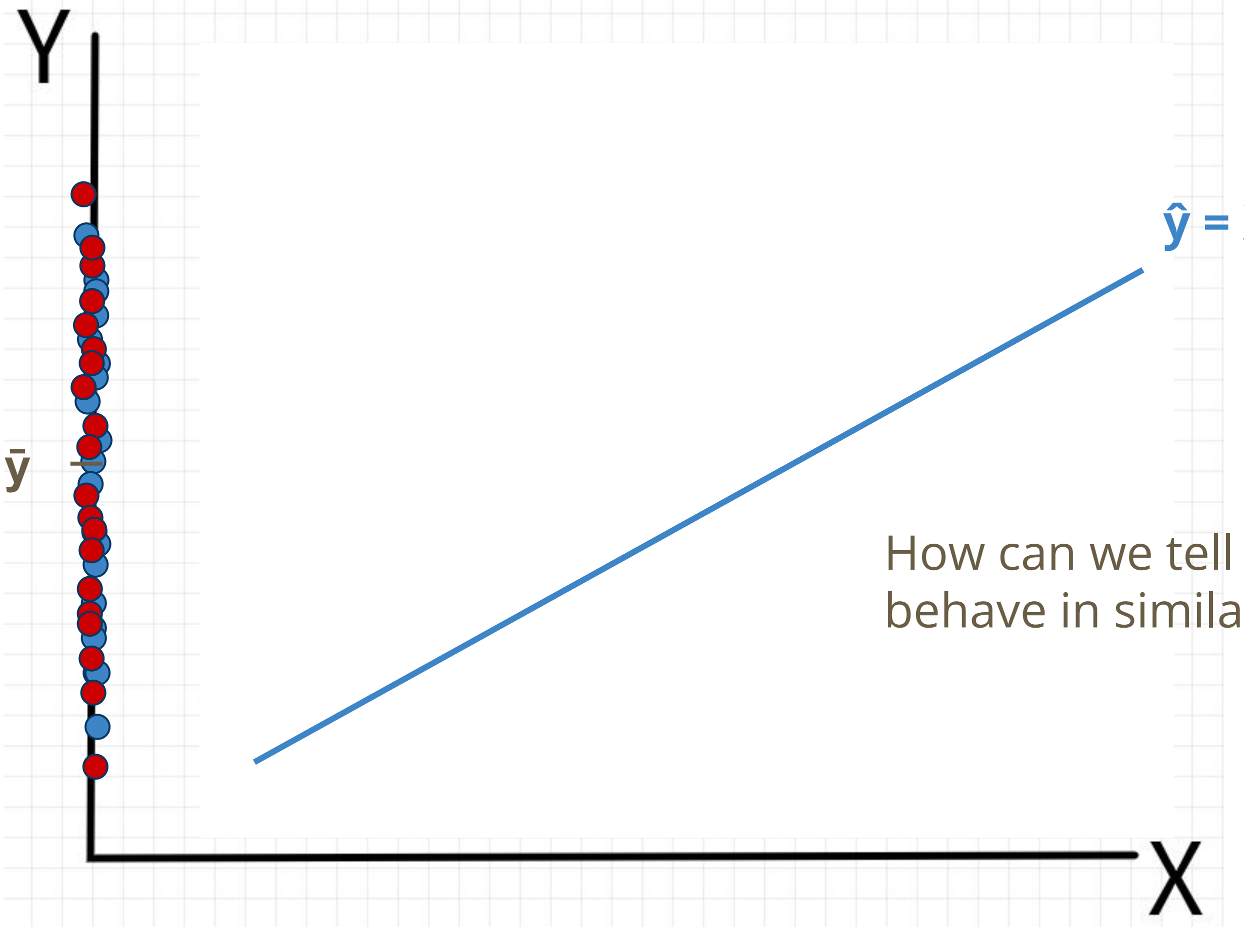

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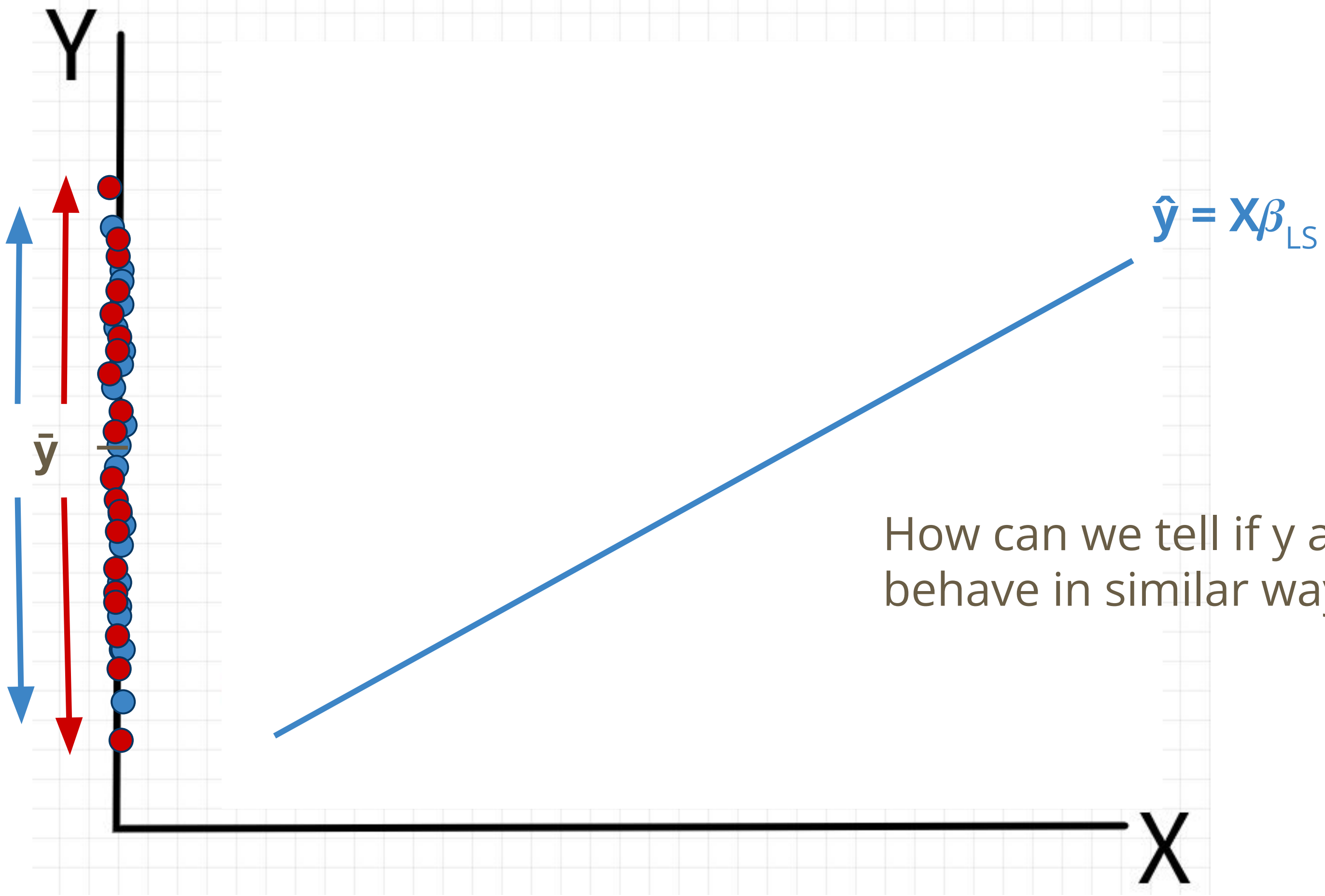


How can we tell if y and ŷ behave in similar ways?

Metric for evaluation the fit of our model?

Is the value of the loss function sufficient? i.e.

$$||y - X\beta||_2^2 = \sum_i^n (y_i - \hat{y}_i)^2$$

Evaluating Our Regression Model

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

This is a measure of the spread of y_i around the mean of y

Evaluating Our Regression Model

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

This is a measure of the spread of y_i around the mean of y

$$ESS = \sum_{i}^{n} (\hat{y_i} - \bar{y})^2$$

This is a measure of the spread of our model's estimates of y_i around the mean of y

Evaluating Our Regression Model

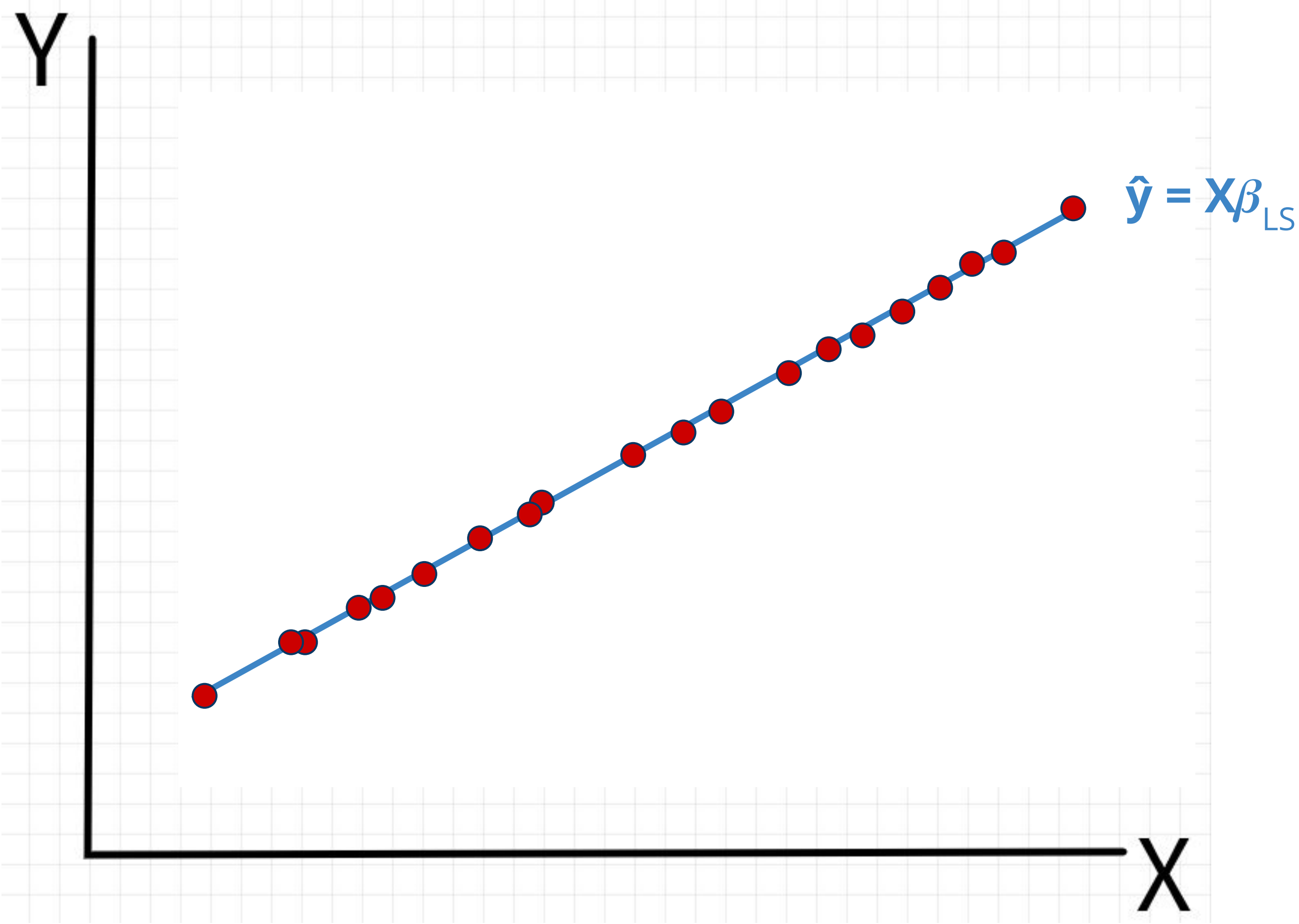
$$TSS = \sum_{i}^{n} (y_i - \bar{y})^2$$

$$R^2 = \frac{ESS}{TSS}$$

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

R^2 measures the fraction of variance that is explained by ŷ (our model)

