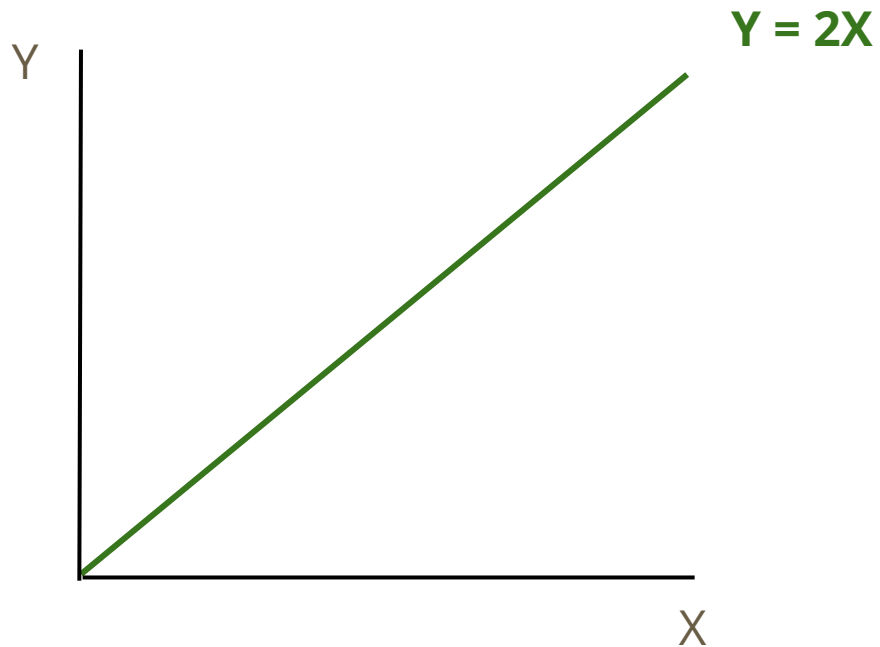
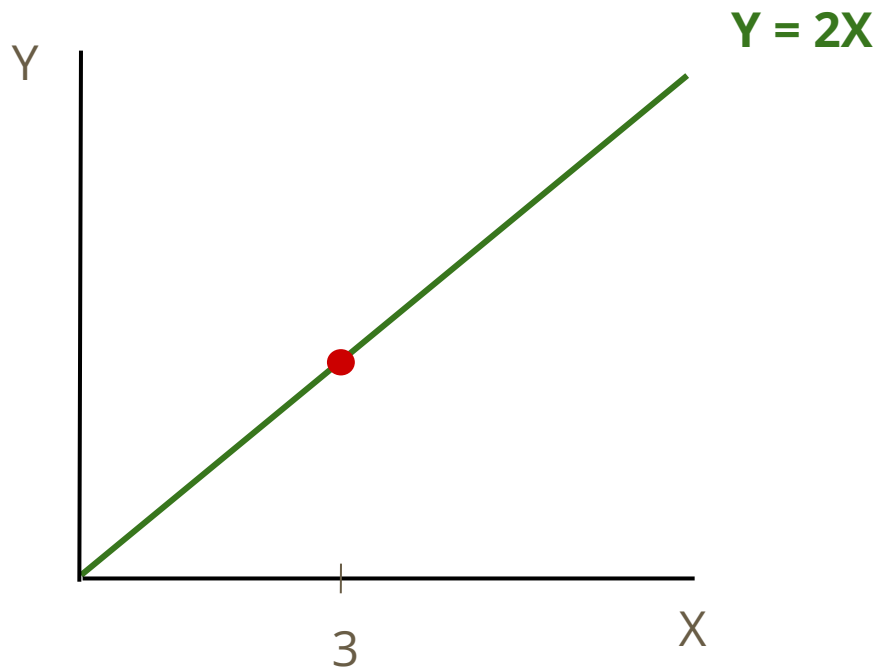

Linear Model Evaluation

— Boston University CS 506 - Lance Galletti —

Linear Function

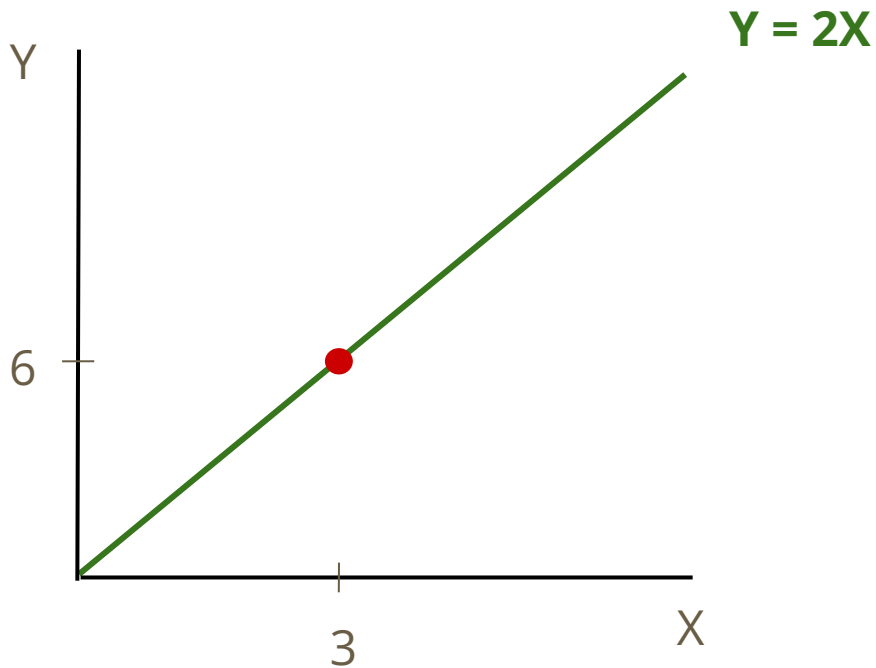


Linear Function

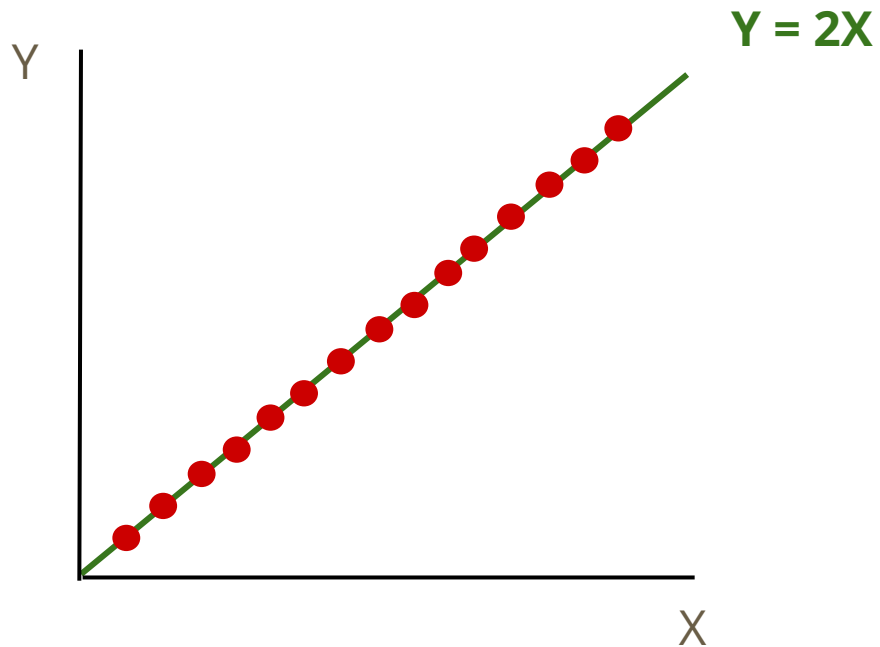


Linear Function

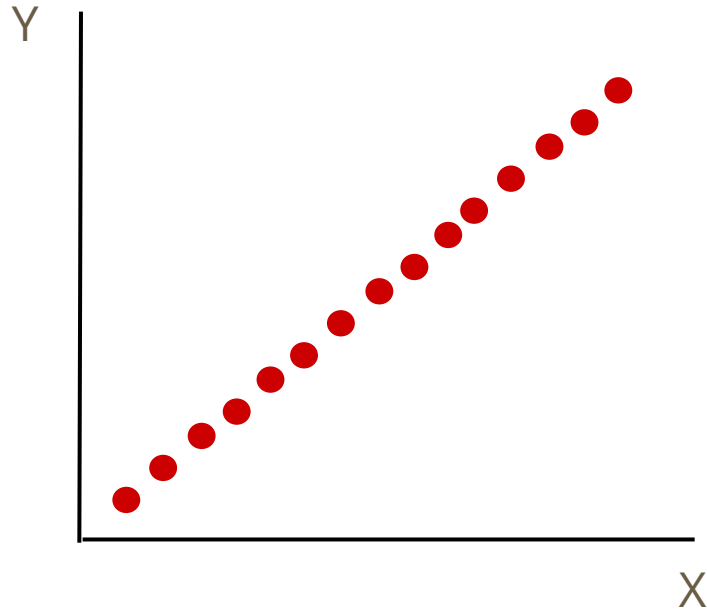
I know for sure what
value of Y I'm gonna get



Linear Function

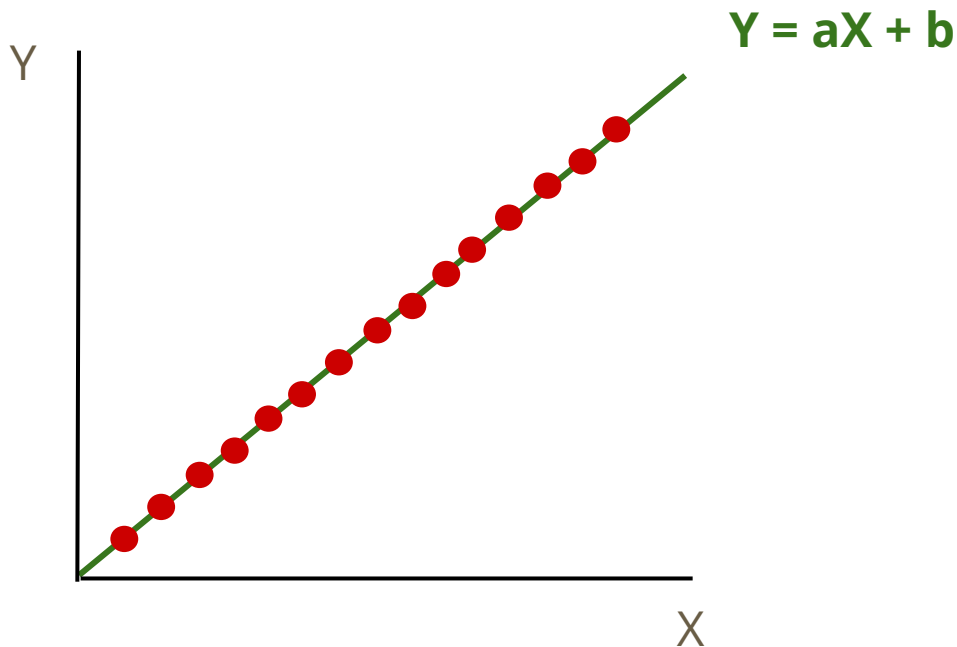


Ideally

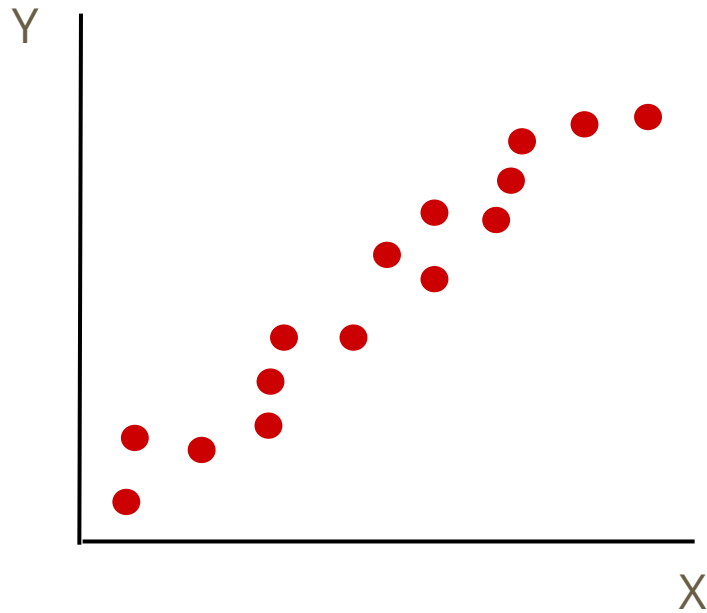


Ideally

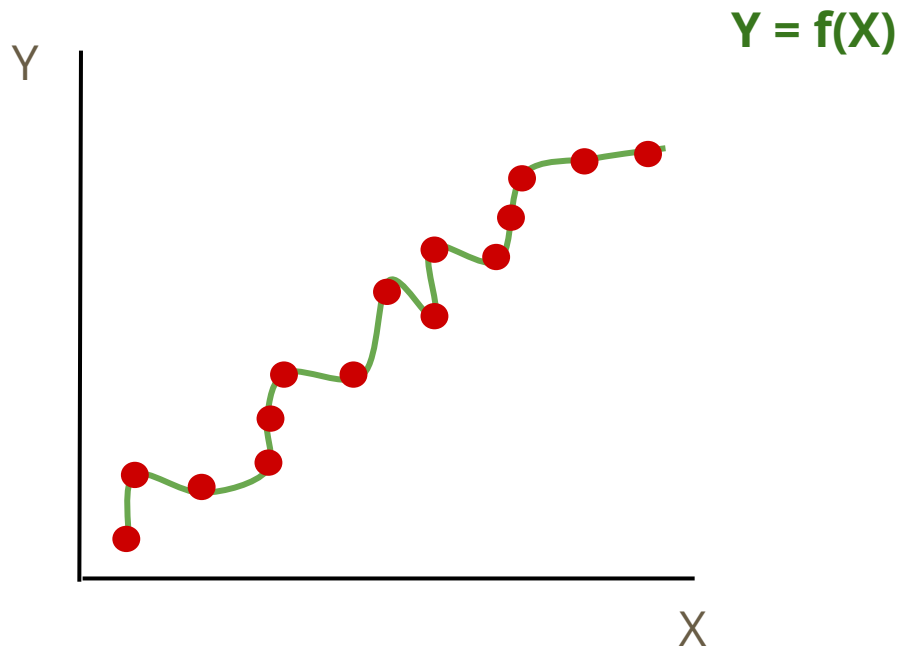
Guess the relationship
(**a** and **b**) from the data