$R^2 = 1$



$R^2 = 0$

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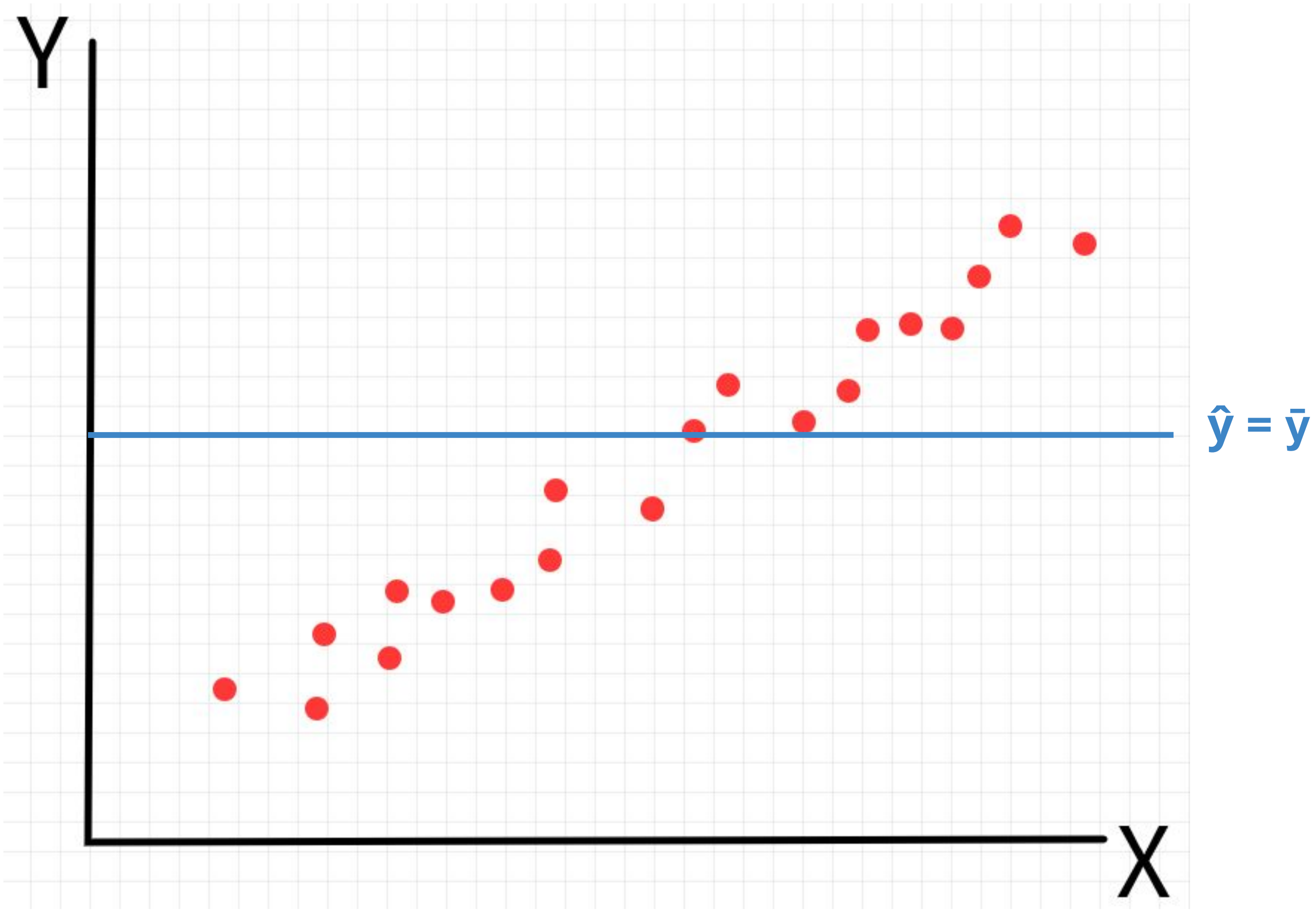
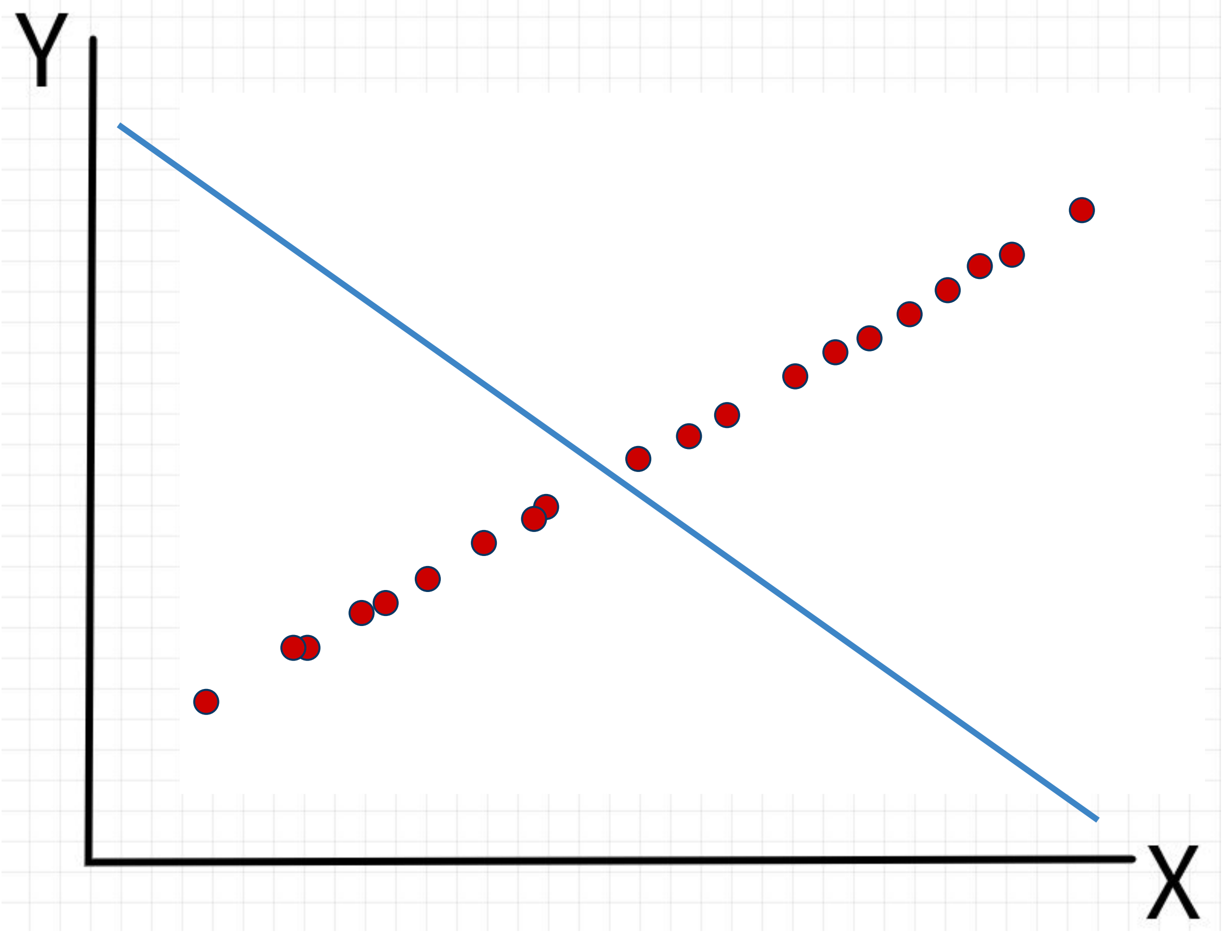
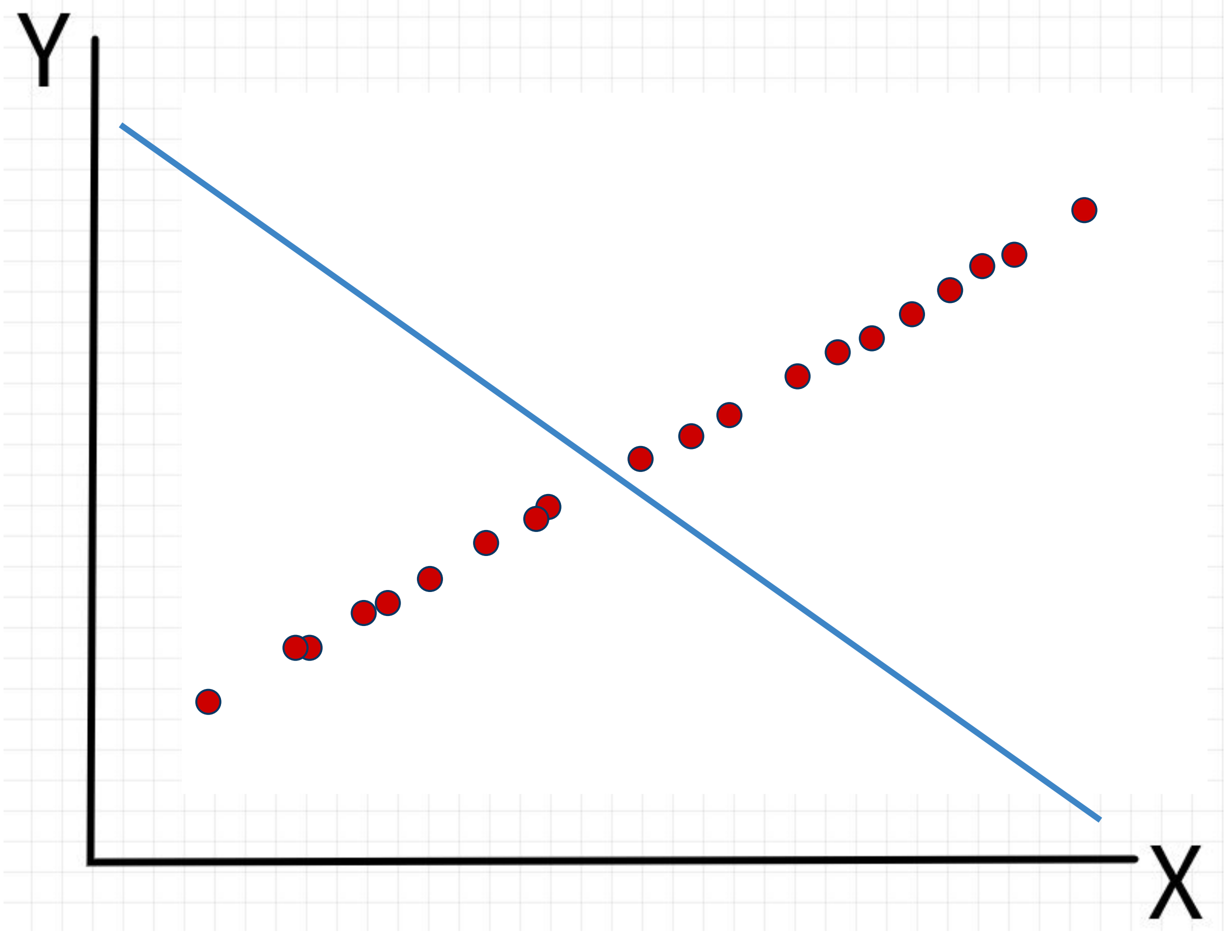




Y
X

$R^2 = 1$



Standard R^2 formula for a linear model

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

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

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

This is what our linear model is minimizing

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

Standard R^2 formula for a linear model

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

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

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

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

This equality only holds for a linear model that minimizes the RSS and is centered around ȳ

Proof

That TSS = ESS + RSS

$$\begin{aligned}
\text{TSS} &= \sum_i (y_i - \bar{y})^2 \\
&= \sum_i (y_i - \hat{y}_i + \hat{y}_i - \bar{y})^2 \\
&= \sum_i (y_i - \hat{y}_i)^2 + \sum_i (\hat{y}_i - \bar{y})^2 + 2\sum_i (y_i - \hat{y}_i)(\hat{y}_i - \bar{y}) \\
&= \text{ESS} + \text{RSS} + 2\sum_i (y_i - \hat{y}_i)(\hat{y}_i - \bar{y}).
\end{aligned}$$

Assume for simplicity that $\hat{\mathbf{y}}_i = \boldsymbol{\beta}_0 + \boldsymbol{\beta}_1 \mathbf{x}_i$

Since $\boldsymbol{\beta}_0$ and $\boldsymbol{\beta}_1$ are least squares estimates, we know they minimize

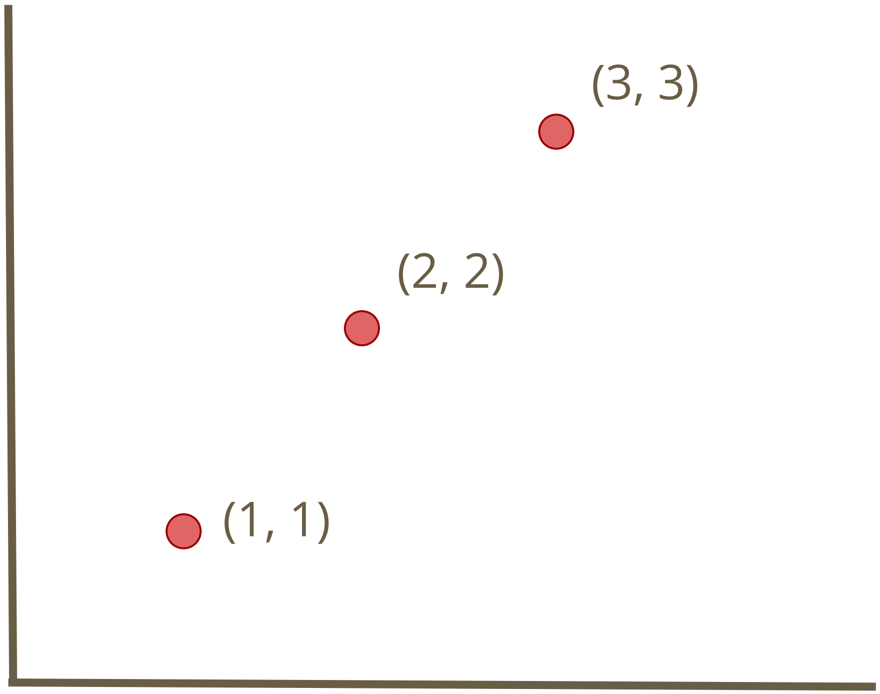
$$\sum_i (y_i - \hat{y}_i)^2$$

By taking derivatives of the above with respect to $\boldsymbol{\beta}_0$ and $\boldsymbol{\beta}_1$ we discover that

$\sum_i (y_i - \hat{y}_i) = 0$ and $\sum_i (y_i - \hat{y}_i)x_i = 0$

$$\begin{aligned}
\sum_i (y_i - \hat{y}_i)(\hat{y}_i - \bar{y}) &= \sum_i (y_i - \hat{y}_i)\hat{y}_i - \bar{y}\sum_i (y_i - \hat{y}_i) \\
&= \hat{\beta}_0 \sum_i (y_i - \hat{y}_i) + \hat{\beta}_1 \sum_i (y_i - \hat{y}_i)x_i - \bar{y}\sum_i (y_i - \hat{y}_i)
\end{aligned}$$

Why this new formula is standard

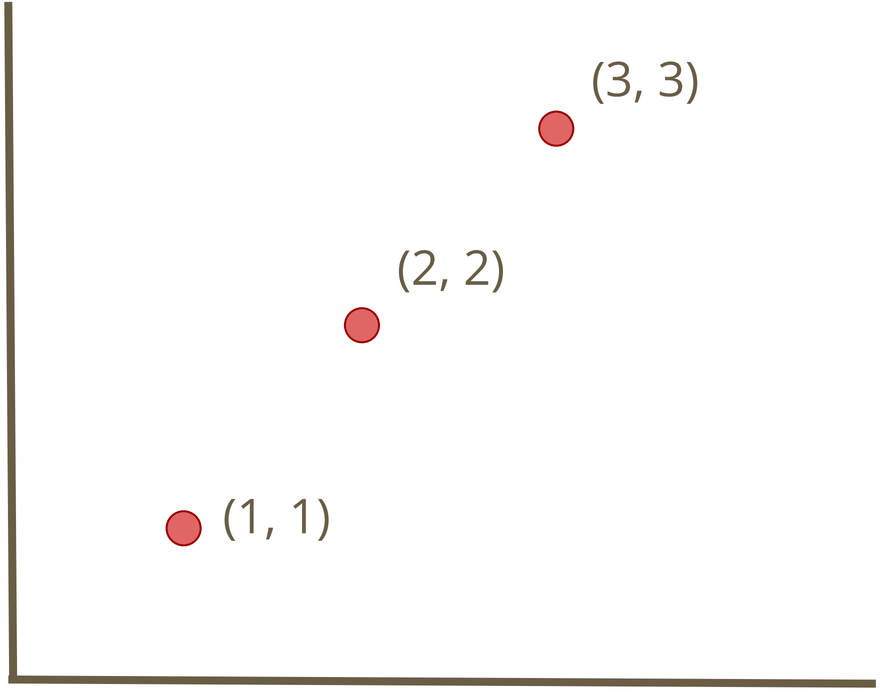


Why this new formula is standard

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

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

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



$$R^2 = \frac{ESS}{TSS}$$

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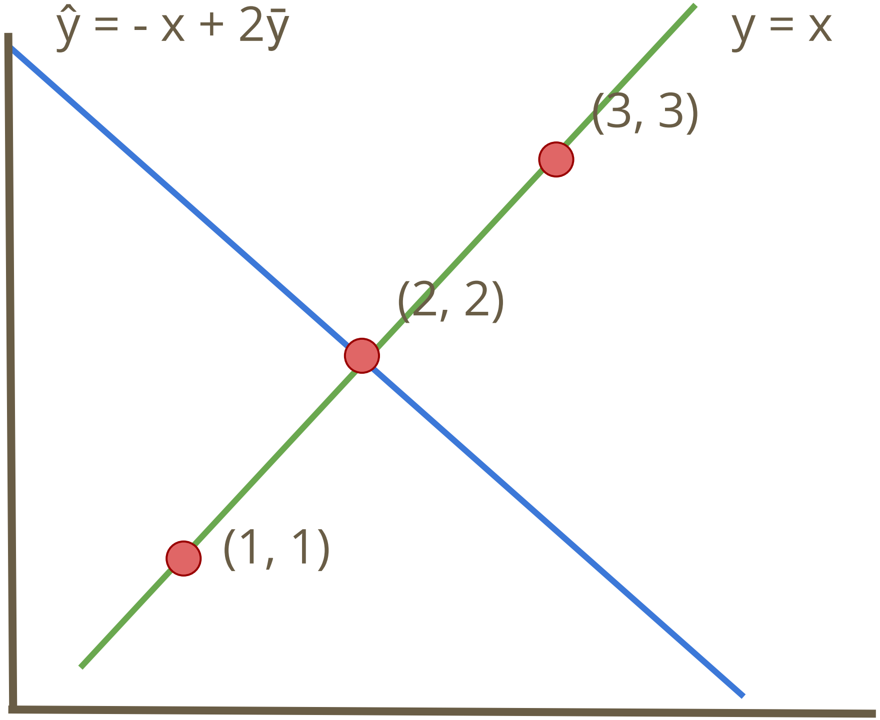

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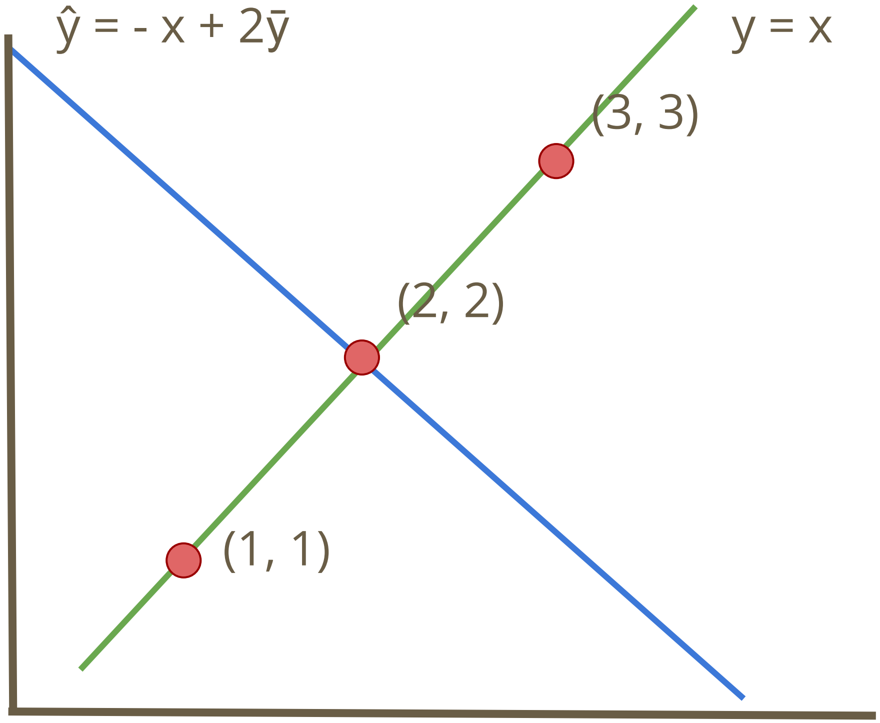