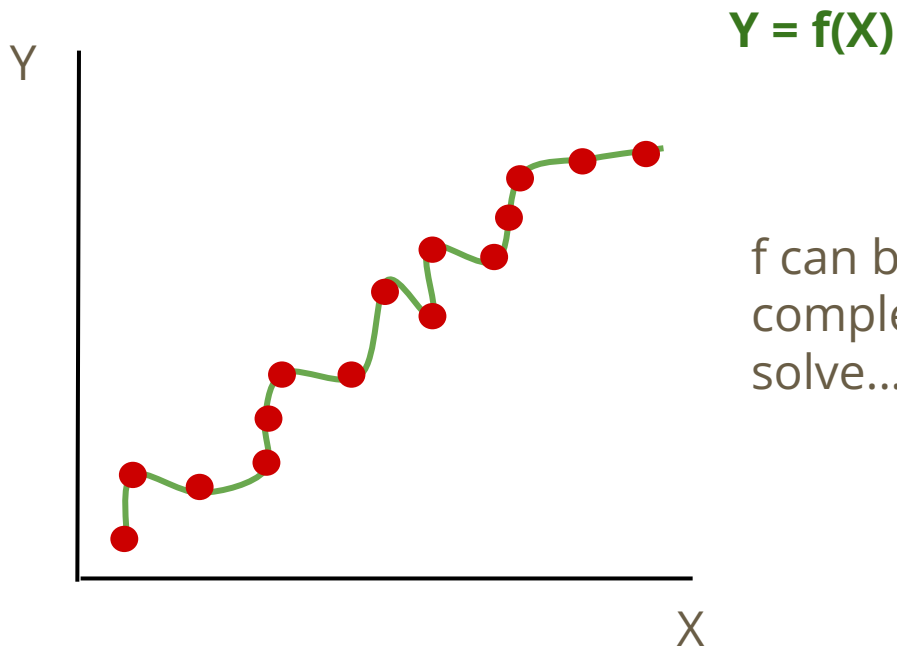
Practically



Practically

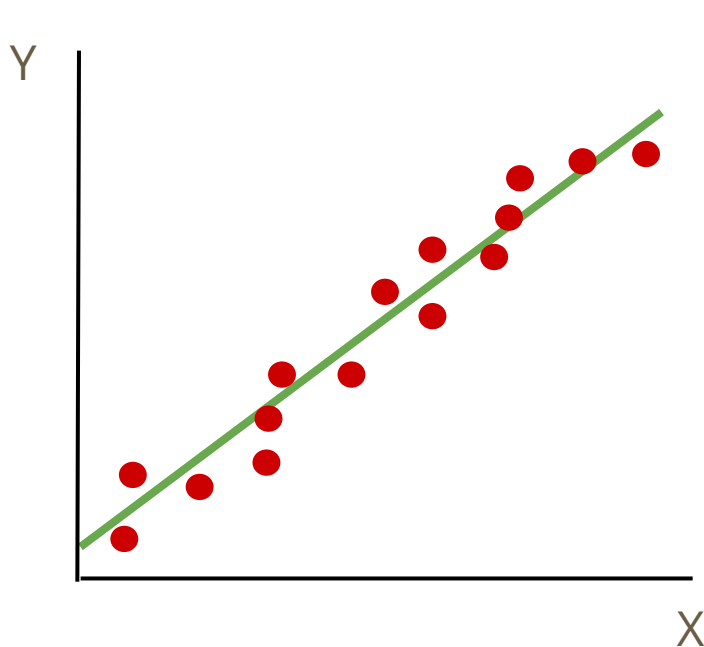


Practically



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

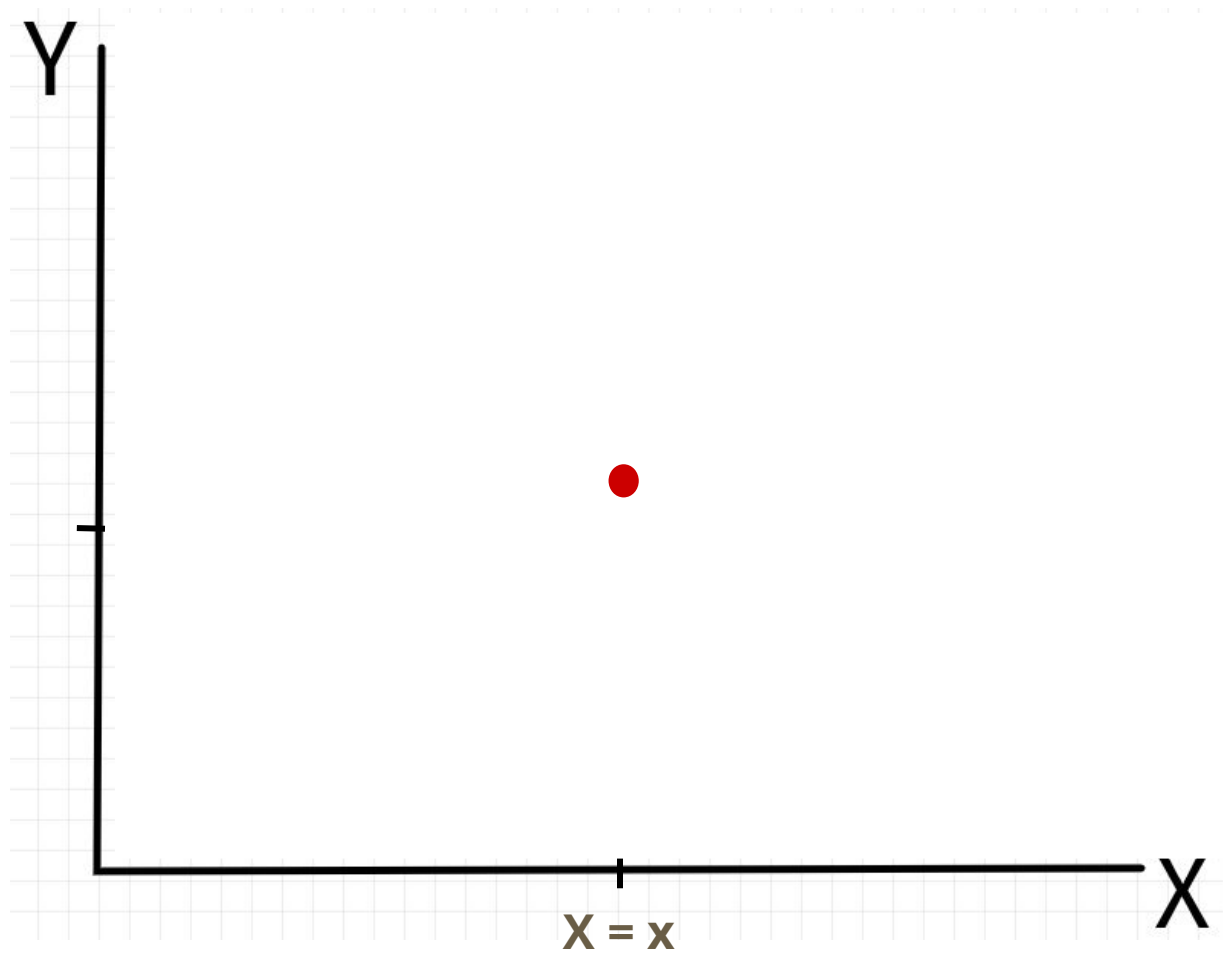
Practically



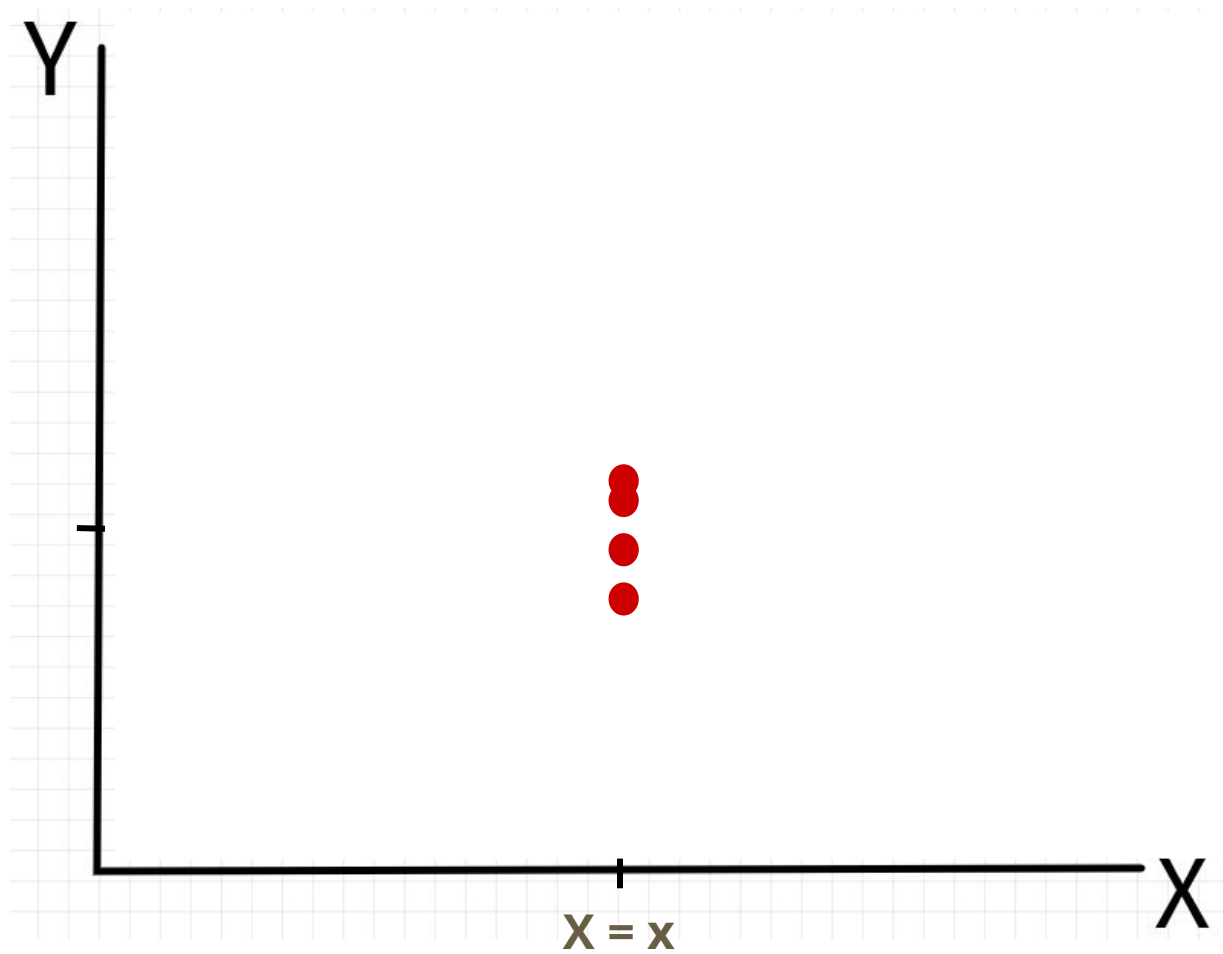
$$Y = f(X) + \text{noise}$$

Assume f is linear and the variation we're seeing is noise

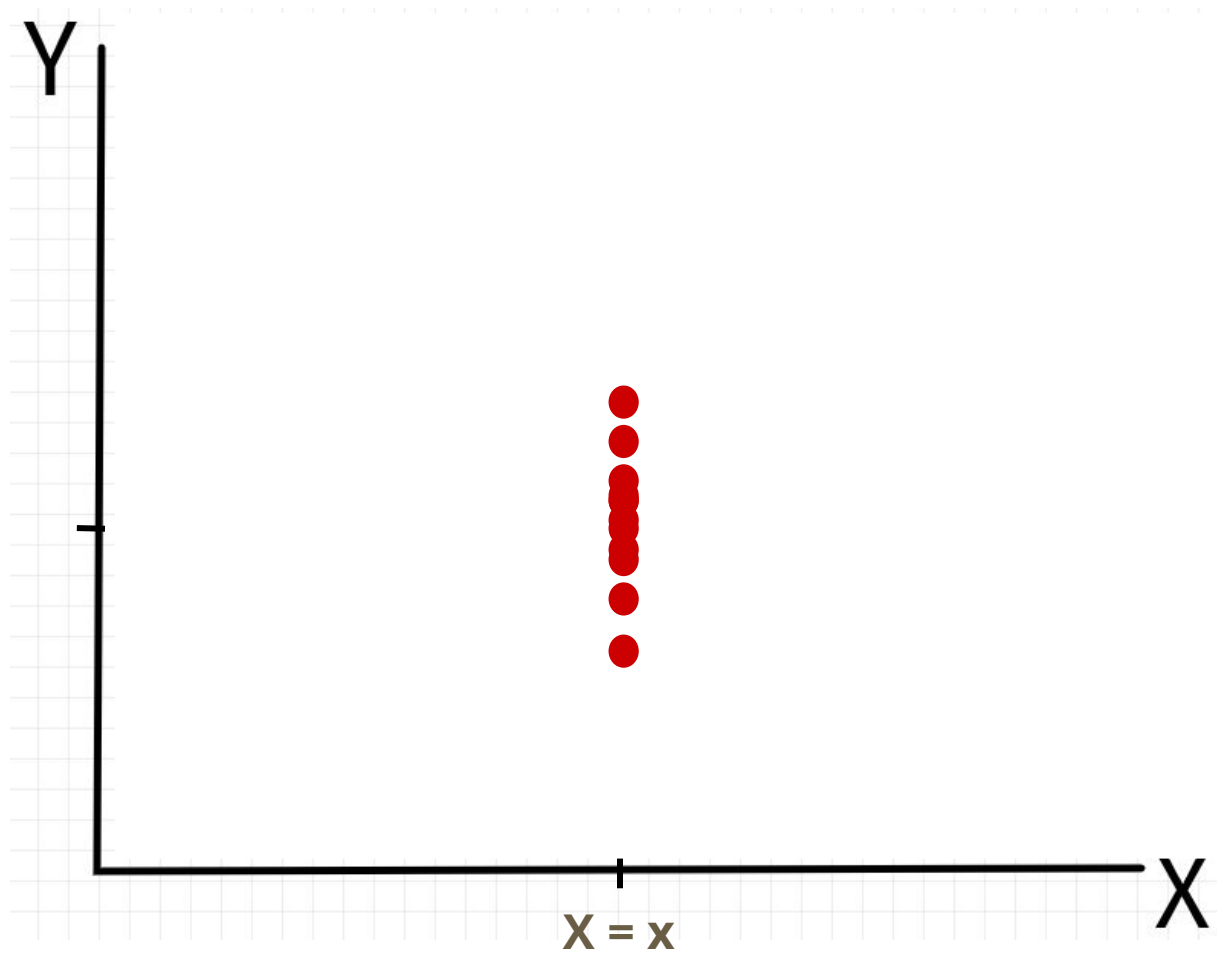
Assumptions



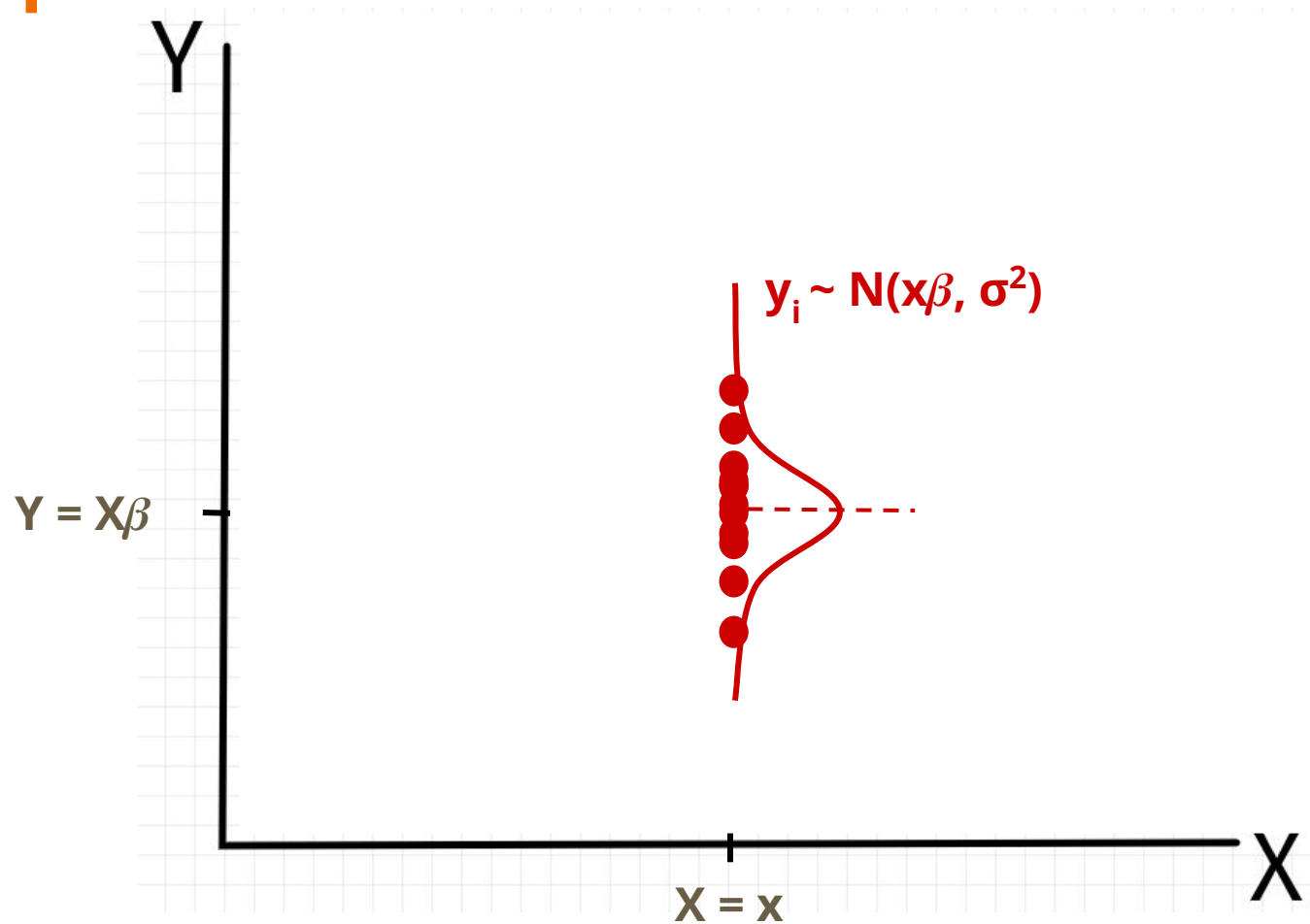
Assumptions



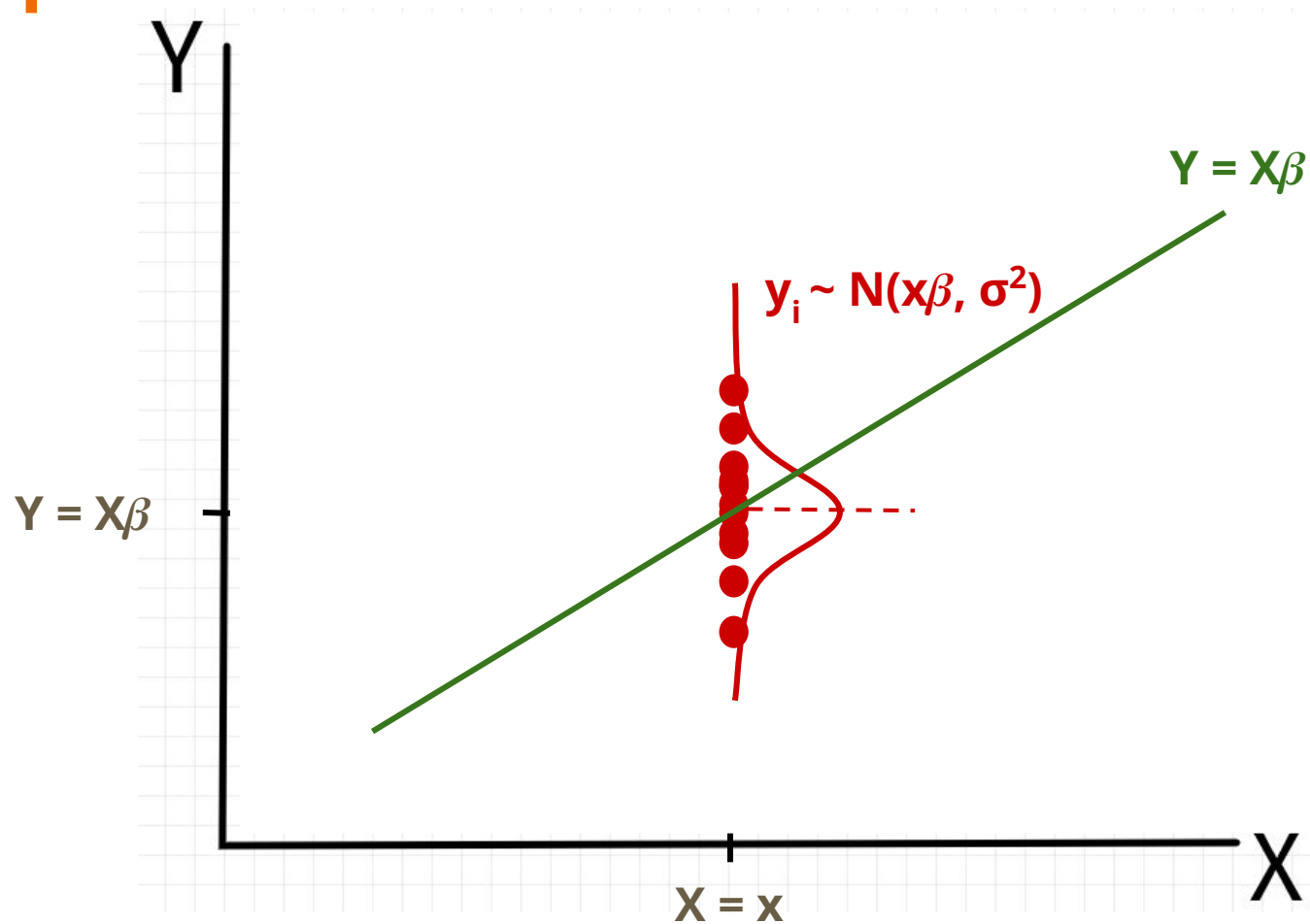
Assumptions



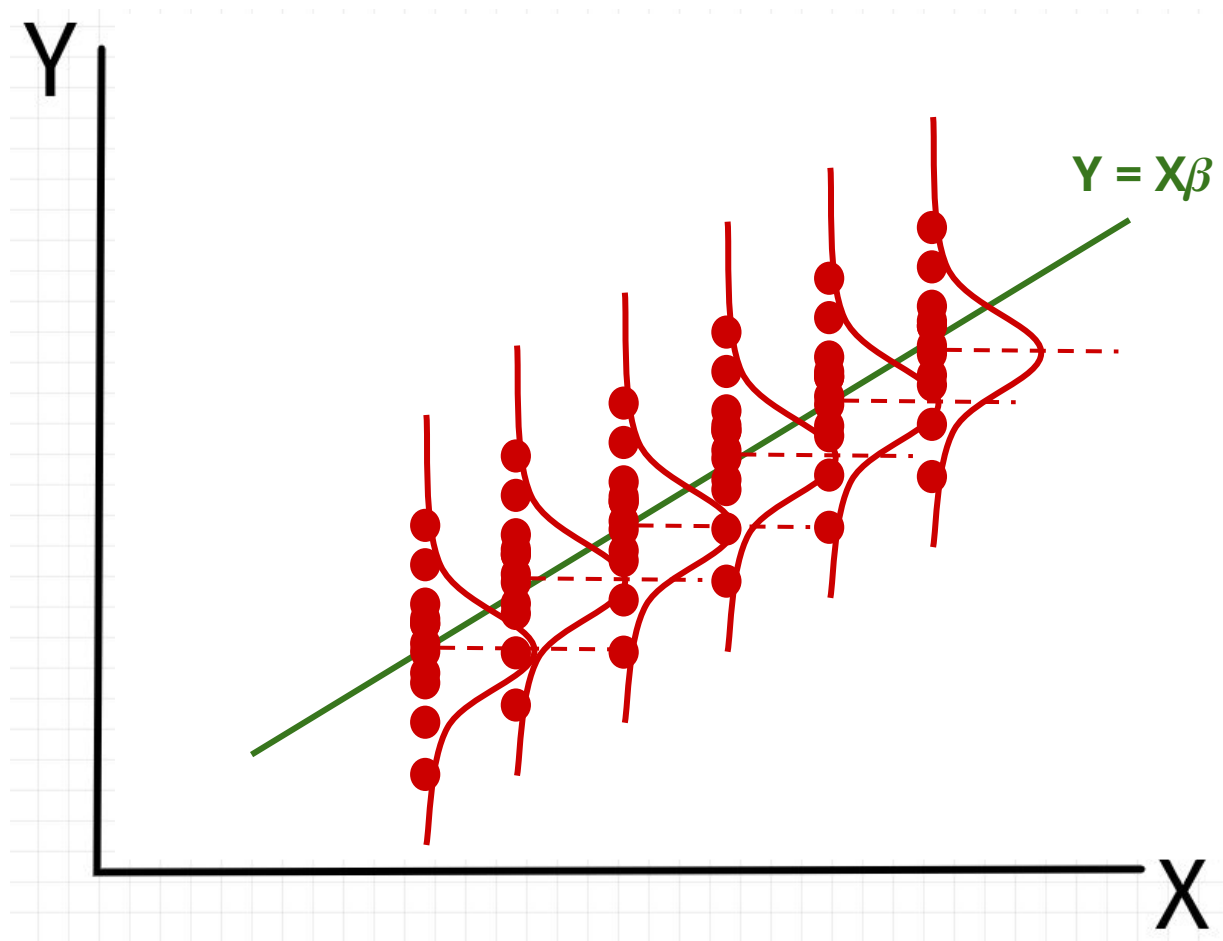
Assumptions



Assumptions