$(\hat{y} - \bar{y})^2$
$= (-x + 2\bar{y} - \bar{y})^2$
$= (-x + \bar{y})^2$
$= (-(y - \bar{y}))^2$
$= (y - \bar{y})^2$

$$R^2 = \frac{ESS}{TSS}$$

Why this new formula is standard

$$TSS = \sum_i^n (y_i - \bar{y})^2$$

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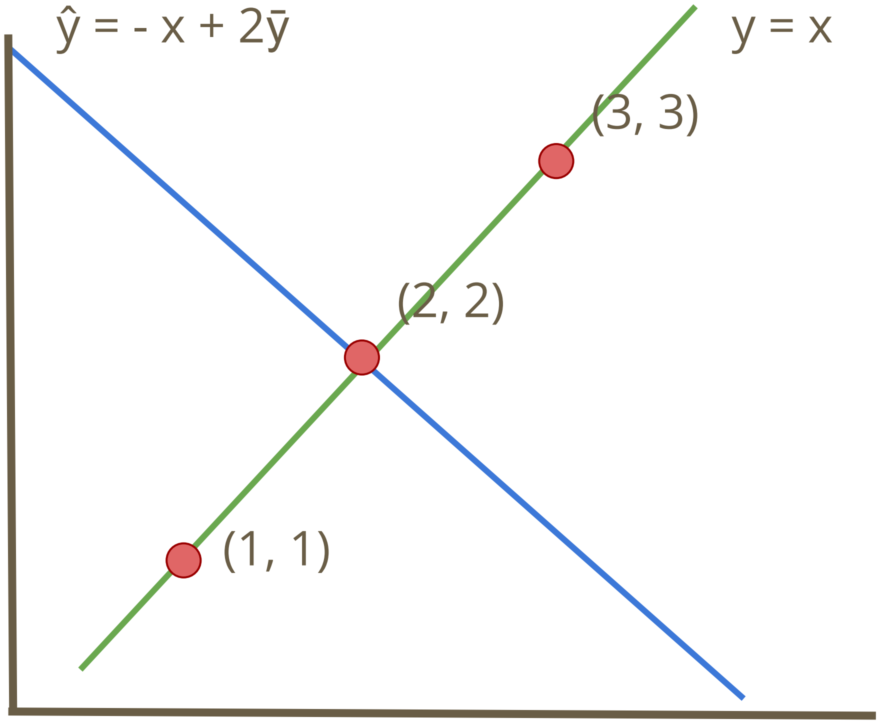

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$= (-x + \bar{y})^2$
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$$R^2 = 1$$

Why this new formula is standard

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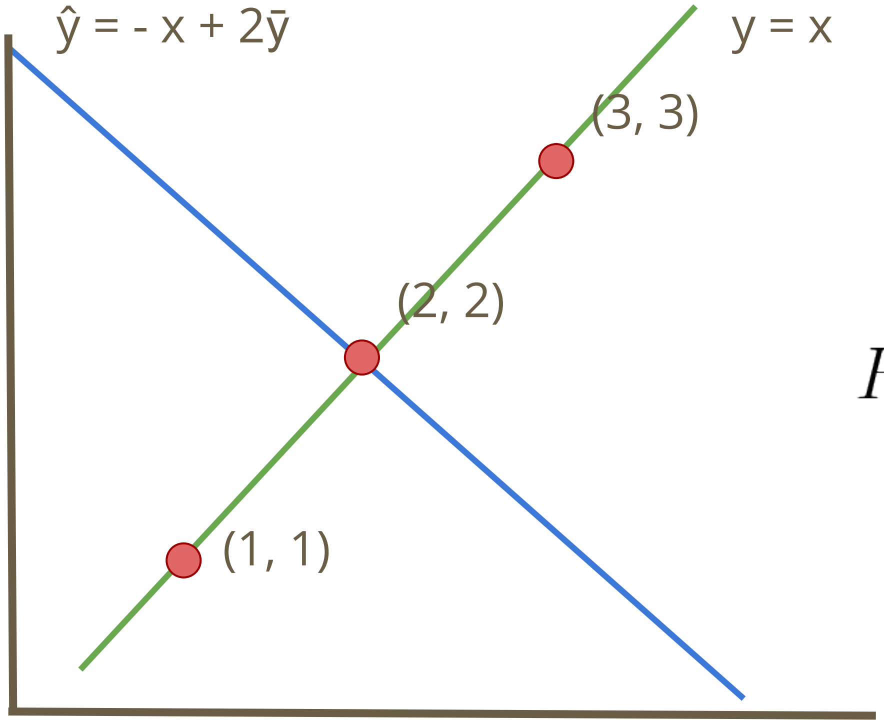

$$R^2 = 1 - \frac{RSS}{TSS}$$

Why this new formula is standard

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

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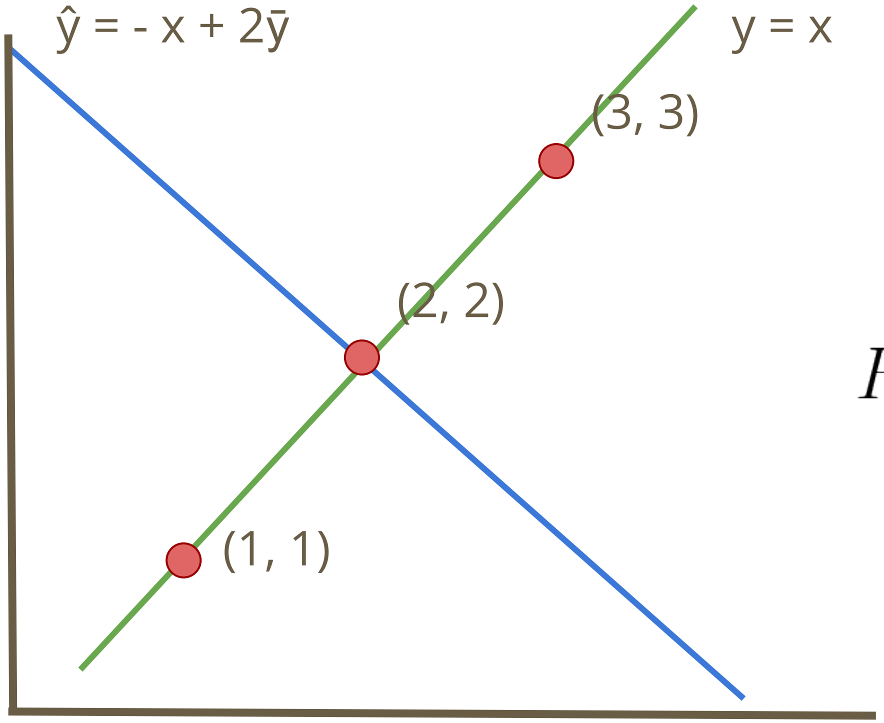

$(y - \hat{y})^2$
$= (x - (-x + 2\bar{y}))^2$
$= (-2x + 2\bar{y})^2$
$= (-2(y - \bar{y}))^2$
$= 4(y - \bar{y})^2$

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

Why this new formula is standard

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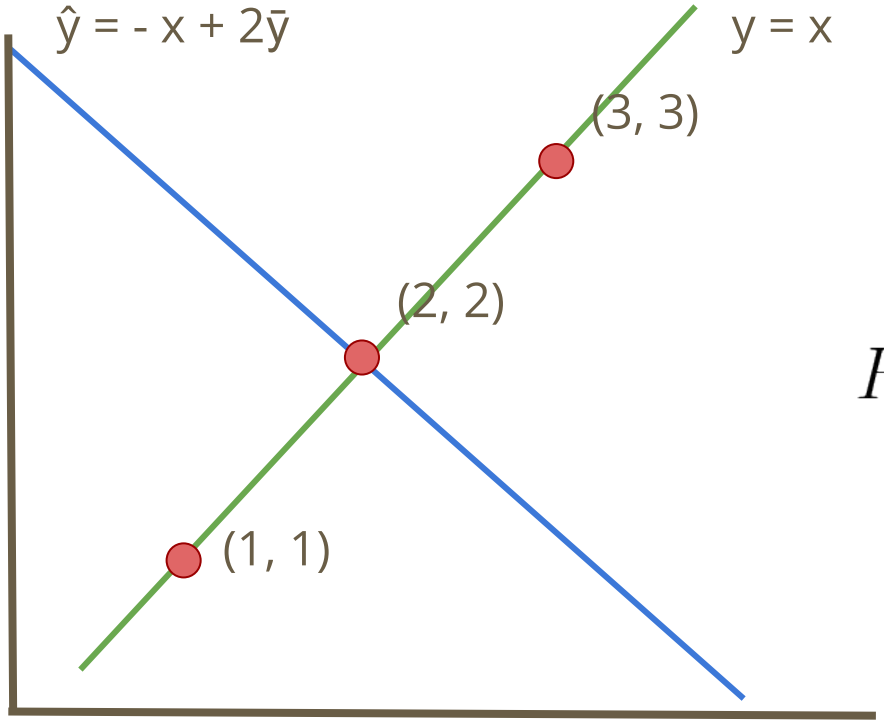

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$$R^2 = 1 - 4$$

Why this new formula is standard

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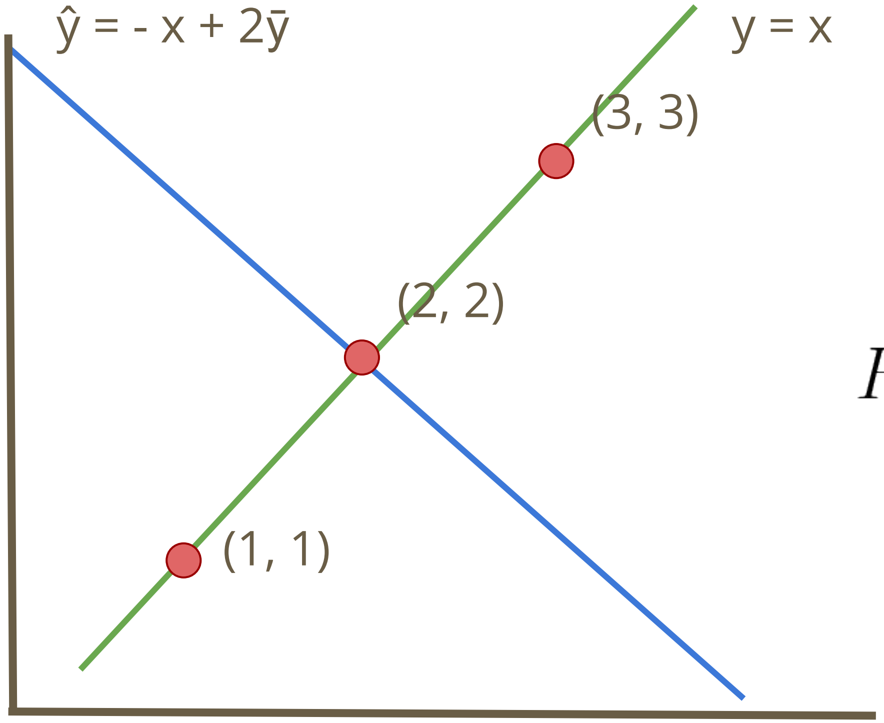