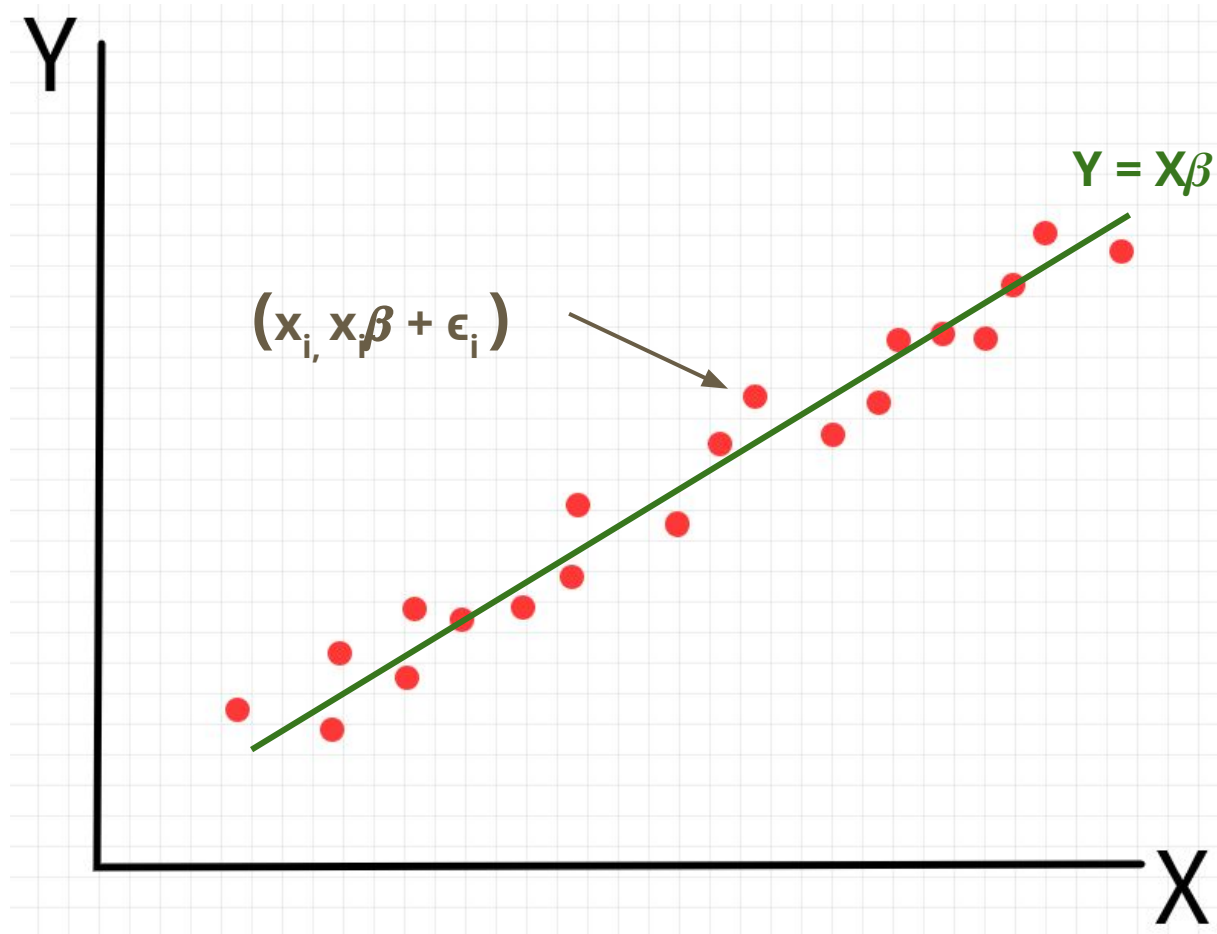
Assumptions



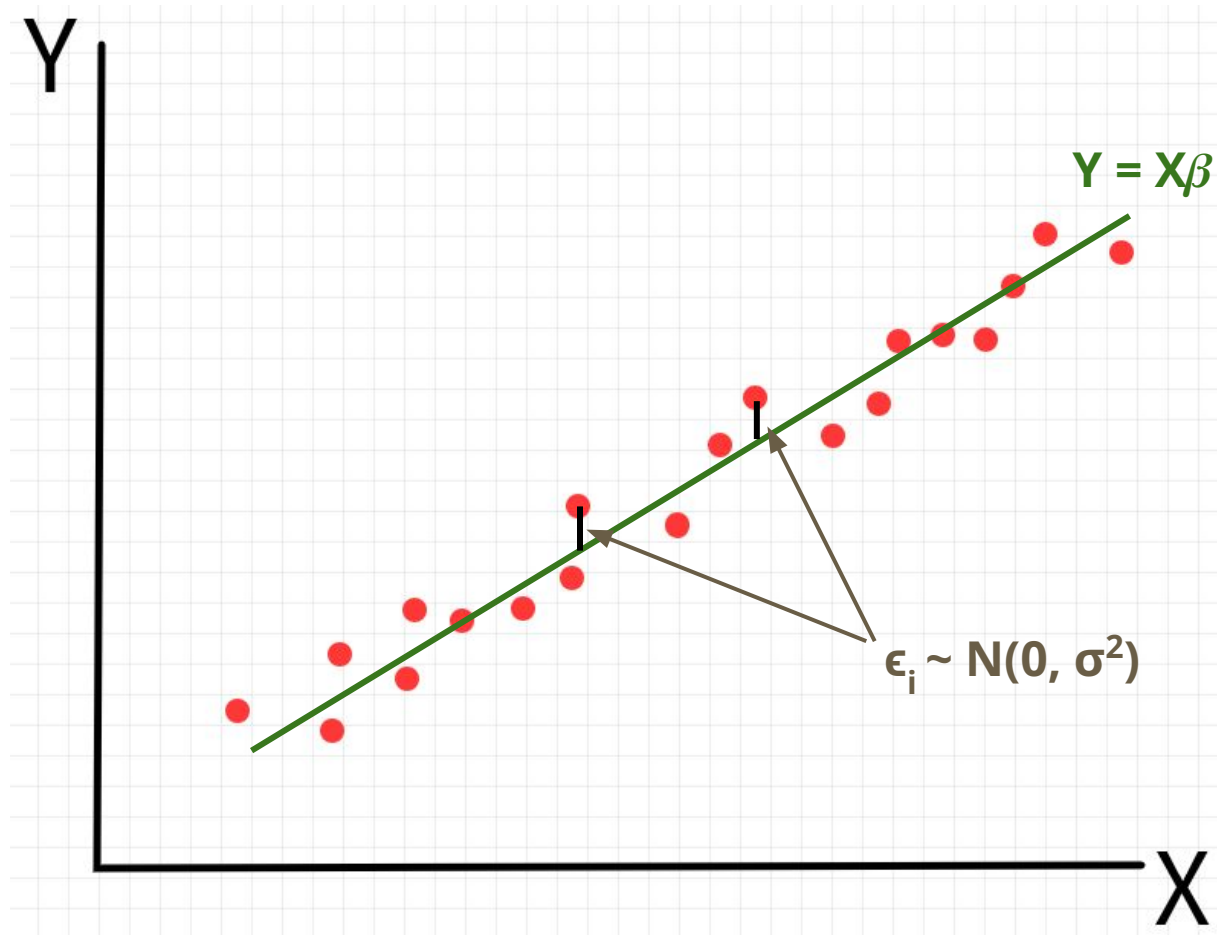
Assumptions



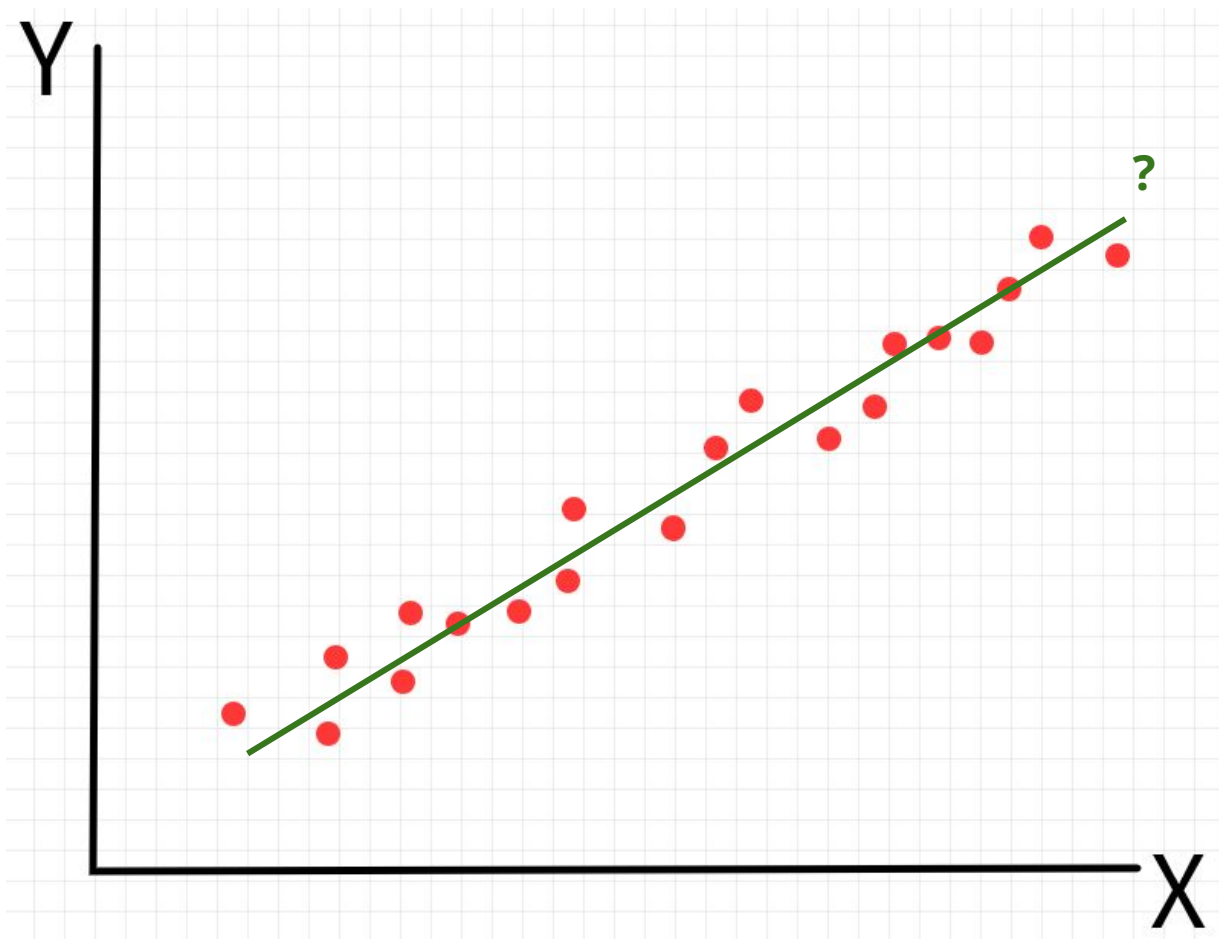
Assumptions



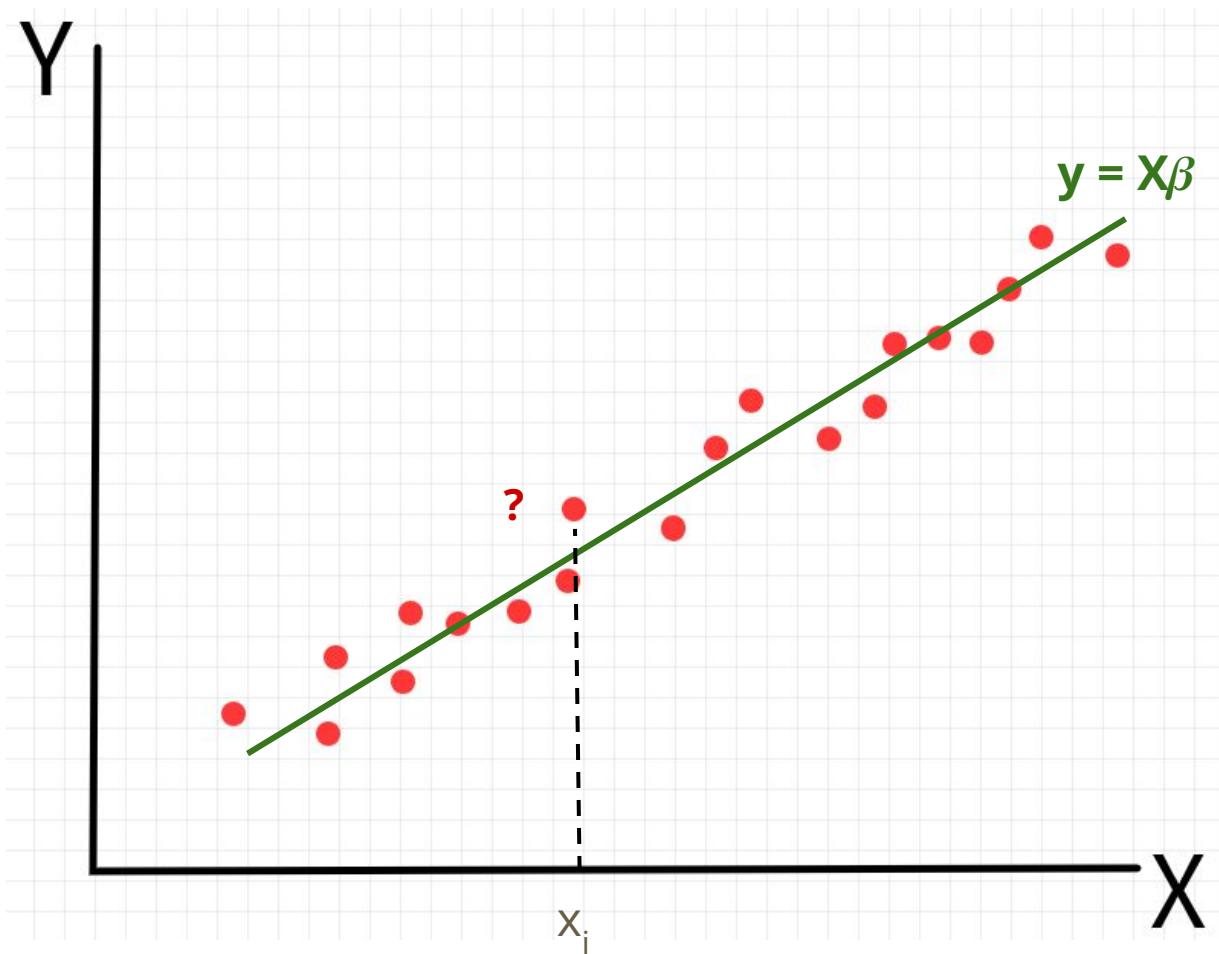
Assumptions

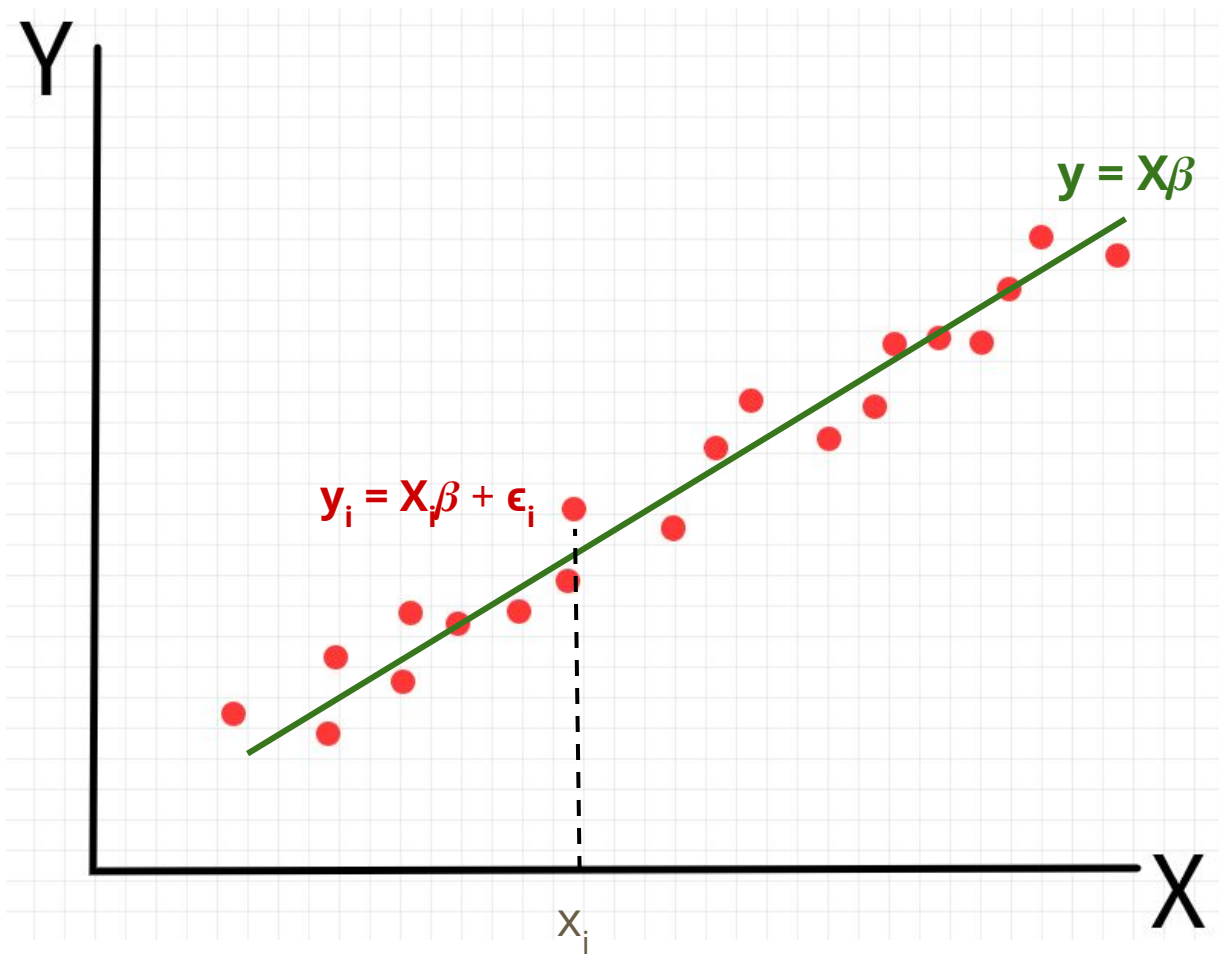


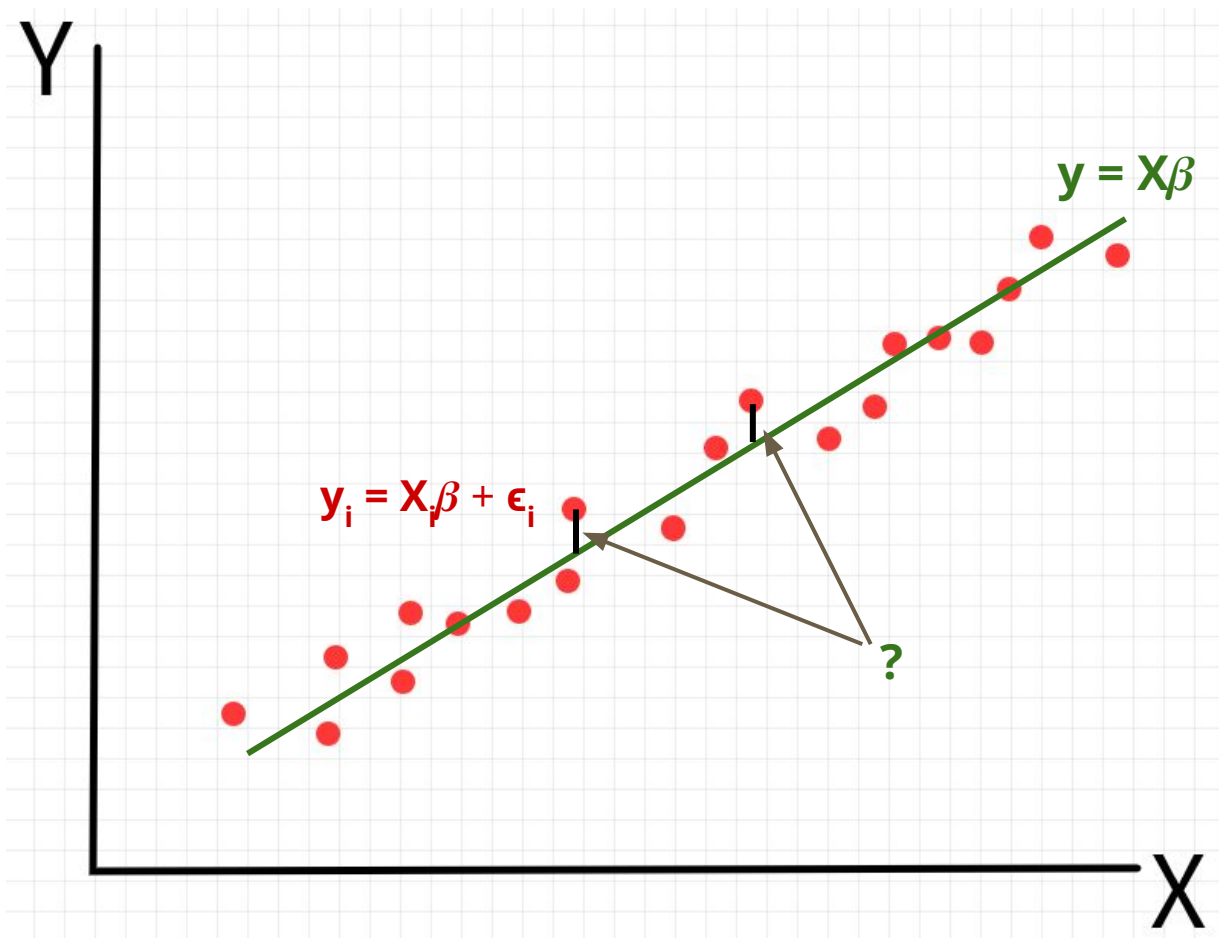
Let's label the diagram

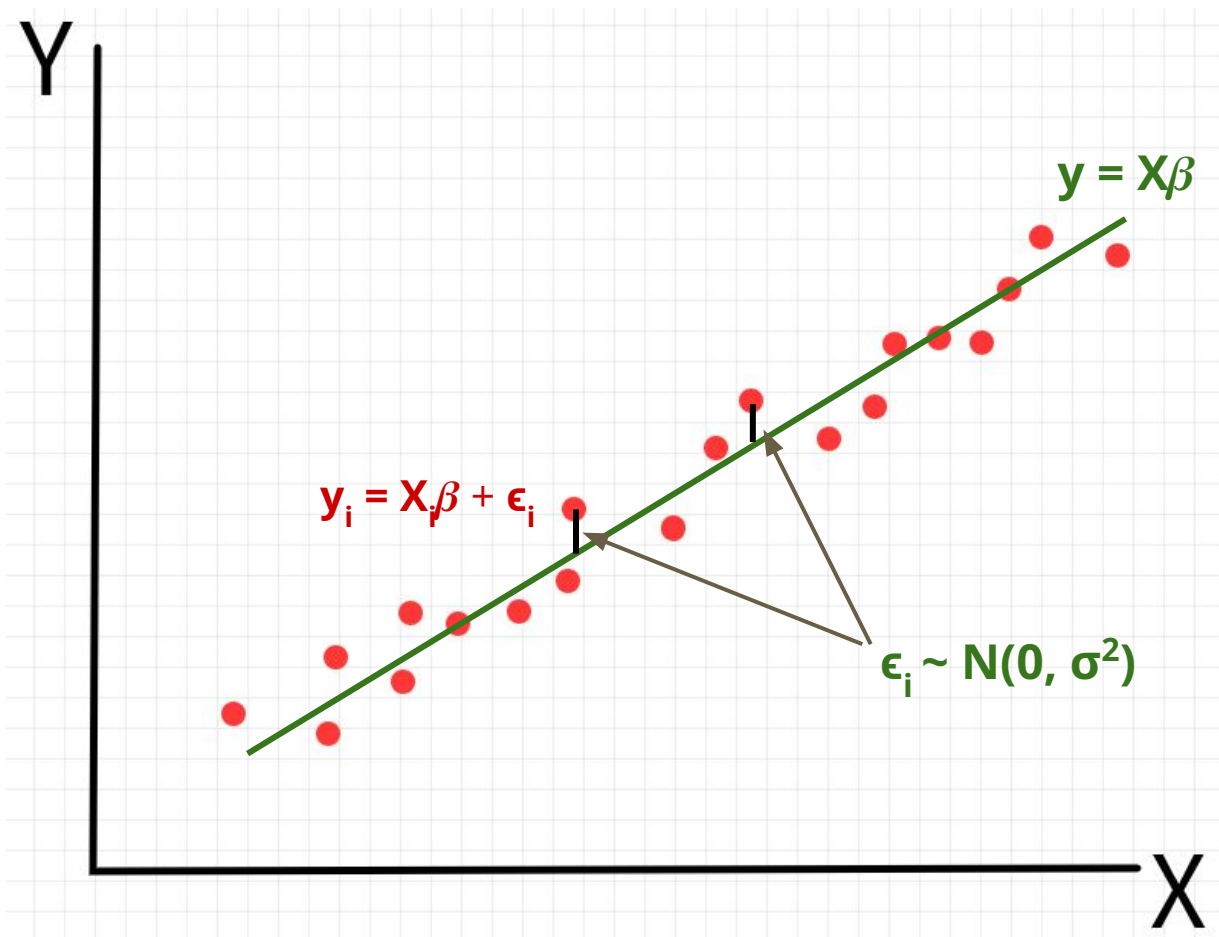


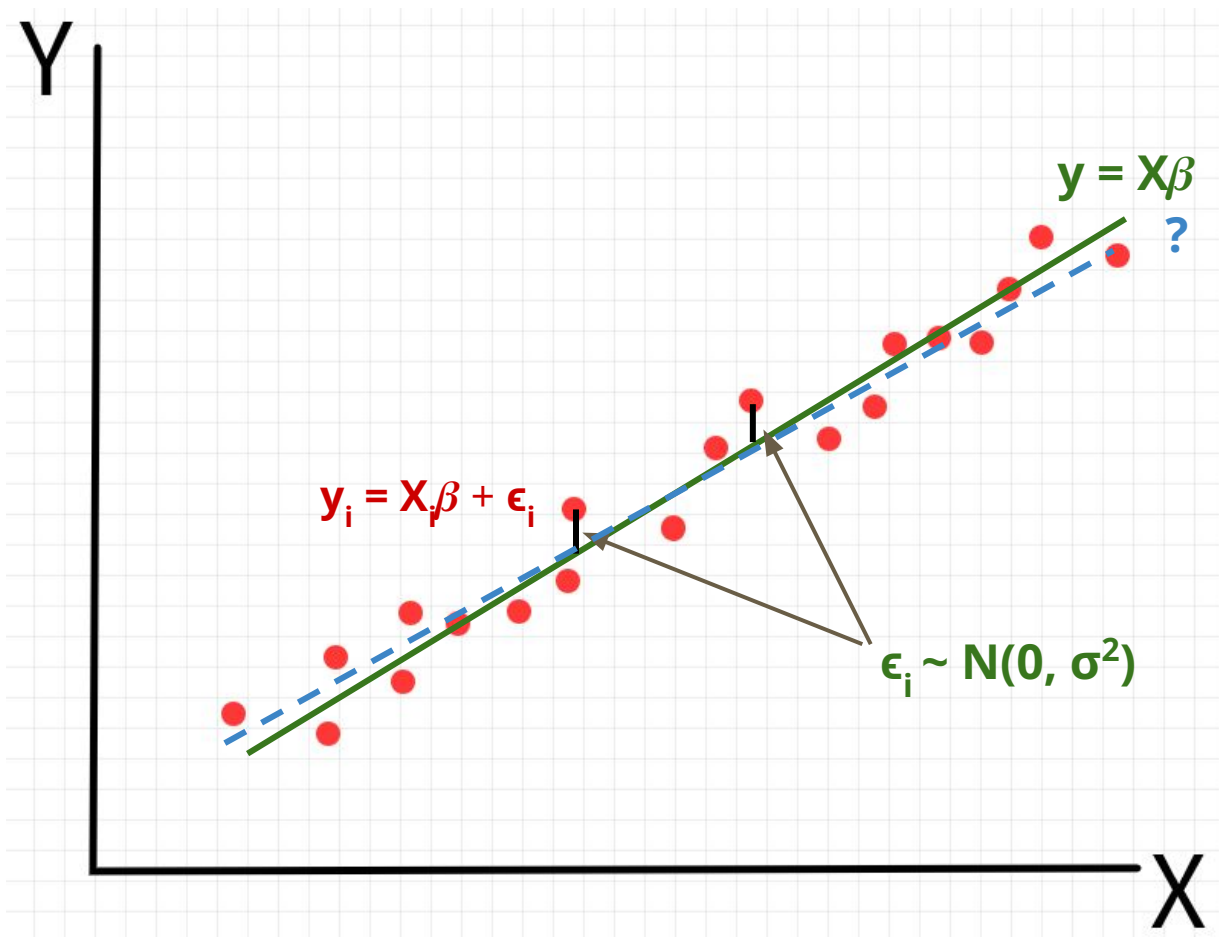


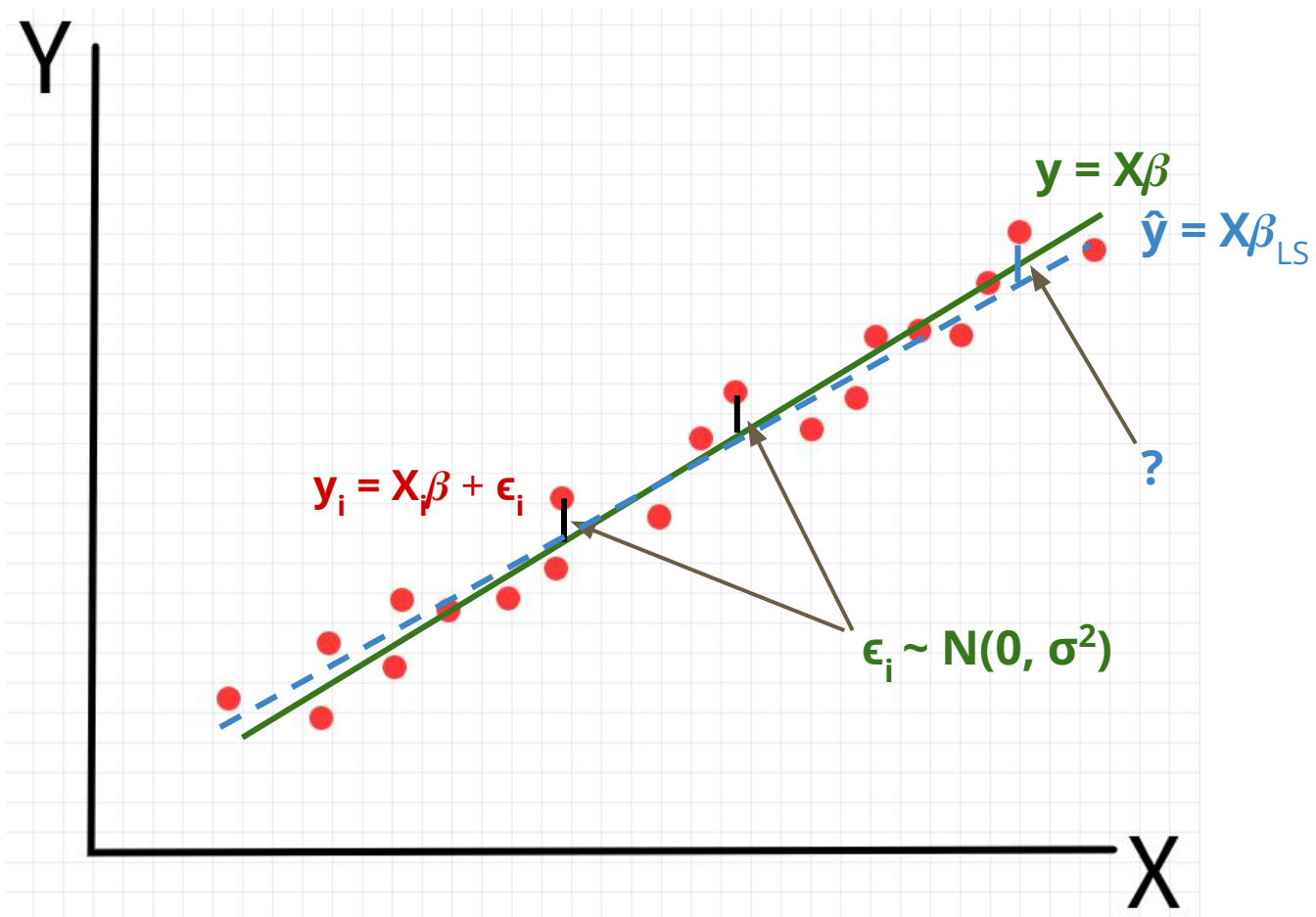


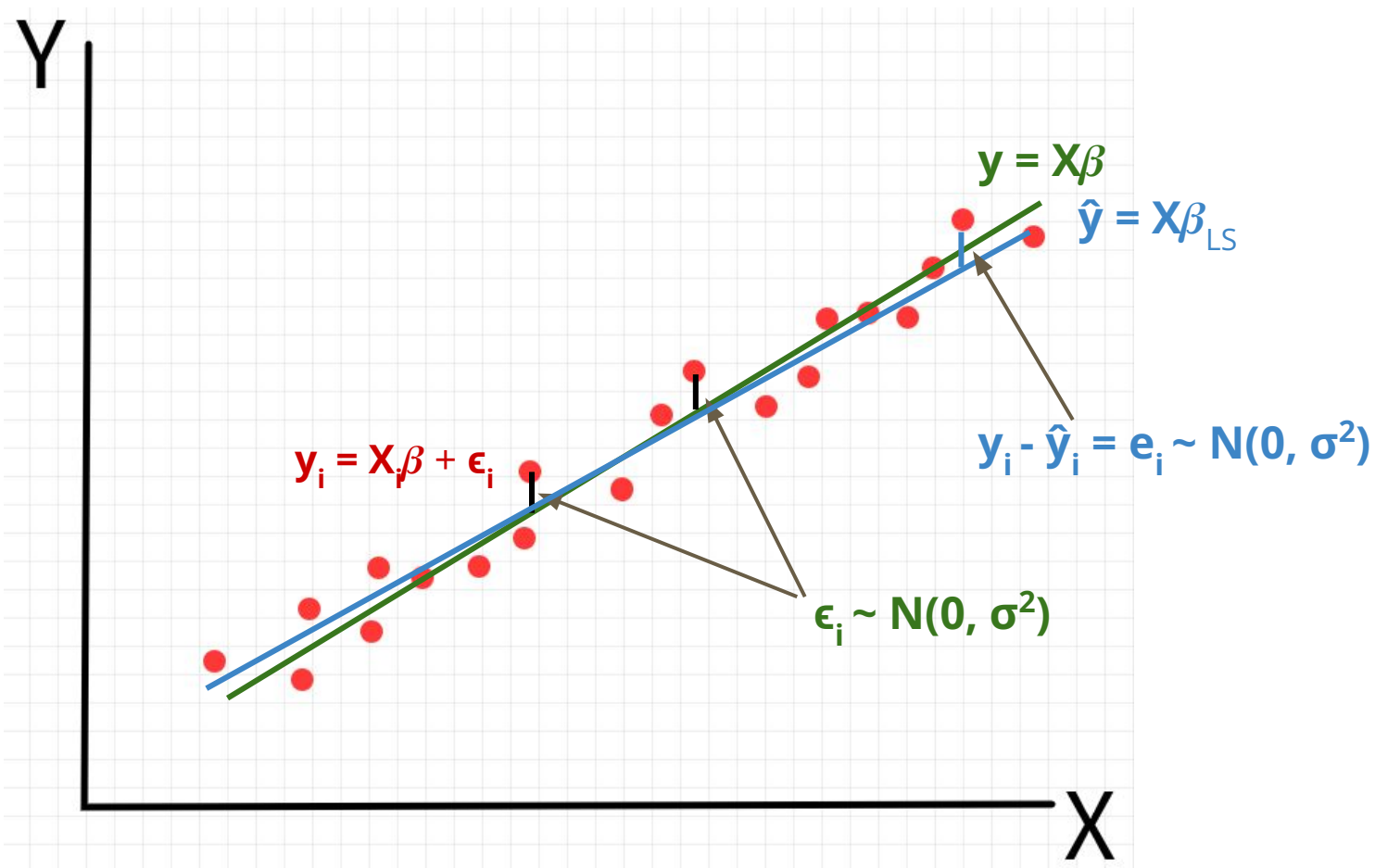


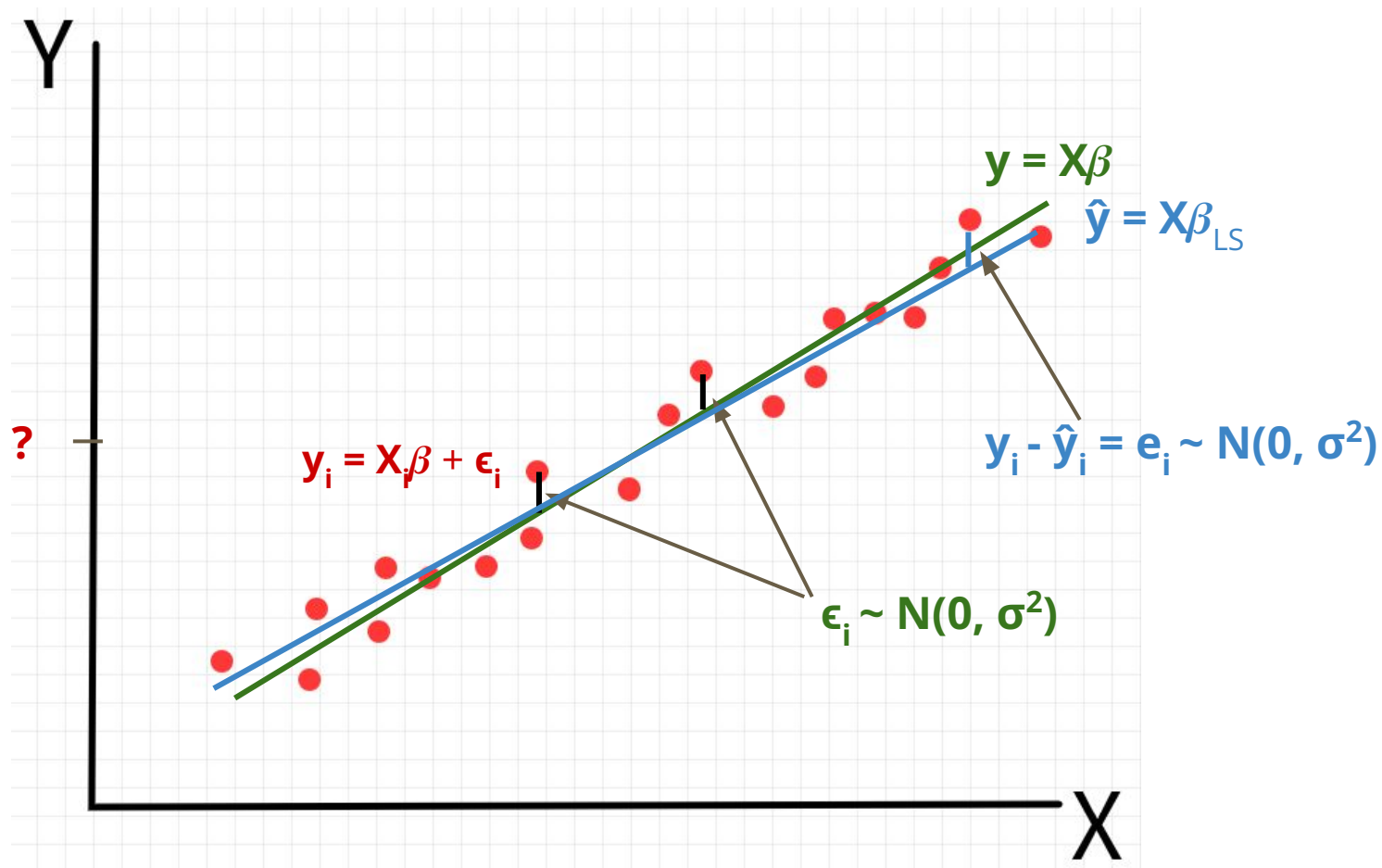


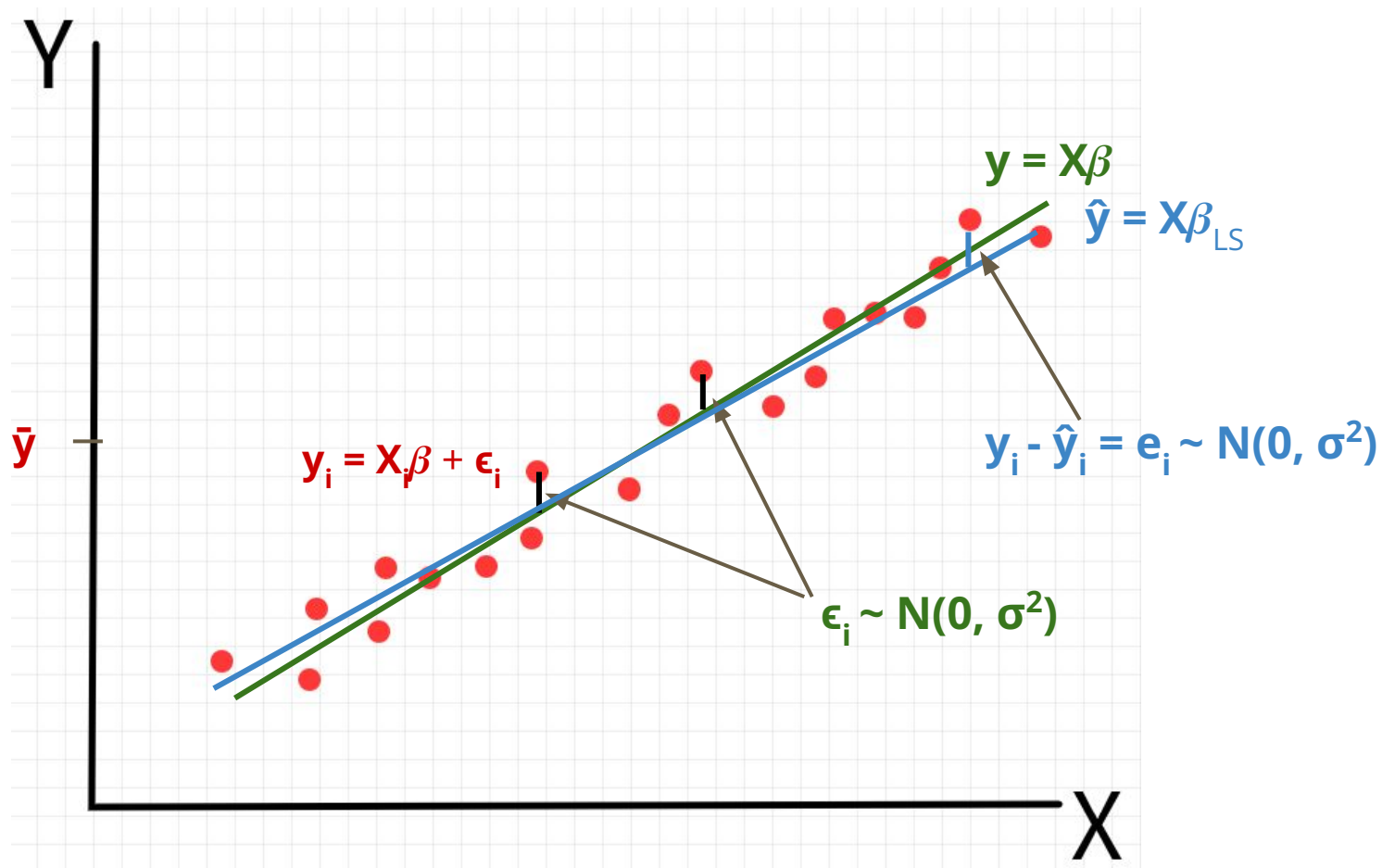