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$R^2 =$ -3

Another example

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

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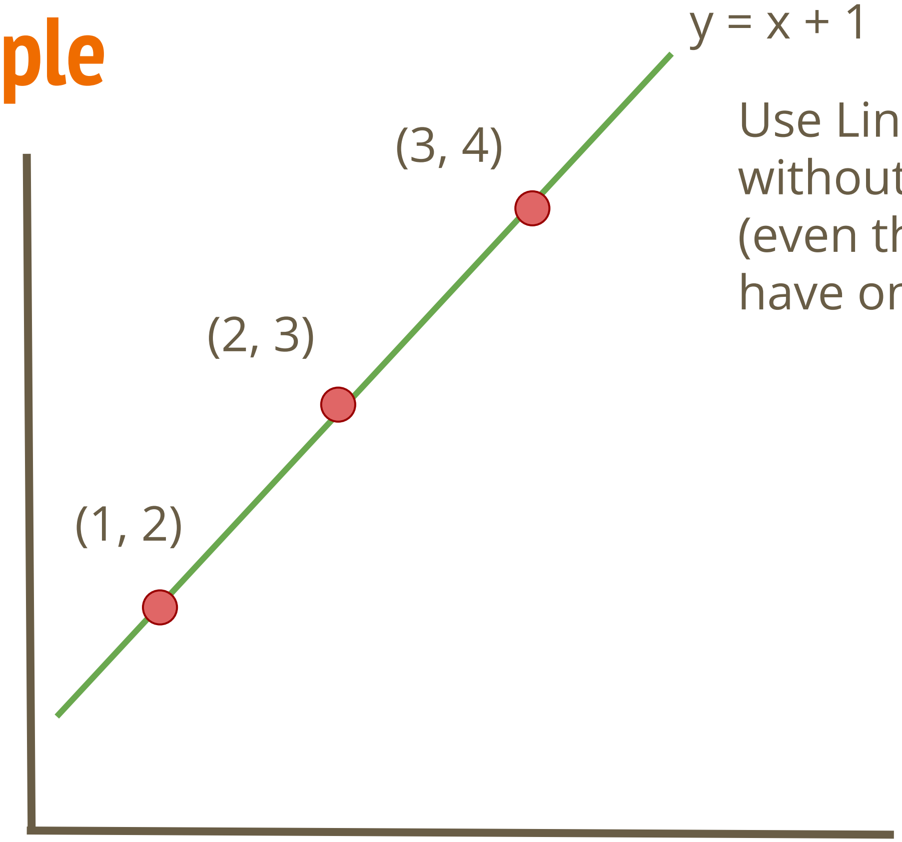
$$ESS = \sum_{i}^{n} (\hat{y}_i - \bar{y})^2$$

$\bar{Y} = 3$



Use Linear Regression without an intercept (even though it should have one in this case)

$$R^2 = \frac{ESS}{TSS}$$

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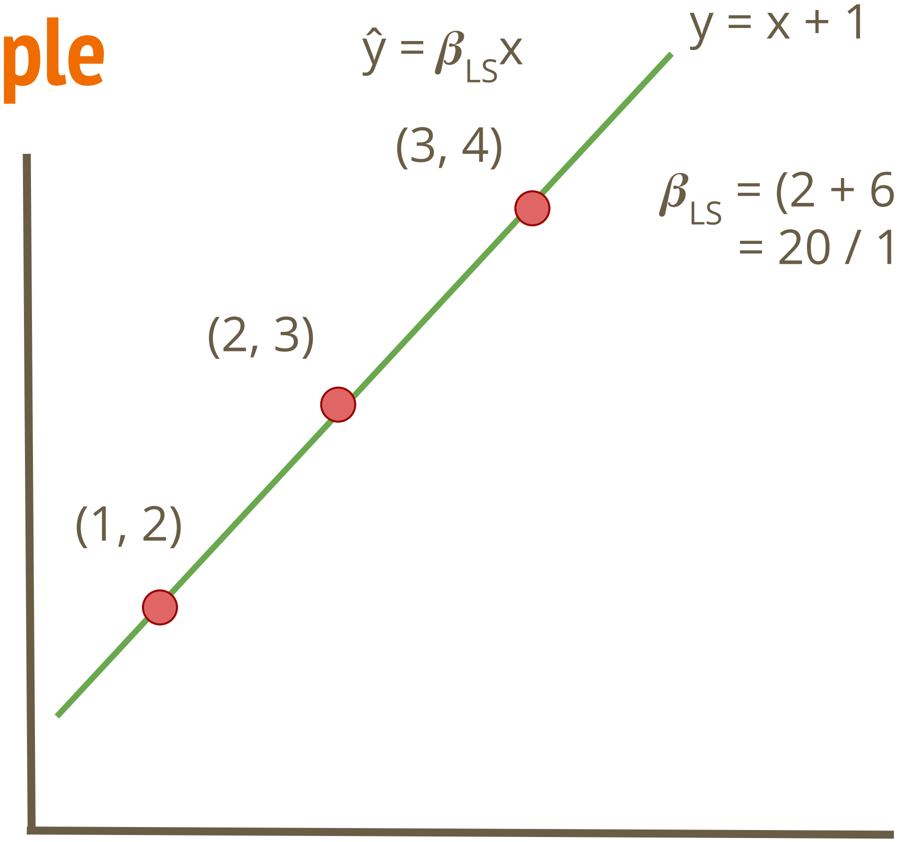

$\beta_{LS} = (2 + 6 + 12) / (1^2 + 2^2 + 3^2)$
$= 20 / 14$ **= 1.43**

$$R^2 = \frac{ESS}{TSS}$$

Another example

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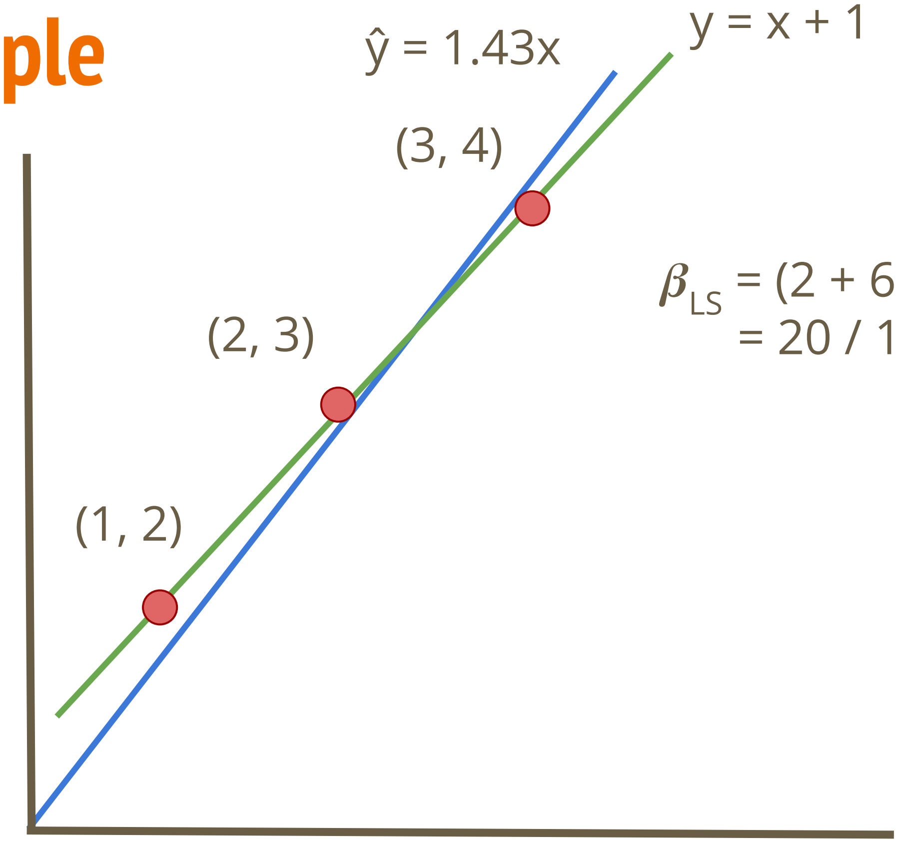

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$$R^2 = \frac{ESS}{TSS}$$

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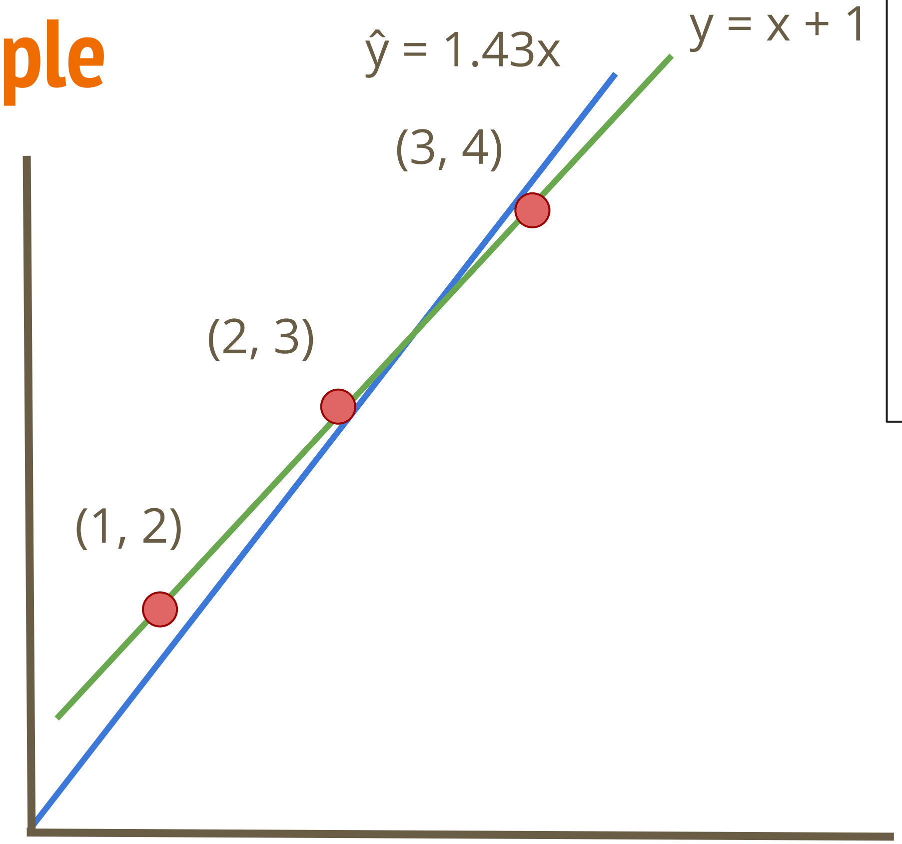

ESS = $(1.43 - 3)^2 + (2.86 - 3)^2 + (4.29 - 3)^2$
= 4.1

TSS = $1^2 + 0^2 + 1^2$
= 2

$$R^2 = \frac{ESS}{TSS}$$

Another example

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

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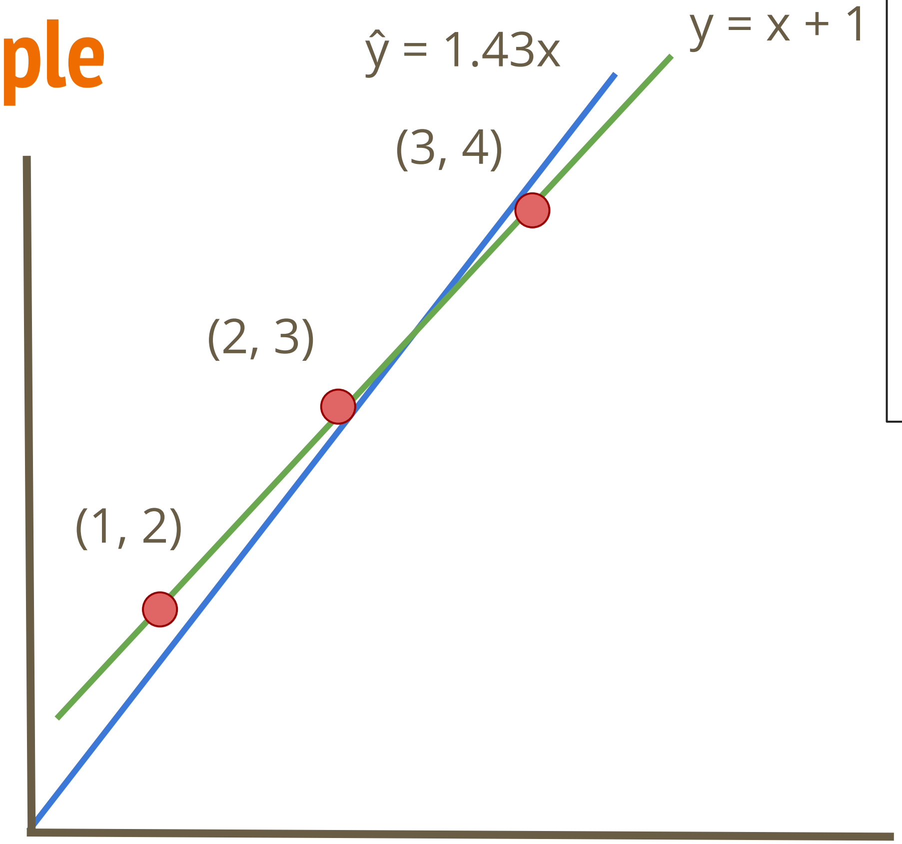