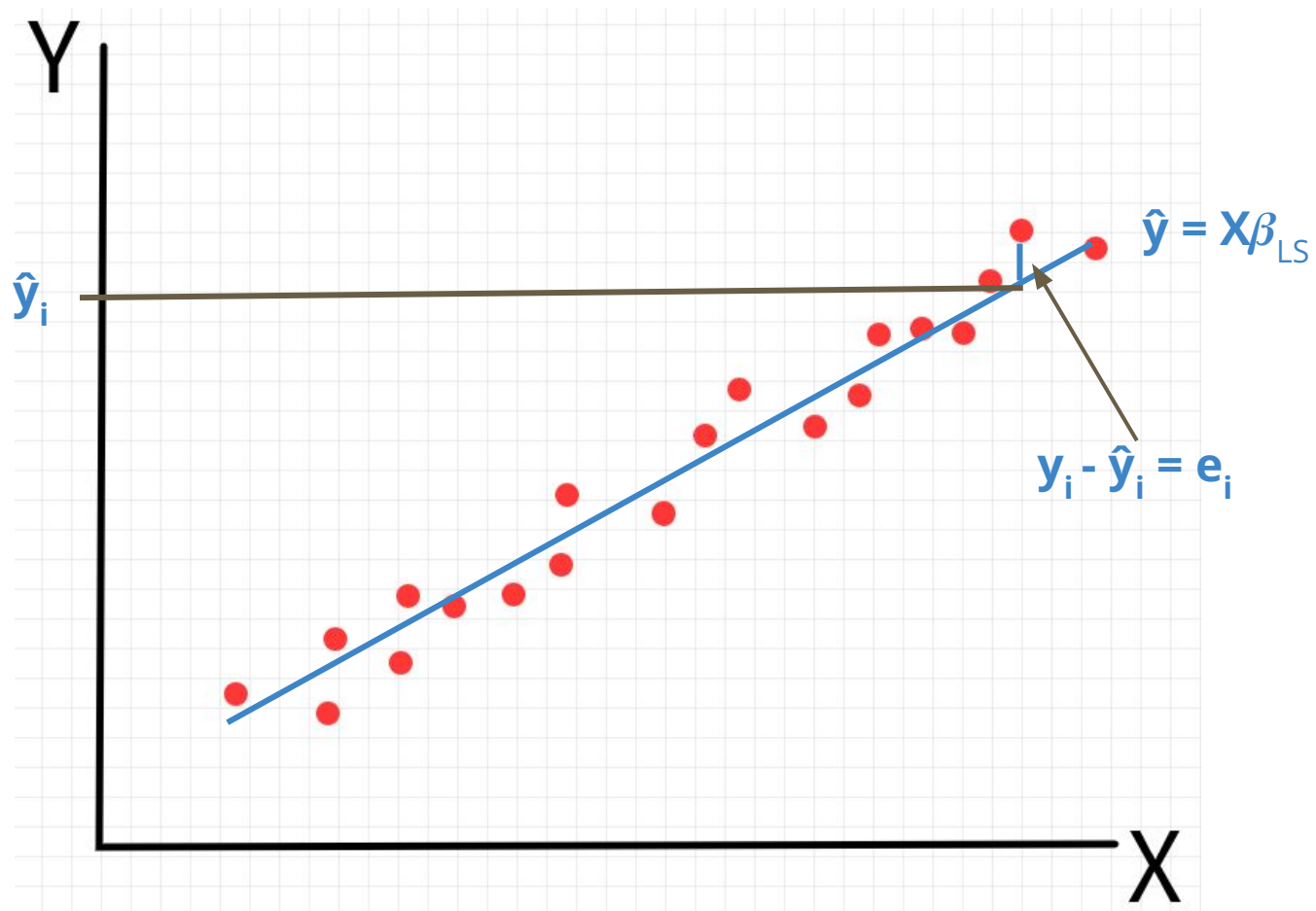












How do we know a linear model is applicable?

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

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Lots of questions secretly hiding in here...

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Lots of questions secretly hiding in here...

1. Is the noise actually normally distributed?

How do we know a linear model is applicable?

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

Lots of questions secretly hiding in here...

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 $\boldsymbol{\epsilon} \sim \mathbf{N}(\mathbf{0}, \sigma^2)$?