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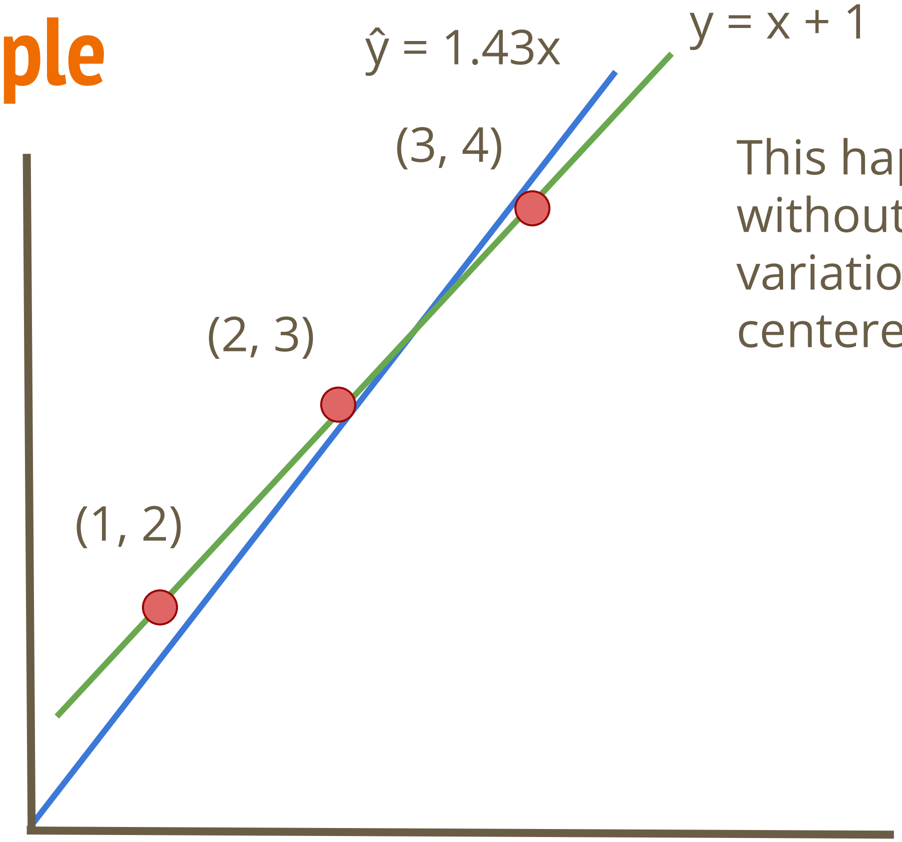

This happens because, without an intercept, variation of ŷ is not centered around Ȳ

$$R^2 = 2$$

Another example

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

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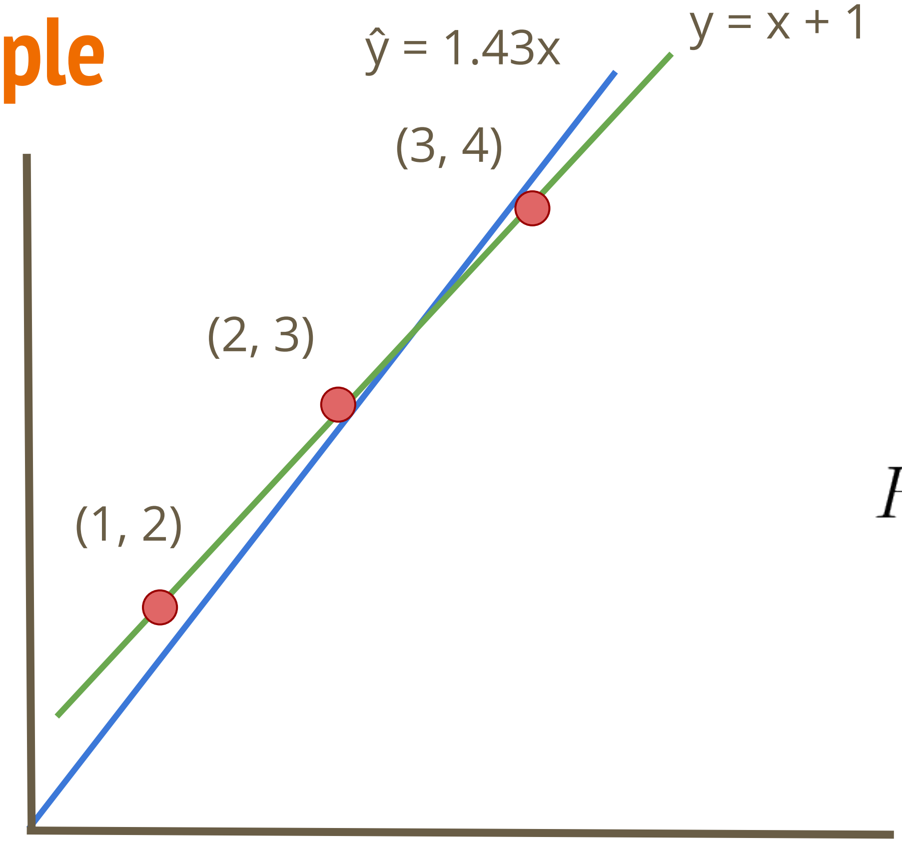

$$R^2 = 1 - \frac{RSS}{TSS}$$

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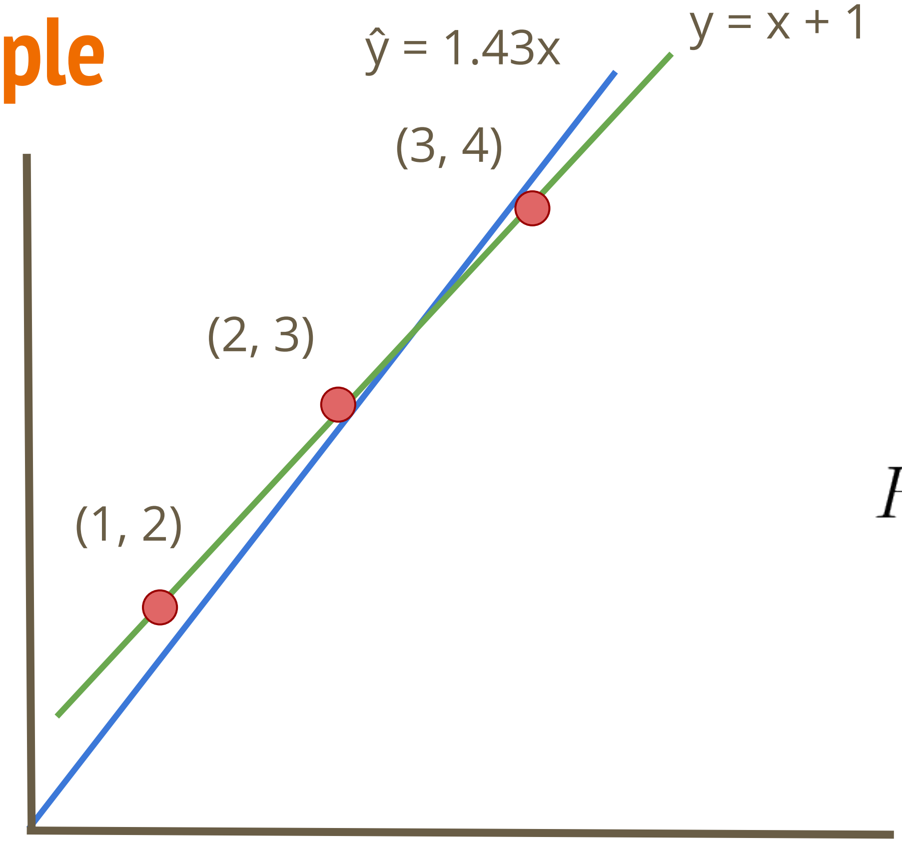

$$R^2 = .98$$

Recap

Variance formula:

- Cannot be negative
- Can be greater than 1
- Only use when $\hat{y}$ is a linear model (minimizing RSS) and is centered around $\bar{Y}$ (i.e. not omitting an intercept for example)

Residual-based R^2 formula

- Can be negative
- Cannot be greater than 1
- Adapts to any model. A linear model that passes through all points will have an R^2 of 1

Evaluating our Regression Model

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.840
Model:                            OLS   Adj. R-squared:                  0.836
Method:                 Least Squares   F-statistic:                     254.1
Date:                Sun, 20 Mar 2022   Prob (F-statistic):           2.72e-39
Time:                        11:36:16   Log-Likelihood:                -482.37
No. Observations:                 100   AIC:                             970.7
Df Residuals:                      97   BIC:                             978.5
Df Model:                           2
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const          2.1912      3.162      0.693      0.490      -4.085       8.467
x1            29.3912      3.274      8.977      0.000      22.893      35.889
x2            78.1391      3.594     21.741      0.000      71.006      85.272
==============================================================================
Omnibus:                        1.279   Durbin-Watson:                   1.824
Prob(Omnibus):                  0.527   Jarque-Bera (JB):                1.065
Skew:                           0.253   Prob(JB):                        0.587
Kurtosis:                       2.999   Cond. No.                         1.38
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Chance or linearity?

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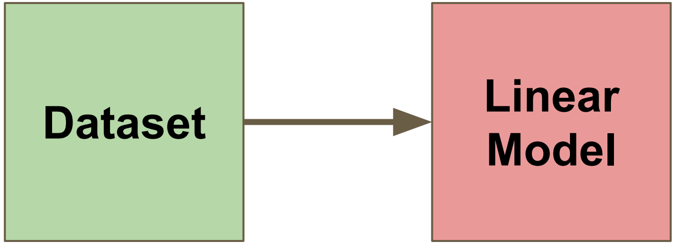
Hypothesis Testing

Dataset

β = ?

Hypothesis Testing



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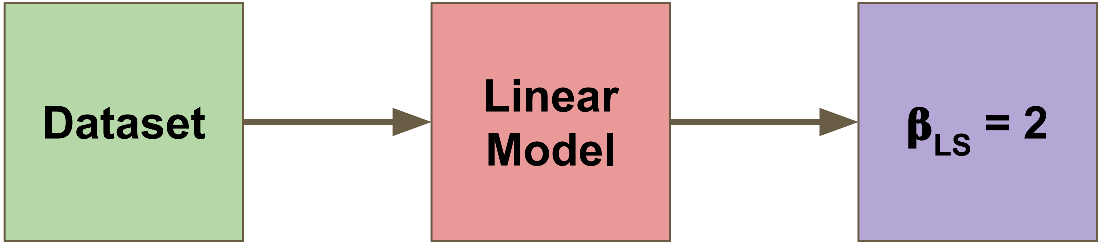
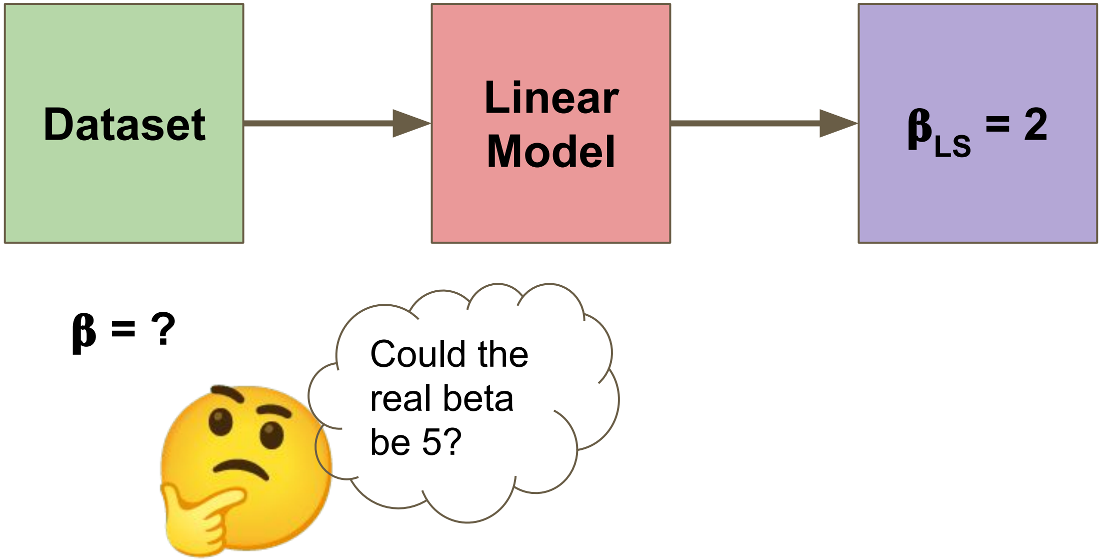
Hypothesis Testing



β = ?

Hypothesis Testing



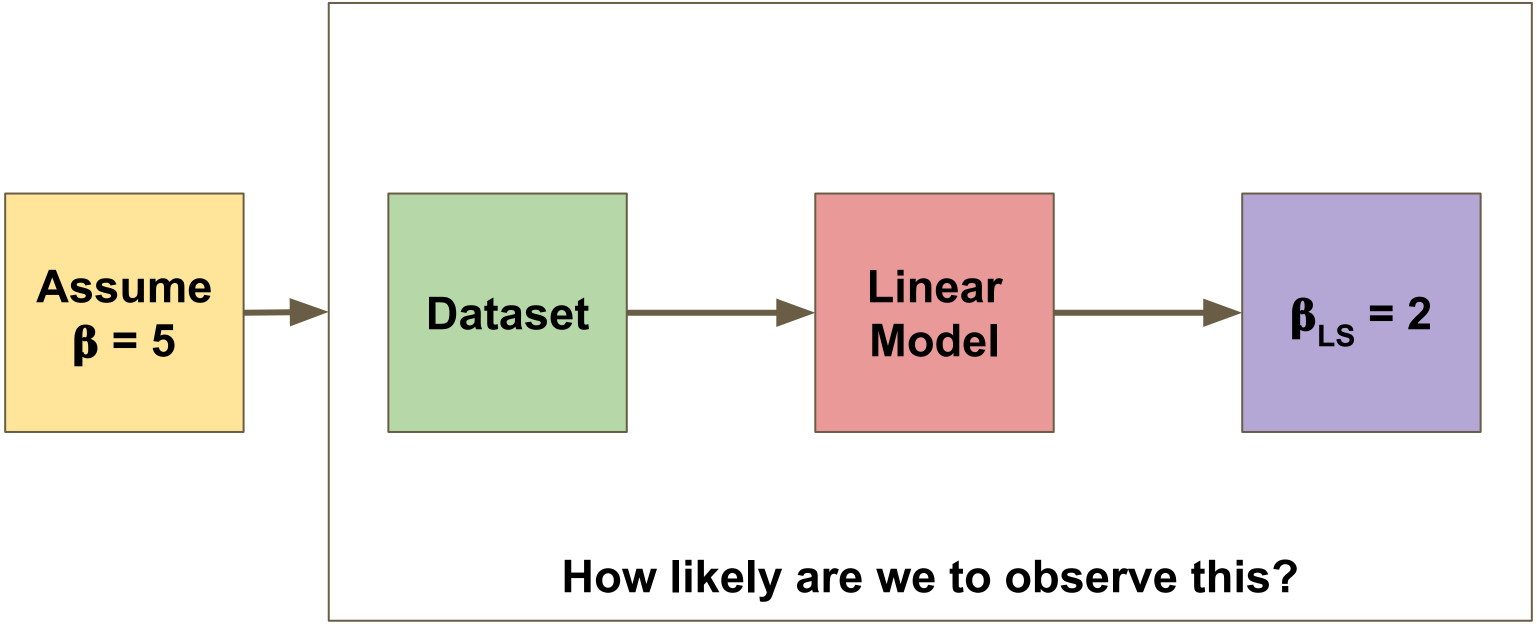
H H H H H H H H

The coin is probably not fair

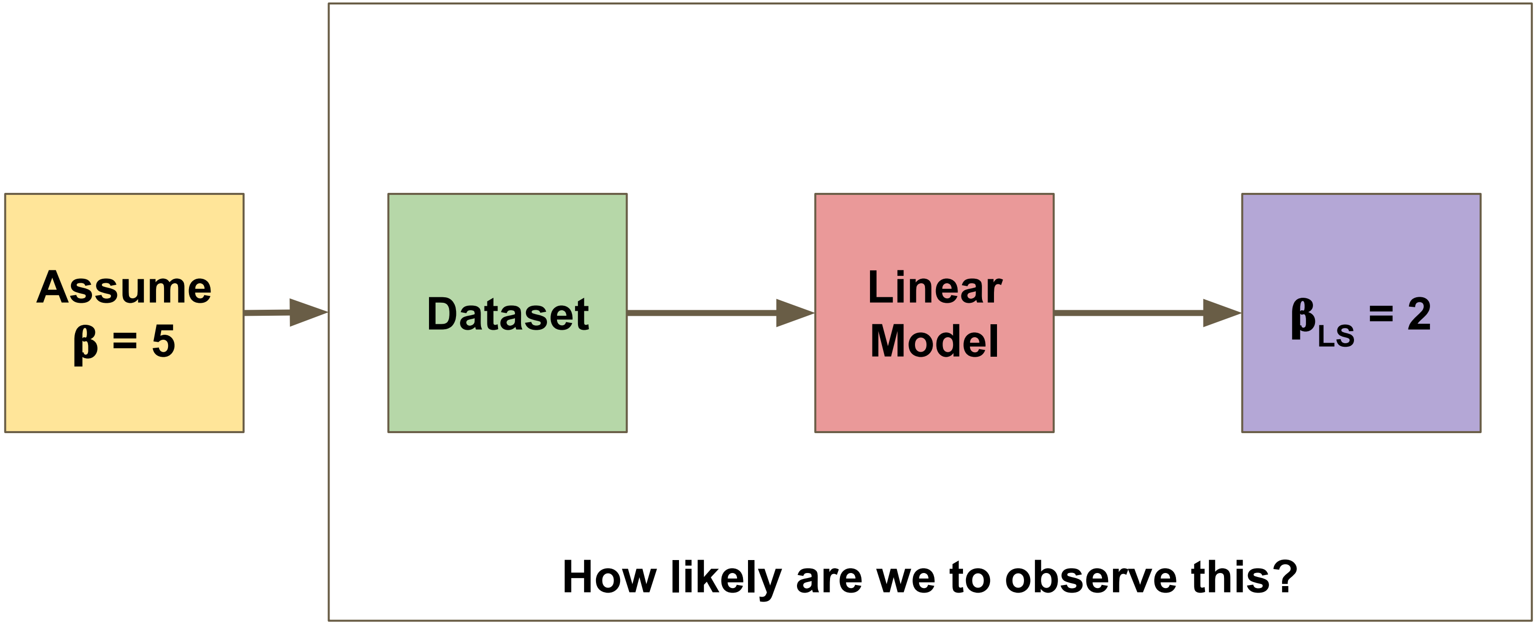
H T H H T H T T

The coin could be fair

Hypothesis Testing

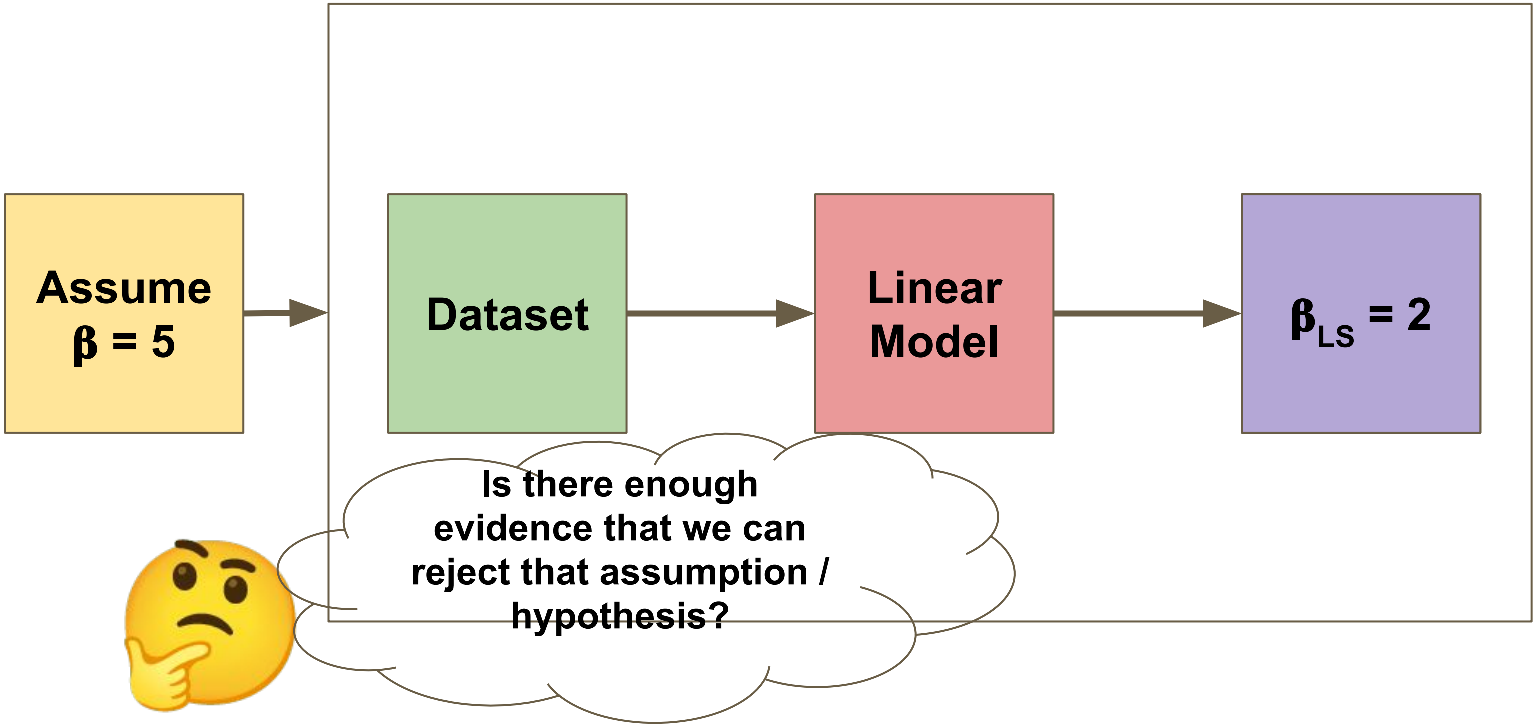


Hypothesis Testing

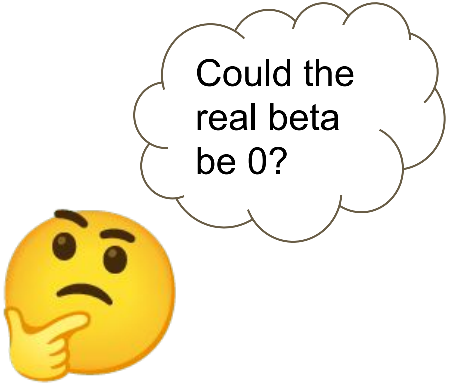


Note: this likeliness is a probability and is called a p-value

Hypothesis Testing



worksheet



Hypothesis Testing

Each parameter of an independent variable **x** has an associated confidence interval and t-value + p-value.