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 $\boldsymbol{\epsilon} \sim \mathbf{N}(\mathbf{0}, \sigma^2)$?

If this is true then: $\mathbf{y}_i - \hat{\mathbf{y}}_i = \mathbf{e}_i \sim \mathbf{N}(0, \sigma^2)$

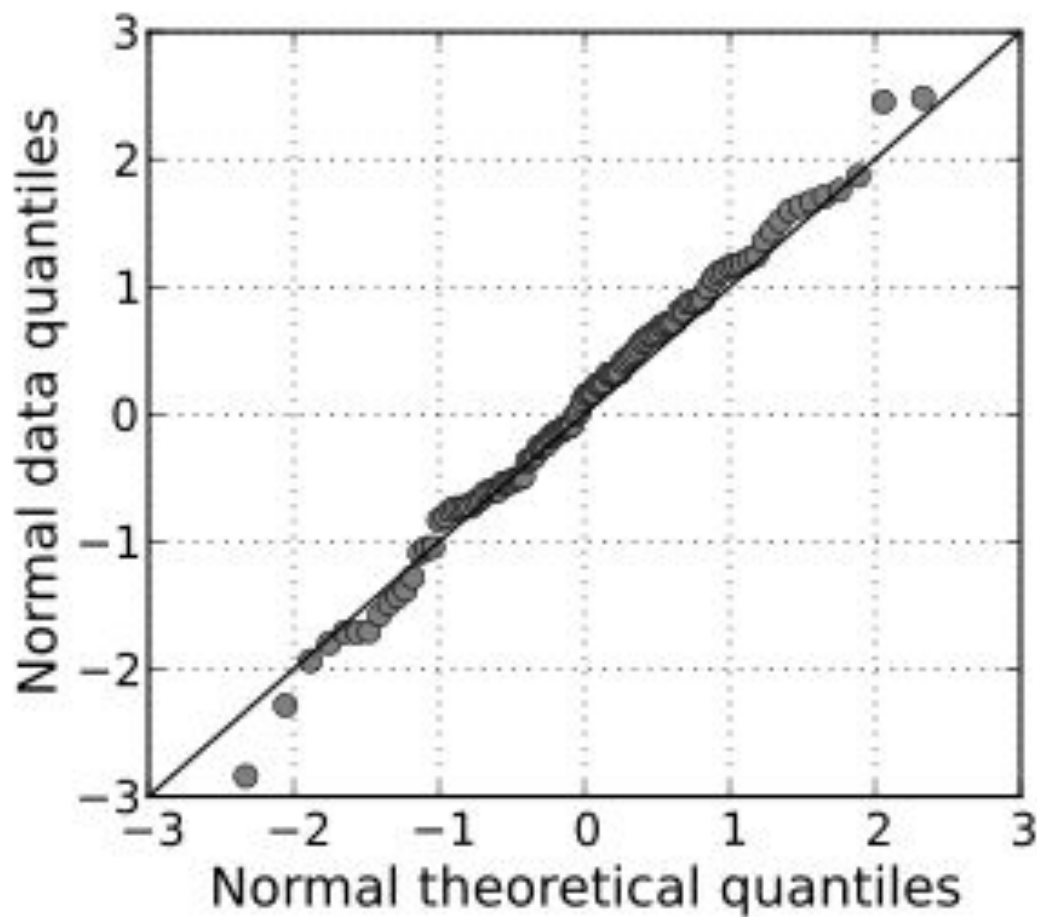
Checking the Normal assumption

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.

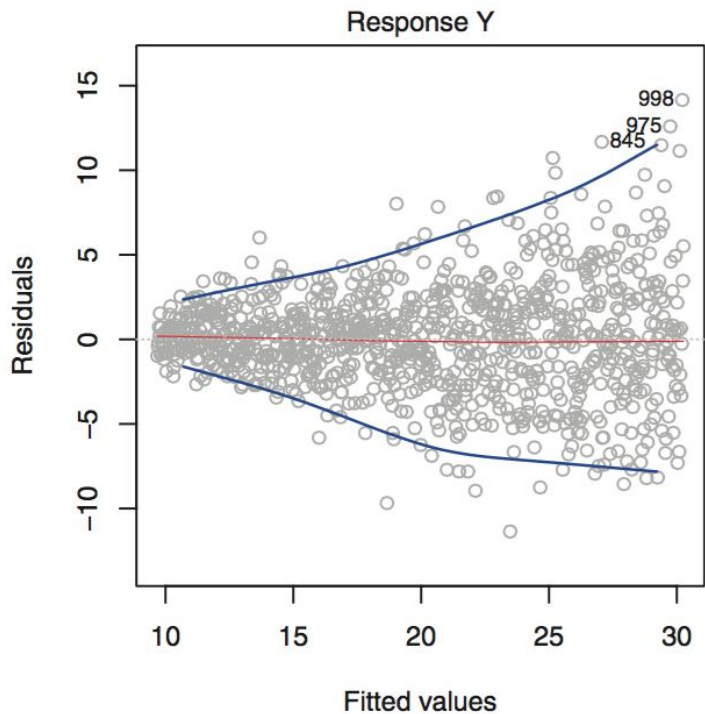
For all quantiles q , if $\text{sample}.q == \text{known_distribution}.q$ then they have the same distribution.

QQ plot



demo

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).