If the parameter / coefficient is not significantly distinguishable from 0 then we cannot assume that there is a significant linear relationship between that independent variable and the observations **y** (i.e. if the interval includes 0 or if the p-value is too large)

Hypothesis Test

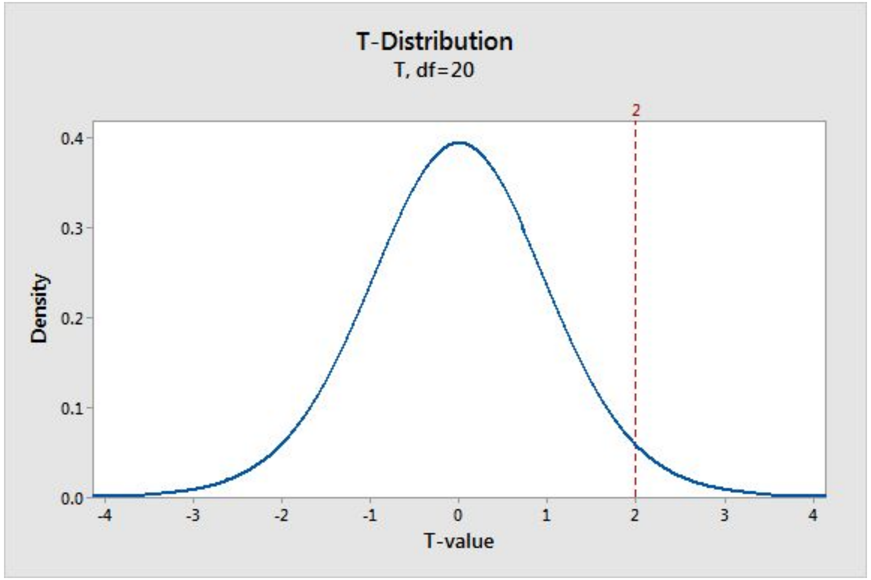
We want to know if there is evidence to reject the hypothesis $H0 : \beta = 0$ (i.e. that there is no linear relation between X and Y) using the information from β hat.

We want to know the largest probability of obtaining the data observed, under the assumption that the null hypothesis is correct.

How do we obtain that probability?

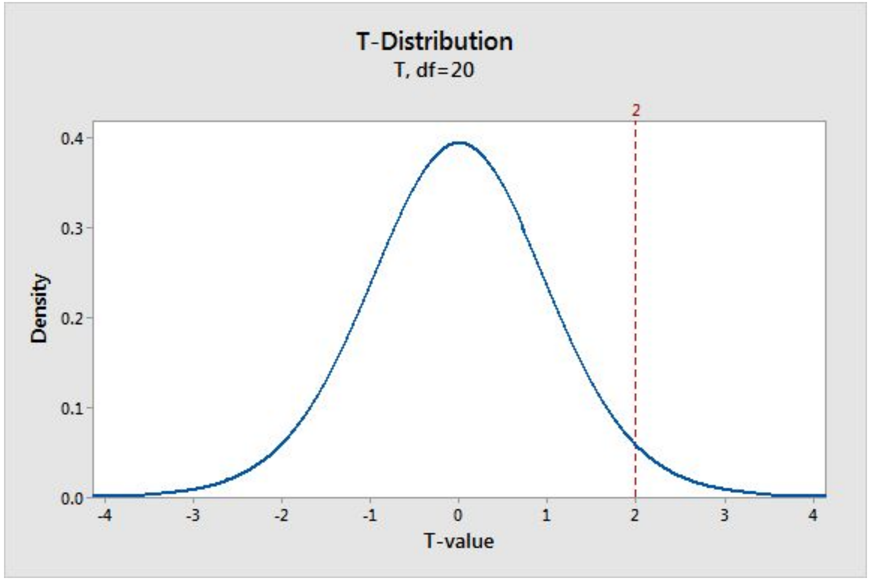
Hypothesis Test

Under the null hypothesis what should be the distribution of the normalized estimates? T-distribution (parametrized by the sample size)



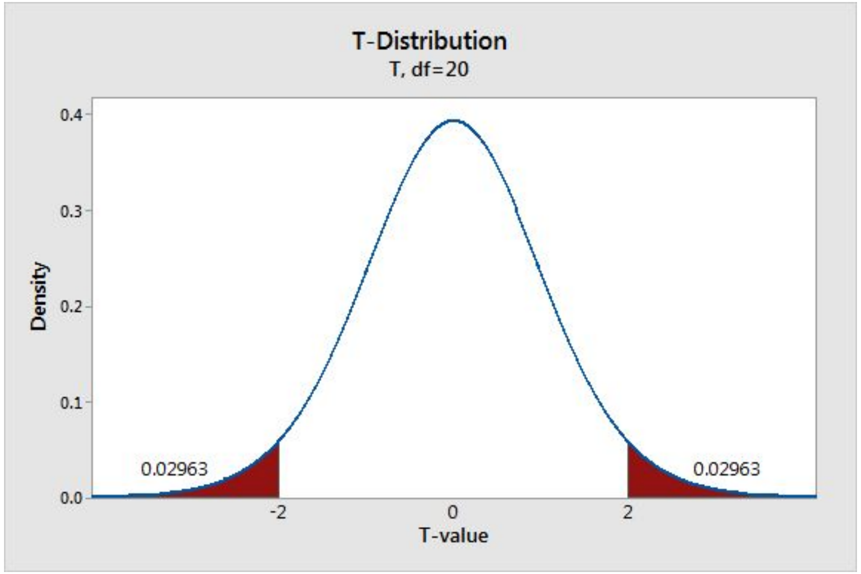
Hypothesis Test

We can then compute the t-value that corresponds to the sample we observed.



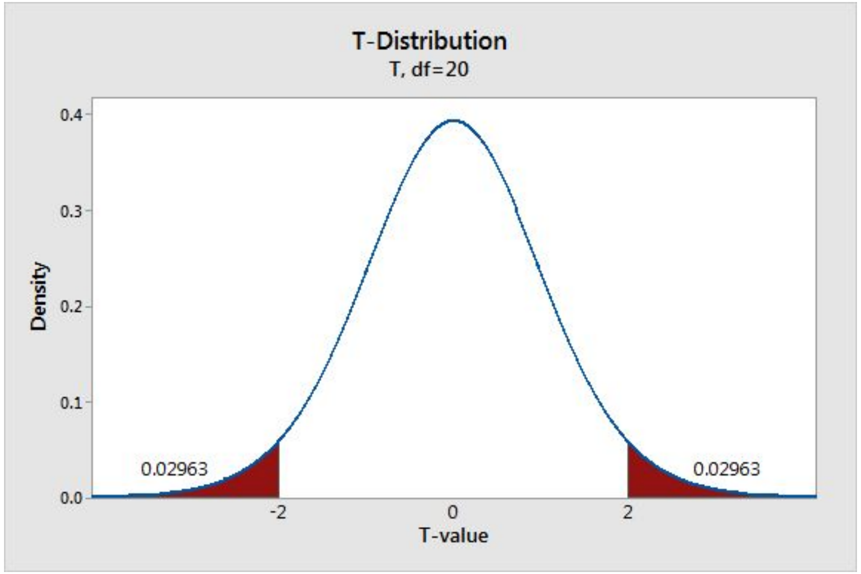
Hypothesis Test

And then compute the probability of observing estimates of β at least as extreme as the one observed. (i.e. trying to find evidence against H0)



Hypothesis Test

This probability is called a p-value.



Hypothesis Test

A p-value **smaller than a given threshold** would mean the data was unlikely to be observed under H0 so we can reject the hypothesis H0. If not, then we lack the evidence to reject H0.

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Hypothesis Test

Which parameters should we not include in our linear model?

	coef	std err	t	P>|t|	[0.025	0.975]
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Skew:                           0.253   Prob(JB):                        0.587
Kurtosis:                       2.999   Cond. No.                         1.38
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```

Confidence Intervals

Goal: for a given confidence level (let's say 90%), construct an interval around an estimate such that, if the estimation process were repeated indefinitely, the interval would contain the true value (that the estimate is estimating) 90% of the time.

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const	2.1912	3.162	0.693	0.490	-4.085	8.467
x1	29.3912	3.274	8.977	0.000	22.893	35.889
x2	78.1391	3.594	21.741	0.000	71.006	85.272

Z-values

These are the number of standard deviations from the mean of a N(0,1) distribution required in order to contain a specific % of values were you to sample a large number of times.

To find the .95 z-value (the value z such that 95% of the observations lie within z standard deviations of the mean ($\mu \pm z * \sigma$)) you need to solve:

$$\int_{-z}^{z} \frac{1}{2\pi} e^{-\frac{1}{2}x^2} dx = .95$$

Z-values

The .95 z-value is 1.96.

This means 95% of observations from a $N(\mu, \sigma)$ lie within 1.96 standard deviations of the mean ($\mu \pm 1.960 * \sigma$)

If we get a sample from a $N(\mu, \sigma)$ of size n, how would we create a confidence interval around the estimated mean?

Confidence Intervals

How do we build a confidence interval?

Assume $\mathbf{Y_i \sim N(5, 25)}$, for $\mathbf{1 \leq i \leq 100}$ and $\mathbf{y_i = \mu + \epsilon}$ where $\mathbf{\epsilon \sim N(0, 25)}$. Then the Least Squares estimator of $\boldsymbol{\mu}$ ($\boldsymbol{\mu_{LS}}$) is

the sample mean $\bar{y}$

What is the 95% confidence interval for $\boldsymbol{\mu_{LS}}$?

$$SE(\mu_{LS}) = \sigma_\epsilon / \sqrt{n} = 5 / \sqrt{100} = .5$$

$$CI_{.95} = [\bar{y} - 1.96 \times SE(\mu_{LS}), \bar{y} + 1.96 \times SE(\mu_{LS})]$$
$$= [\bar{y} - 1.96 \times .5, \bar{y} + 1.96 \times .5]$$

Z-value for 95% Confidence Interval

One more assumption to check...

This is actually the trickiest one: **independence** of observations.

It's implicitly assumed that all noise in our data are independent of each other.

When data is not independent

Example: running times

For a given runner, 10 * 1km splits throughout a 10km run is not the same as 10 independent 1km runs. The kms before are related to the kms to come through some pacing strategy or fatigue or fitness.

Extending our Linear Model

Changing the assumptions we made can drastically change the problem we are solving. A few ways to extend the linear model:

1. Non-constant variance - used in WLS (weighted least squares)
2. Distribution of error is not Normal - used in GLM (generalized linear models)