Evaluating Our Regression Model

Some Notation:

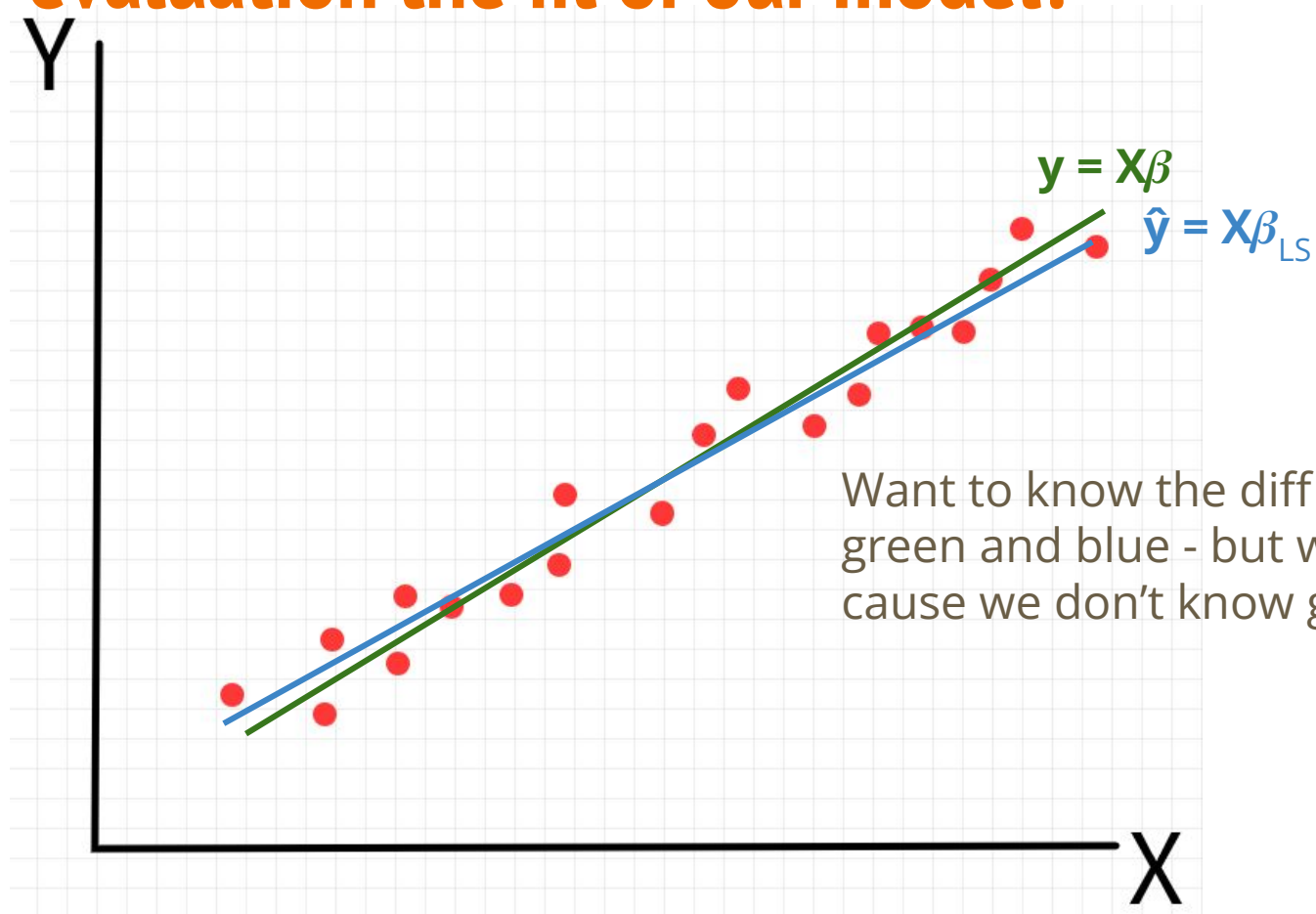
\mathbf{y}_i is the “true” value from our data set (i.e. $\mathbf{x}_i\boldsymbol{\beta} + \boldsymbol{\epsilon}_i$)

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

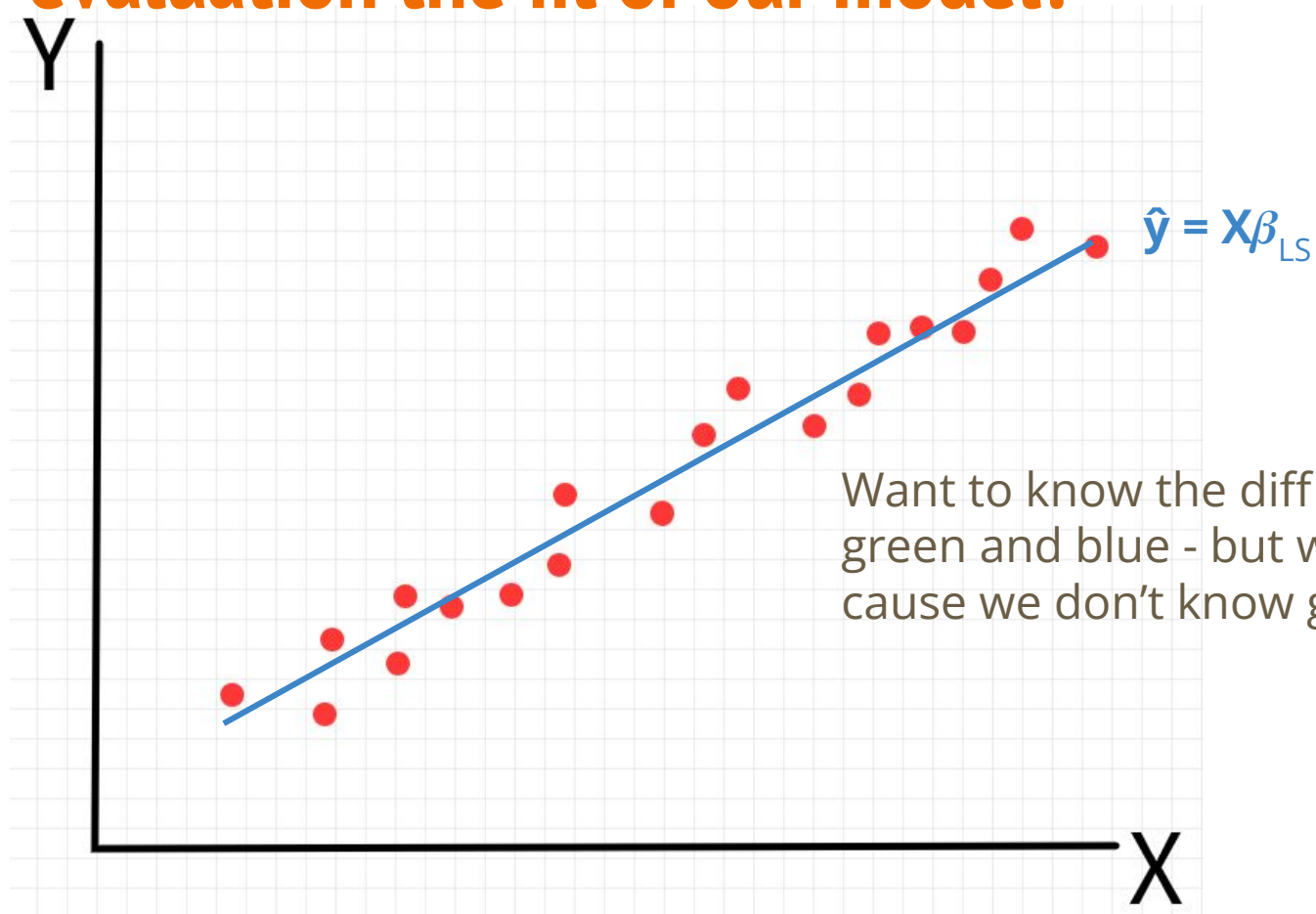
$\bar{\mathbf{y}}$ is the sample mean all \mathbf{y}_i

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

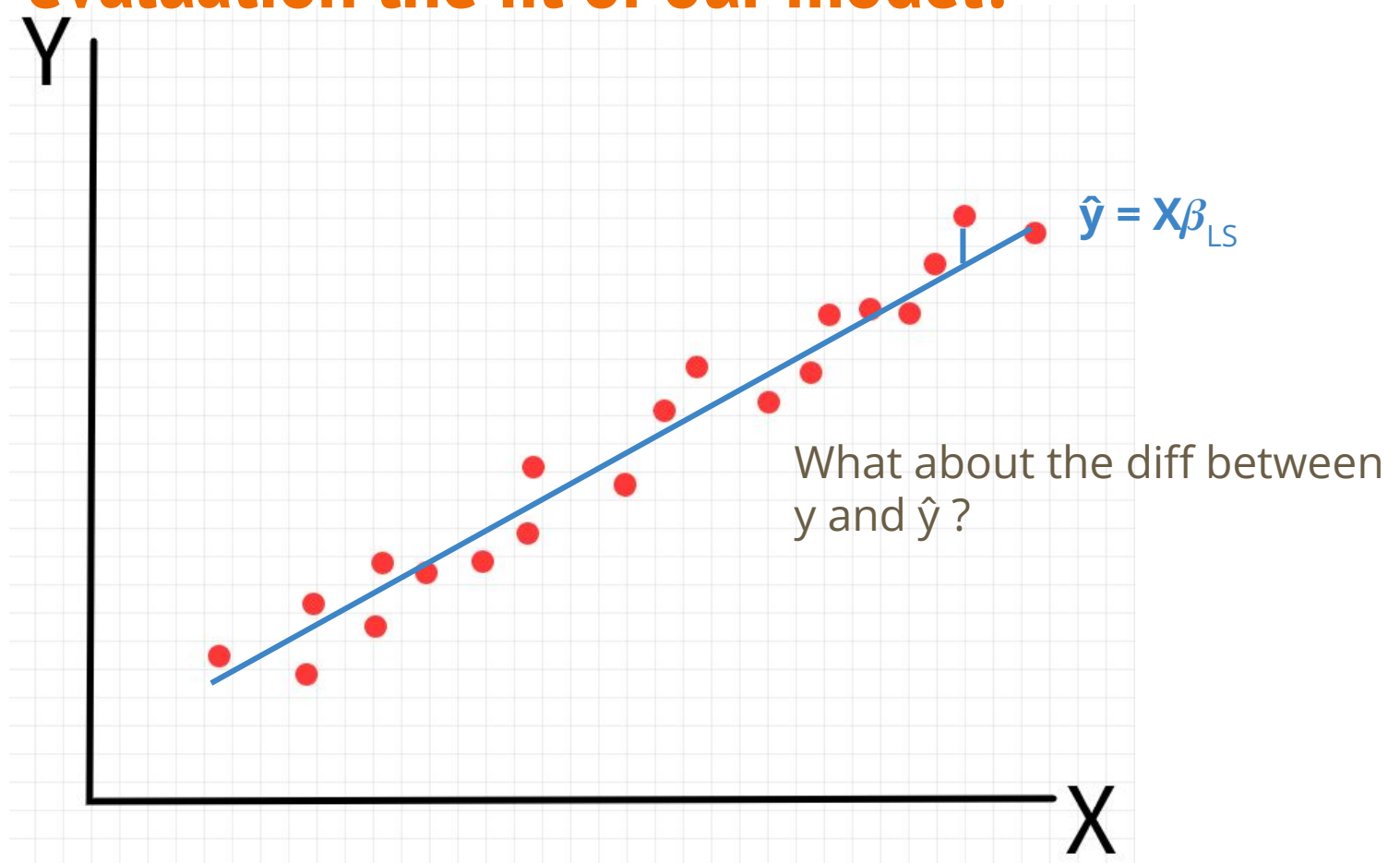
Metric for evaluation the fit of our model?



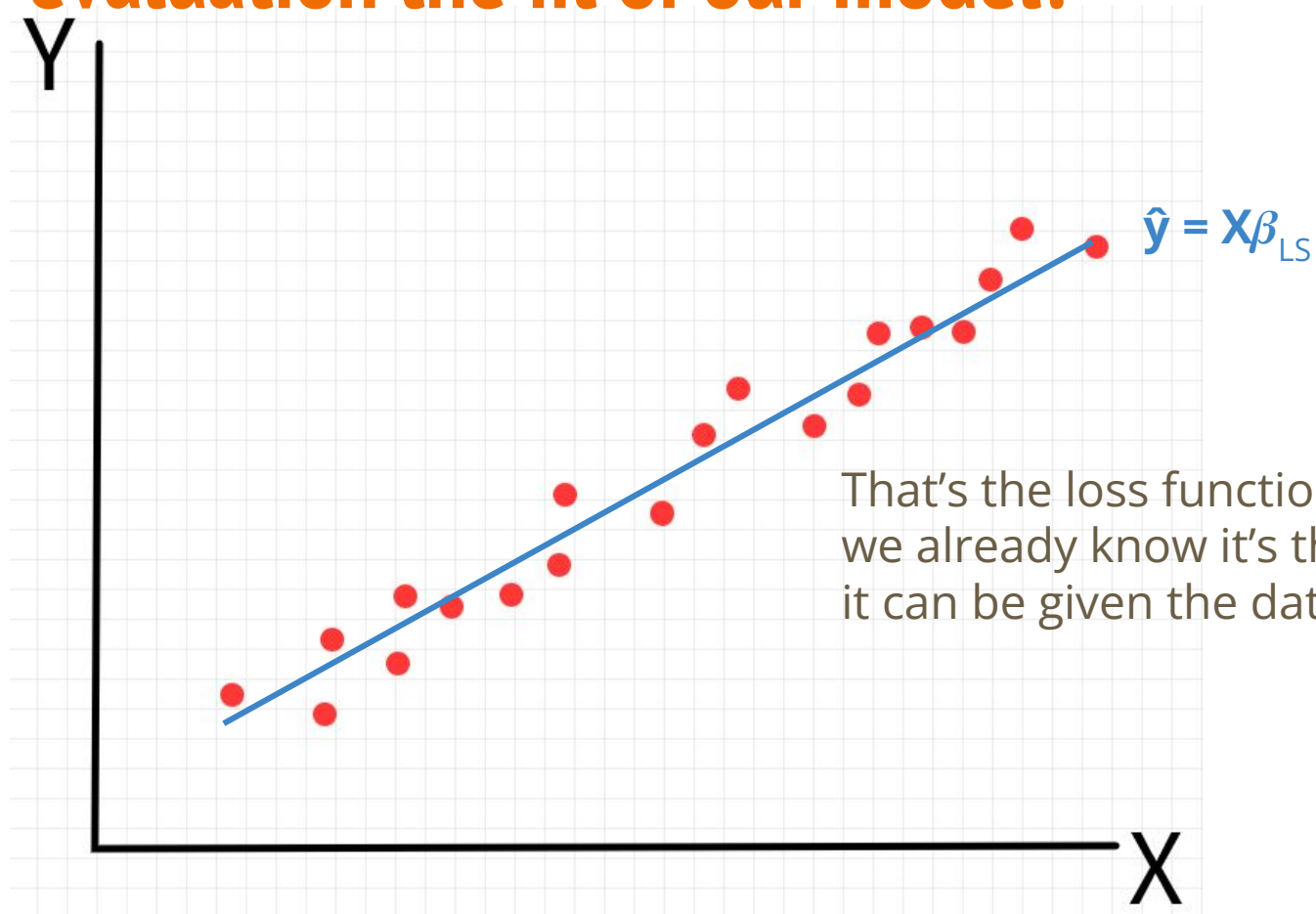
Metric for evaluation the fit of our model?



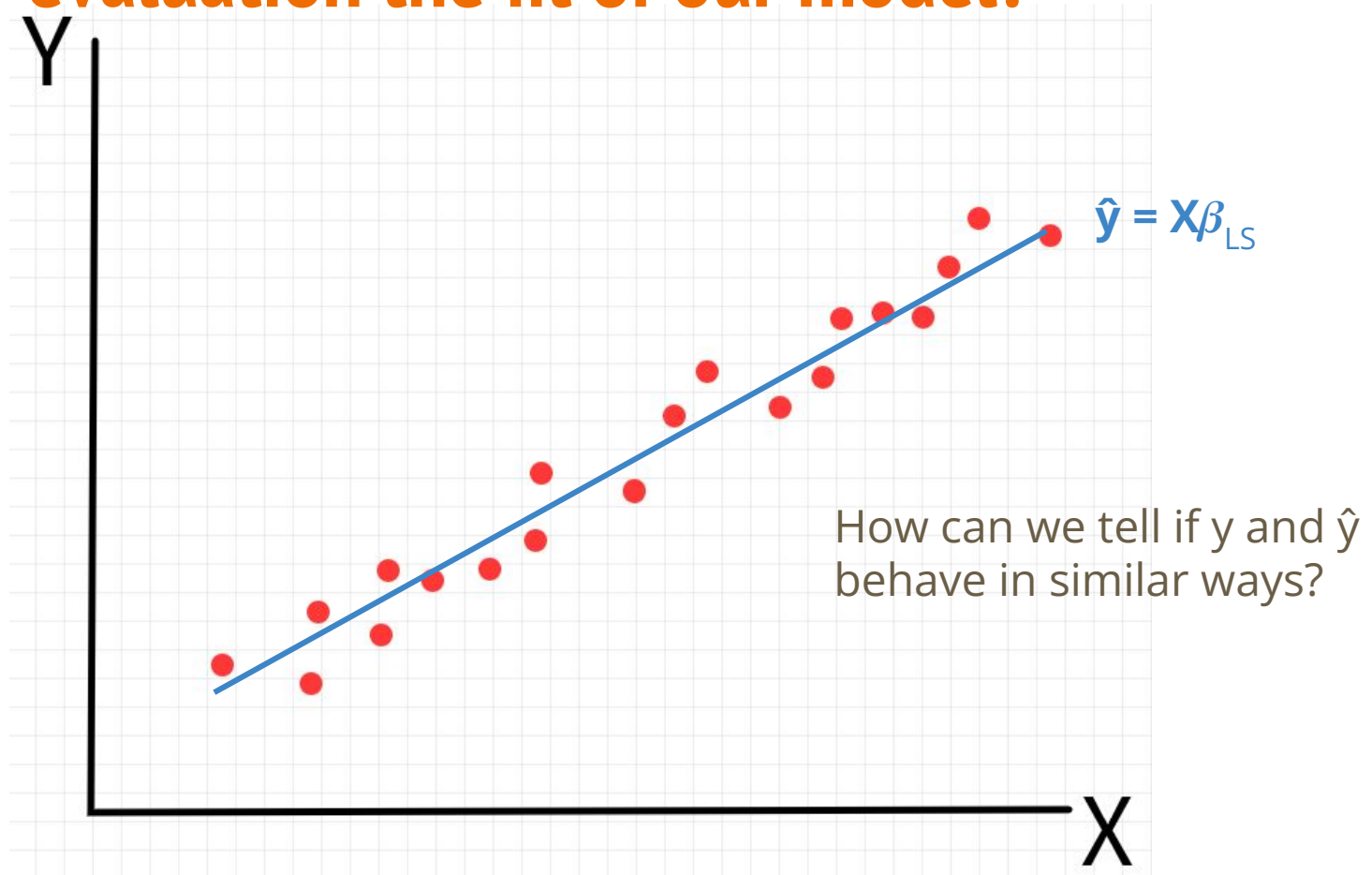
Metric for evaluation the fit of our model?



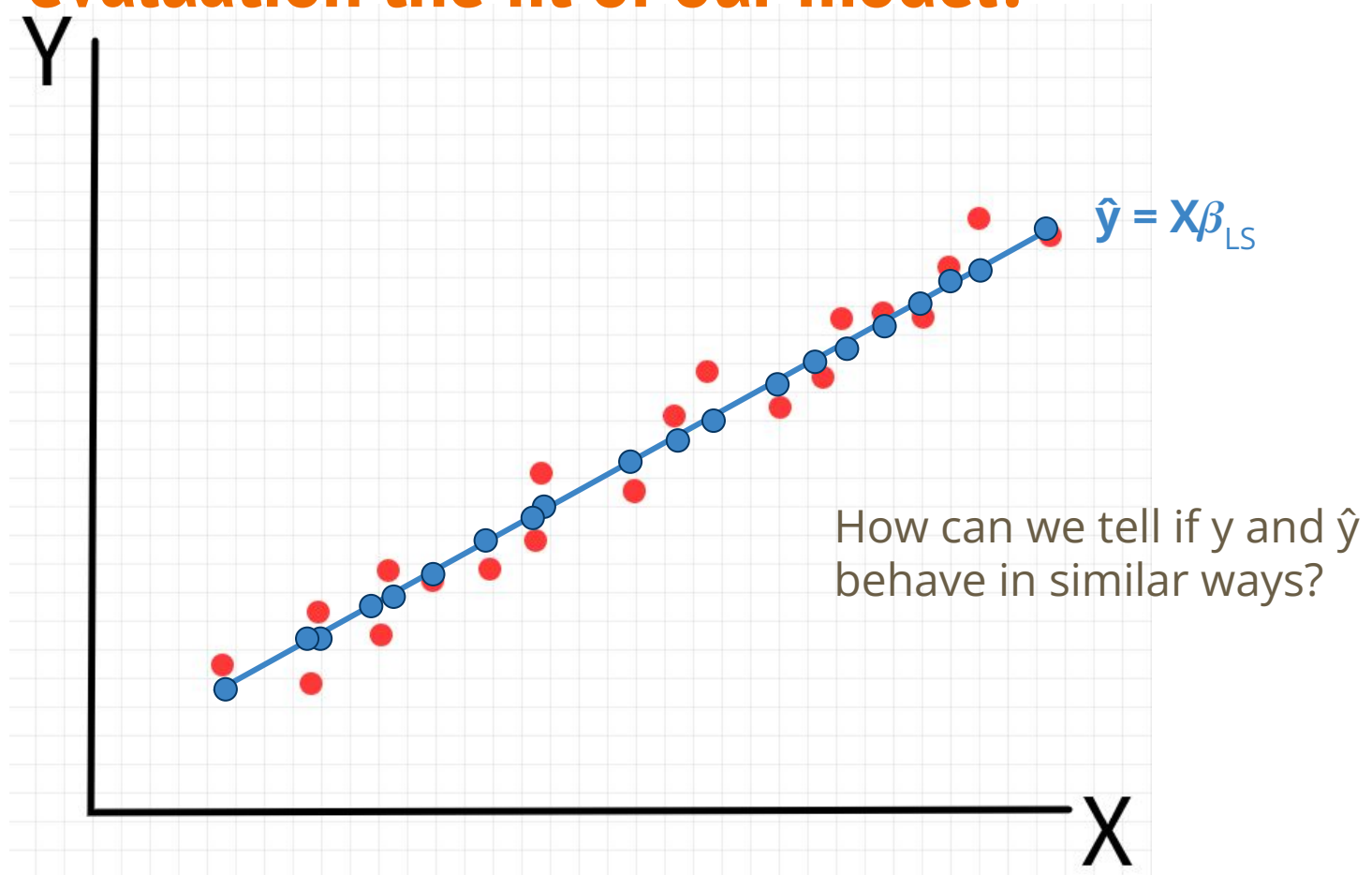
Metric for evaluation the fit of our model?



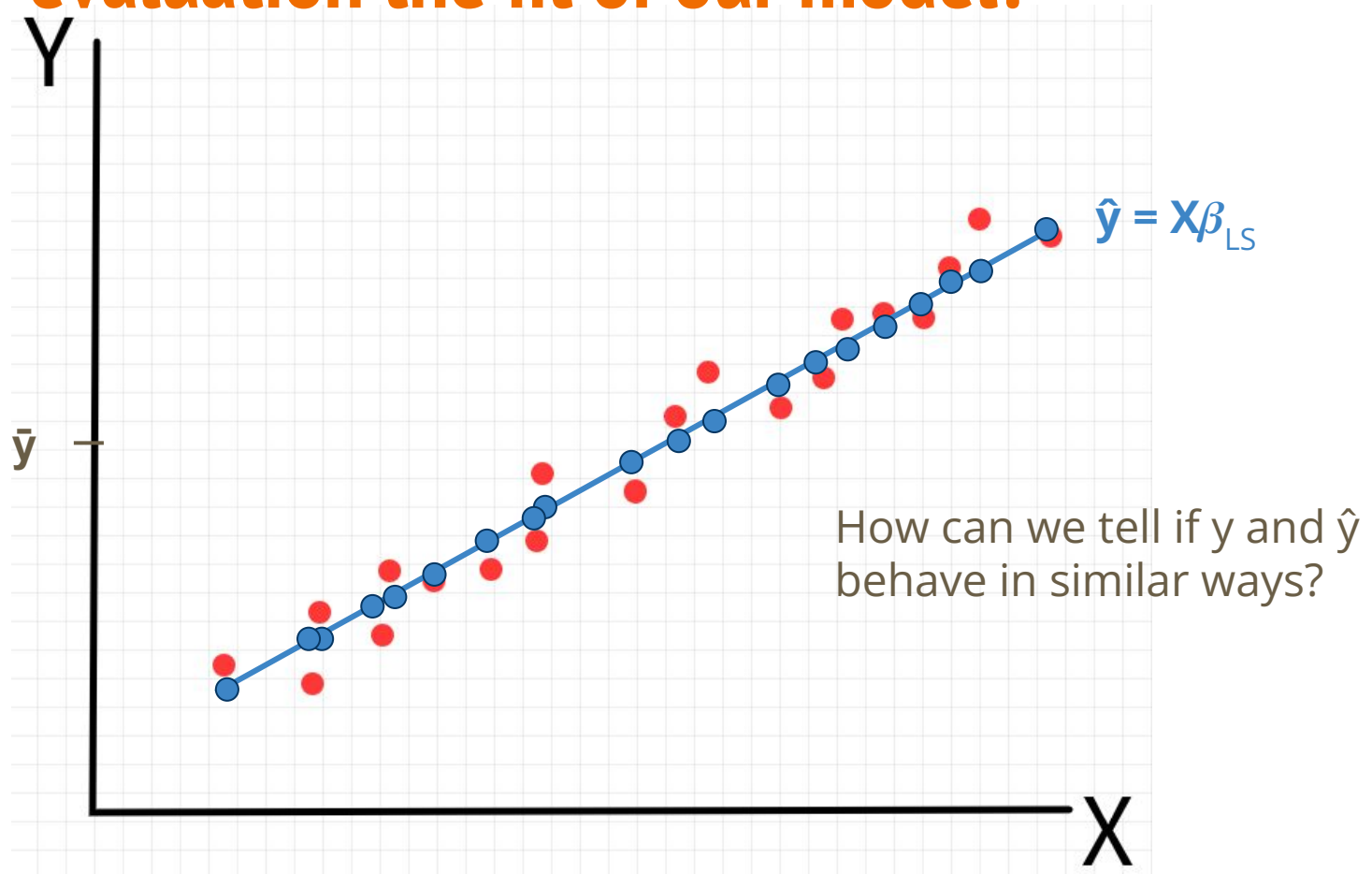
Metric for evaluation the fit of our model?



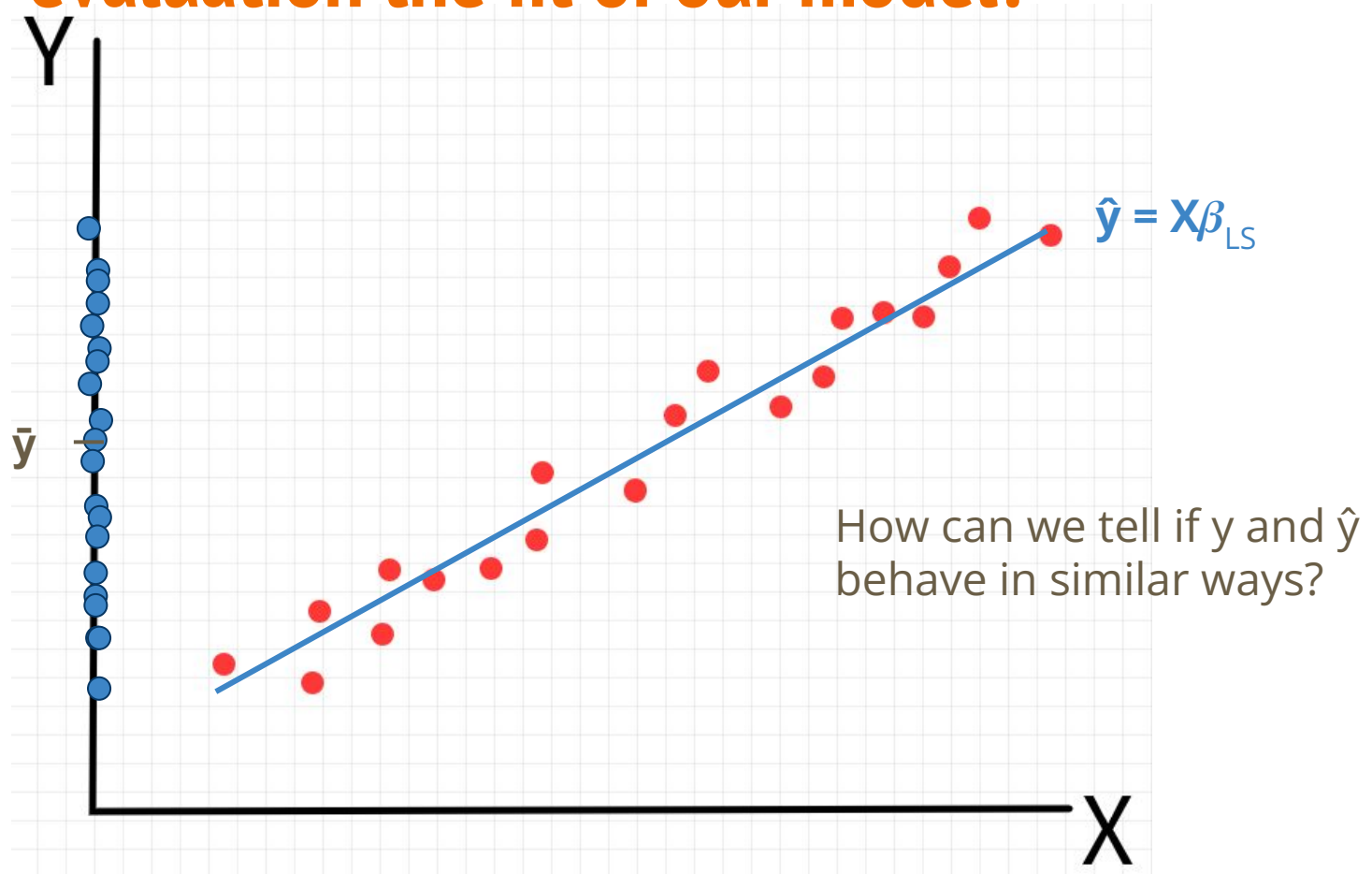
Metric for evaluation the fit of our model?



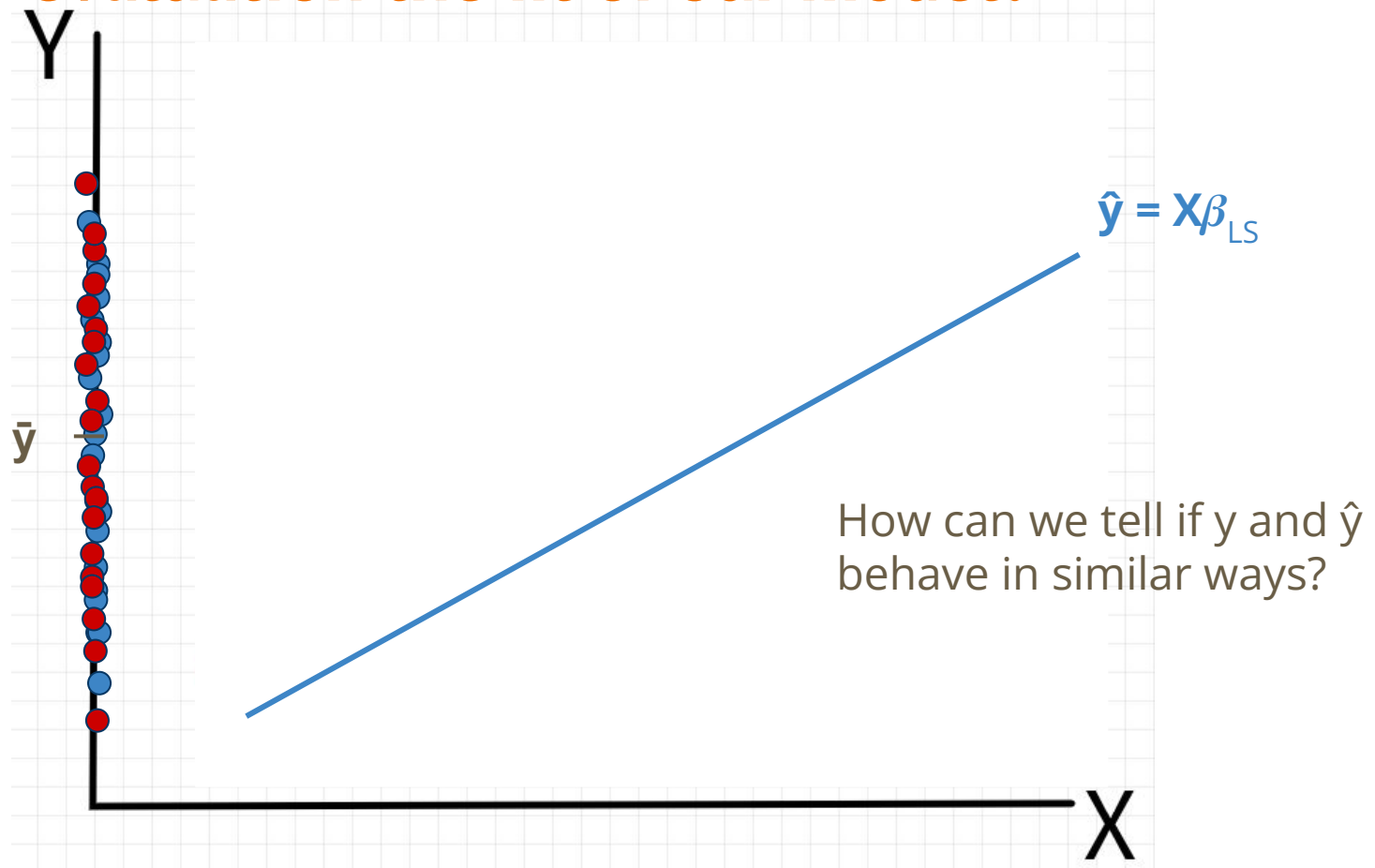
Metric for evaluation the fit of our model?



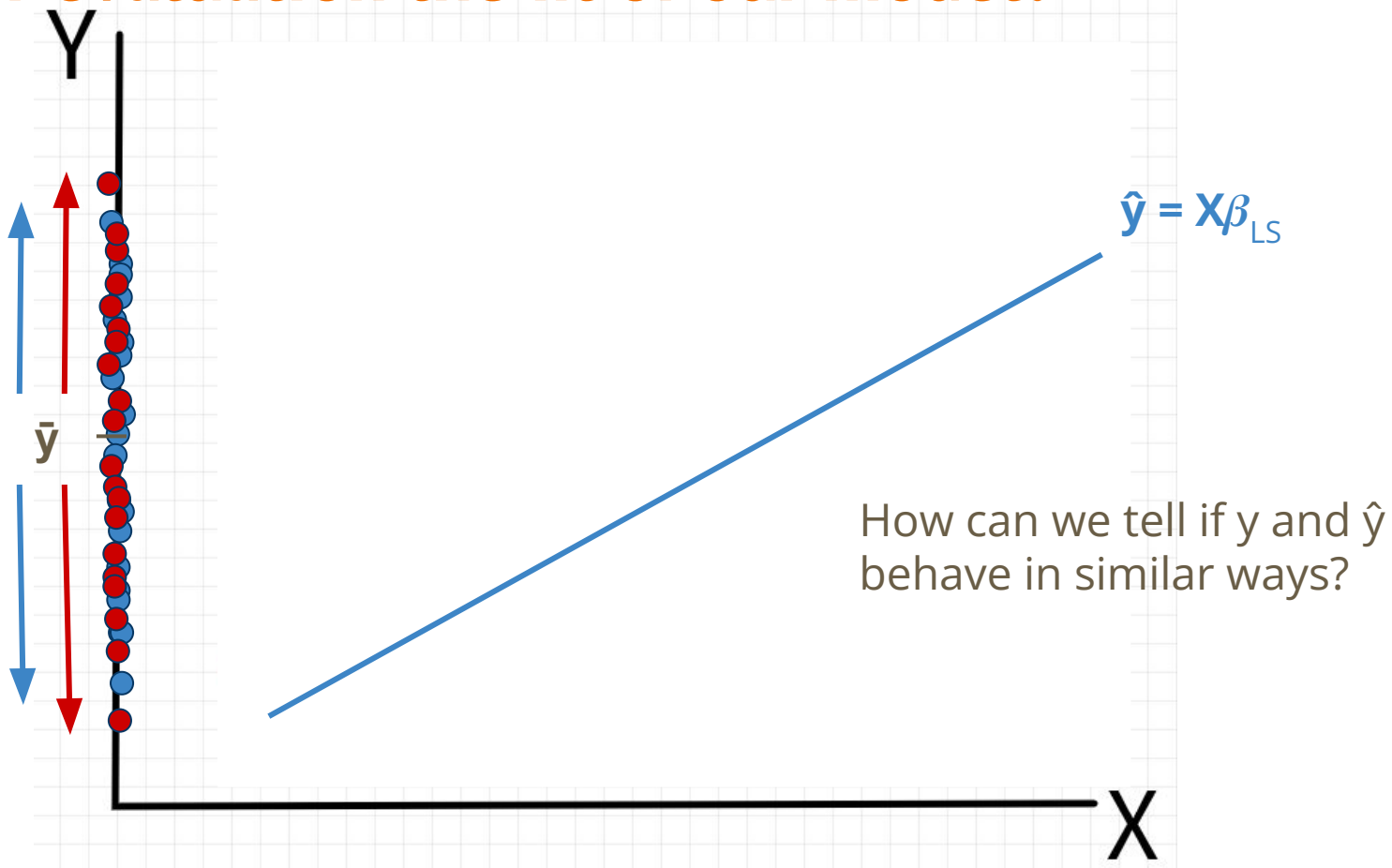
Metric for evaluation the fit of our model?



Metric for evaluation the fit of our model?



Metric for evaluation the fit of our model?



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

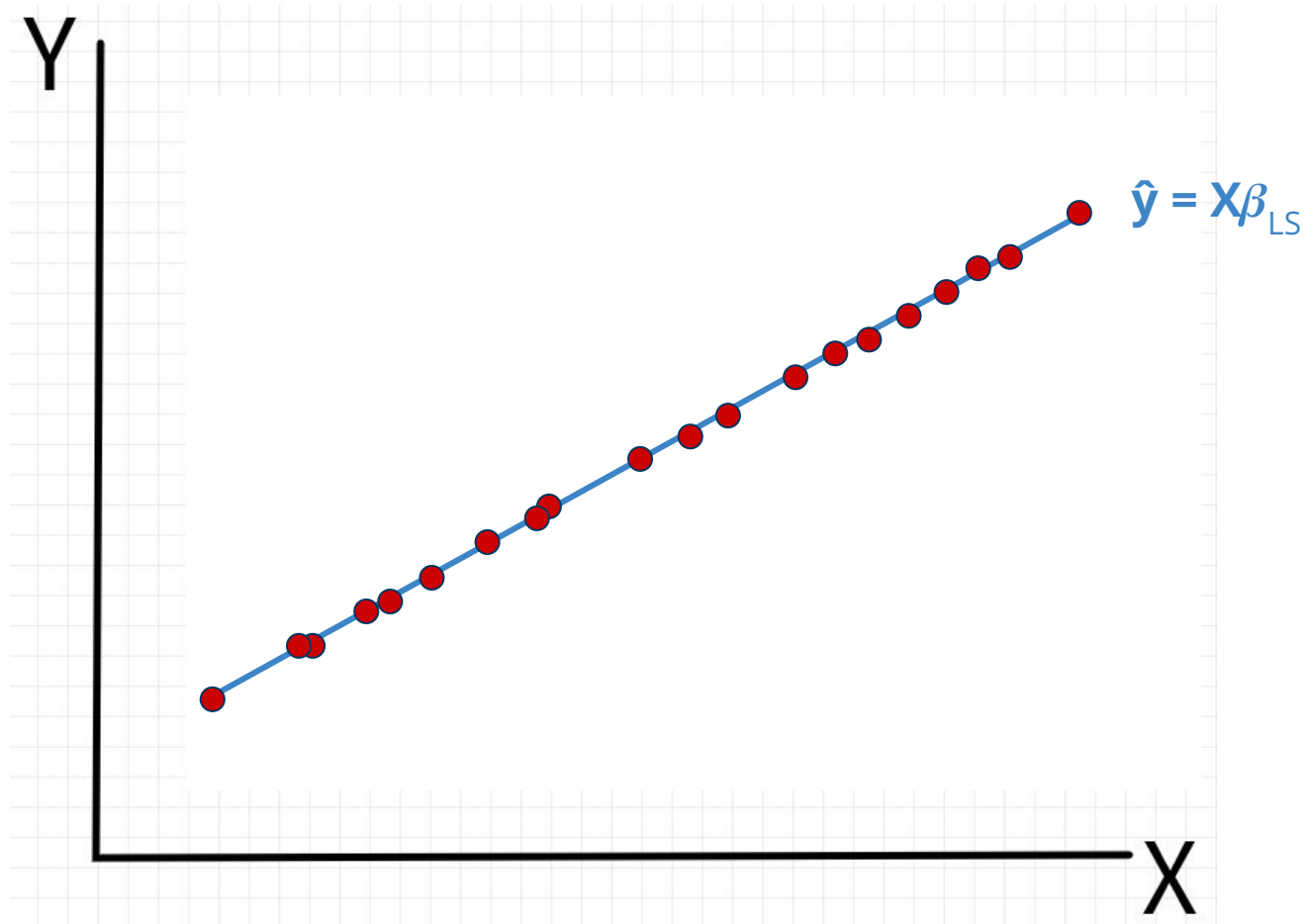
$$TSS = \sum_i^n (y_i - \bar{y})^2$$

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

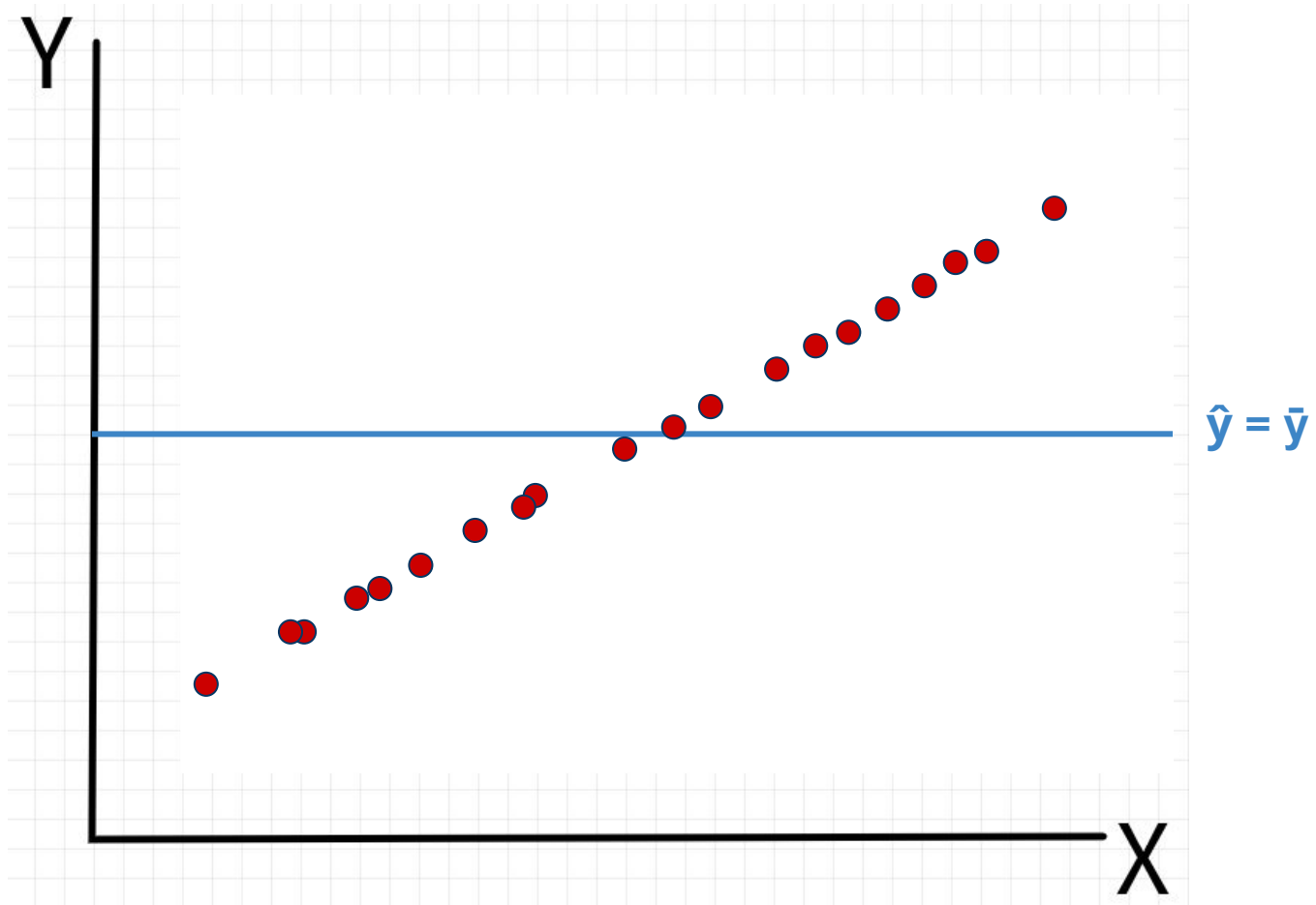
$$ESS = \sum_i^n (\hat{y}_i - \bar{y})^2$$

R^2 measures the fraction of variance that is explained by \hat{y} (our model)

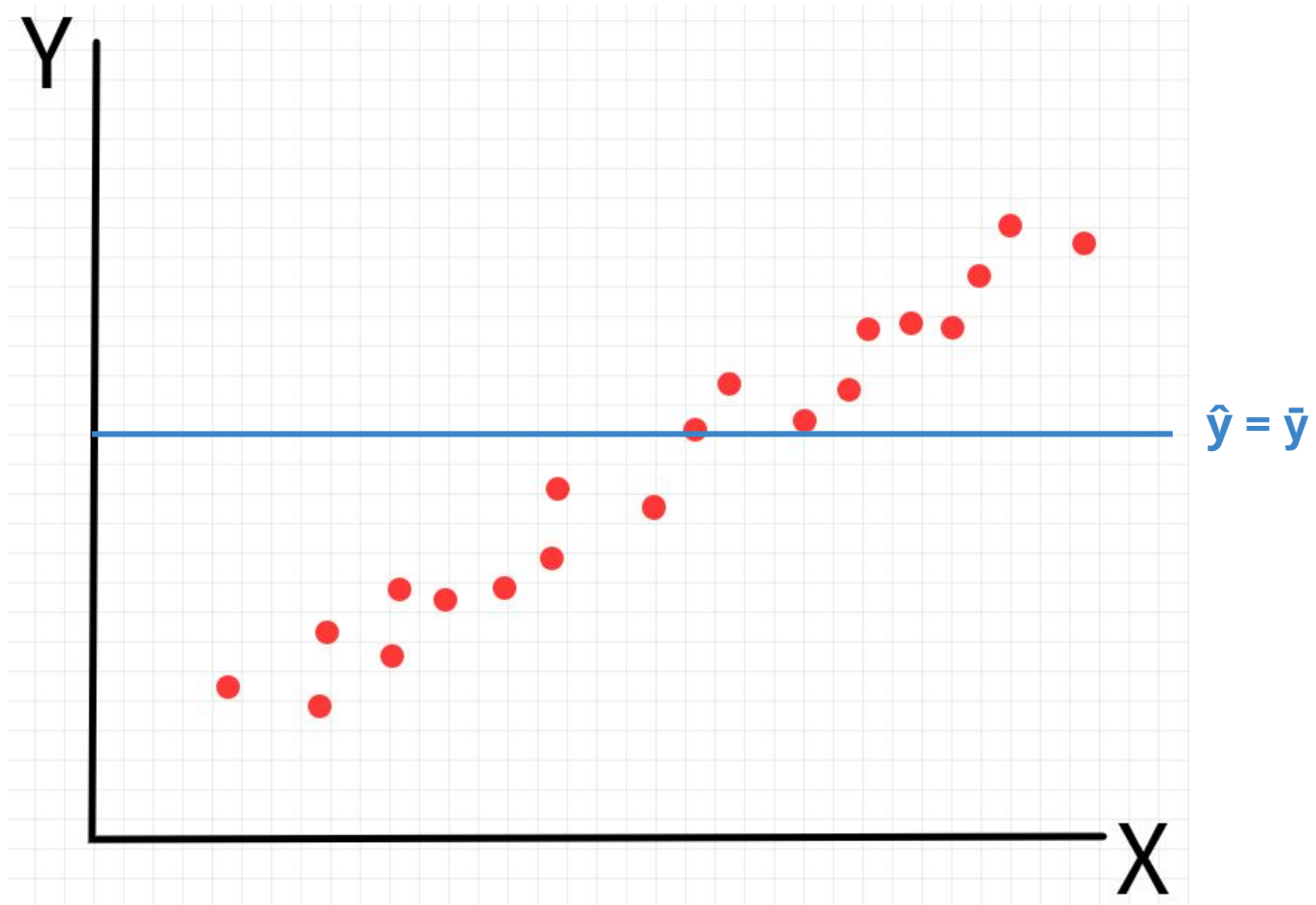
$$R^2 = 1$$



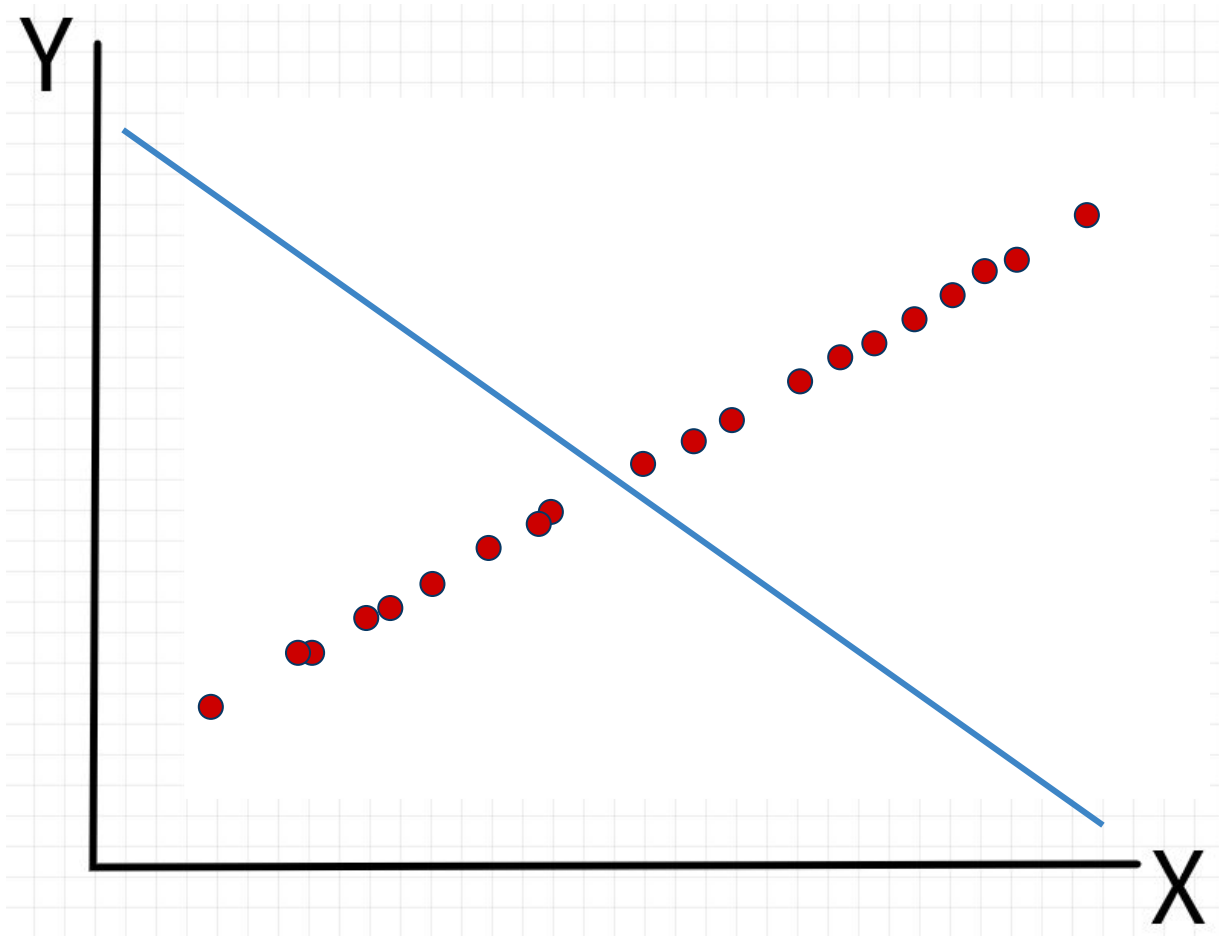
$$R^2 = 0$$



$$R^2 = 0$$



$$R^2 = 1$$



Standard R^2 formula for a linear model

$$TSS = \sum_i^n (y_i - \bar{y})^2 \qquad R^2 = \frac{ESS}{TSS} = 1 - \frac{RSS}{TSS}$$

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

← 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



Proof

That $TSS = ESS + RSS$

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

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

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

$$= ESS + RSS + 2 \sum_i (y_i - \hat{y}_i)(\hat{y}_i - \bar{y}).$$

$$\sum_i (y_i - \hat{y}_i)(\hat{y}_i - \bar{y}) = \sum_i (y_i - \hat{y}_i)\hat{y}_i - \bar{y} \sum_i (y_i - \hat{y}_i)$$

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

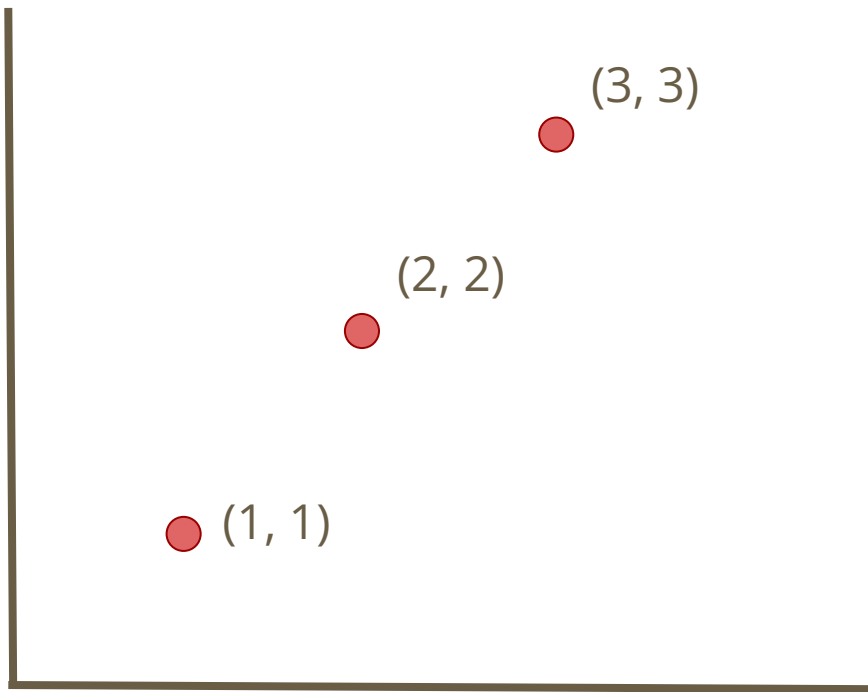
Assume for simplicity that $\hat{y}_i = \beta_0 + \beta_1 x_i$
Since β_0 and β_1 are least squares estimates, we know they minimize

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

By taking derivatives of the above with respect to β_0 and β_1 we discover that

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

Why this new formula is standard

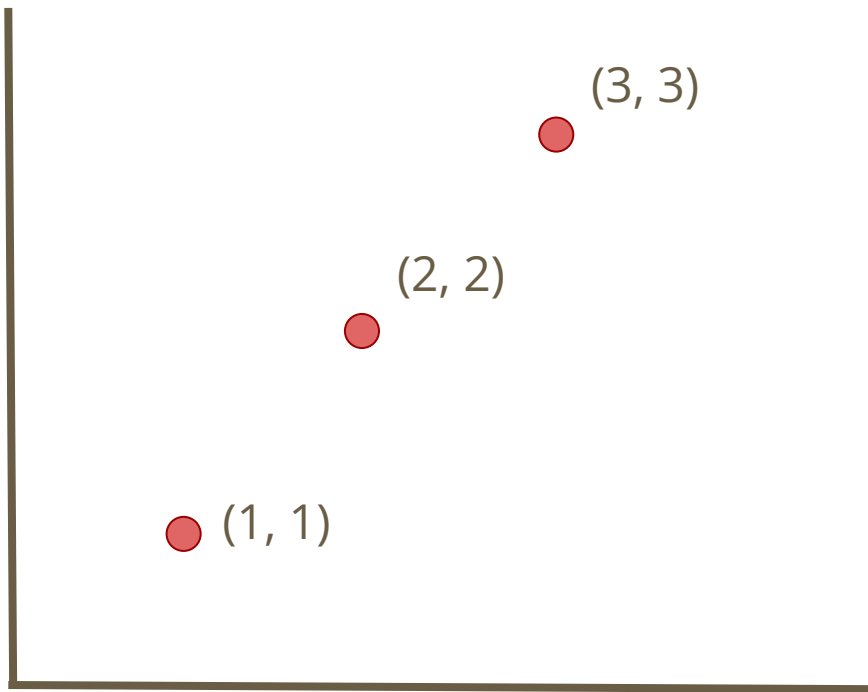


Why this new formula is standard

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

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

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



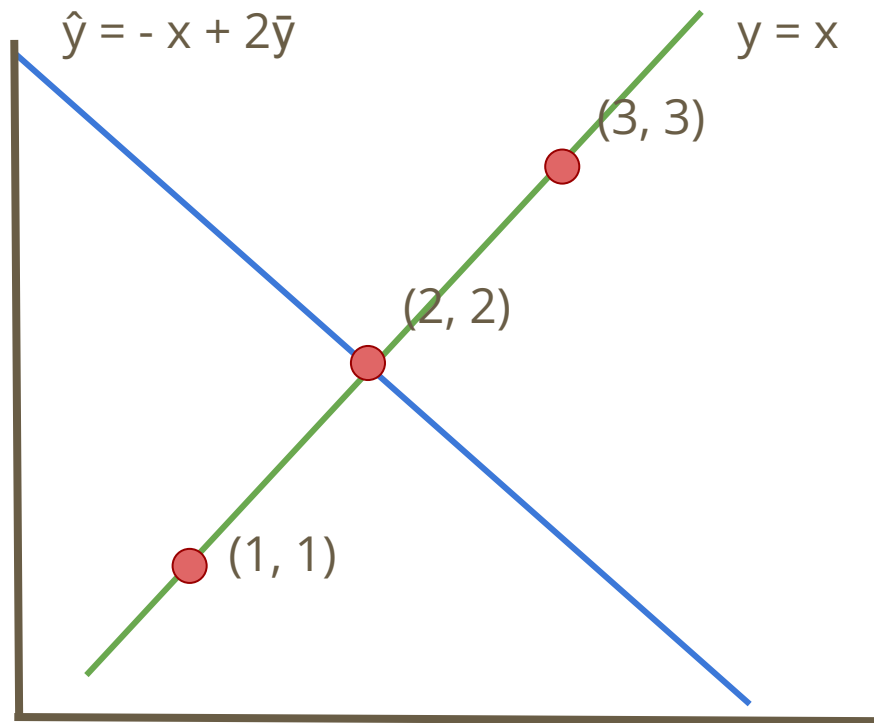
$$R^2 = \frac{ESS}{TSS}$$

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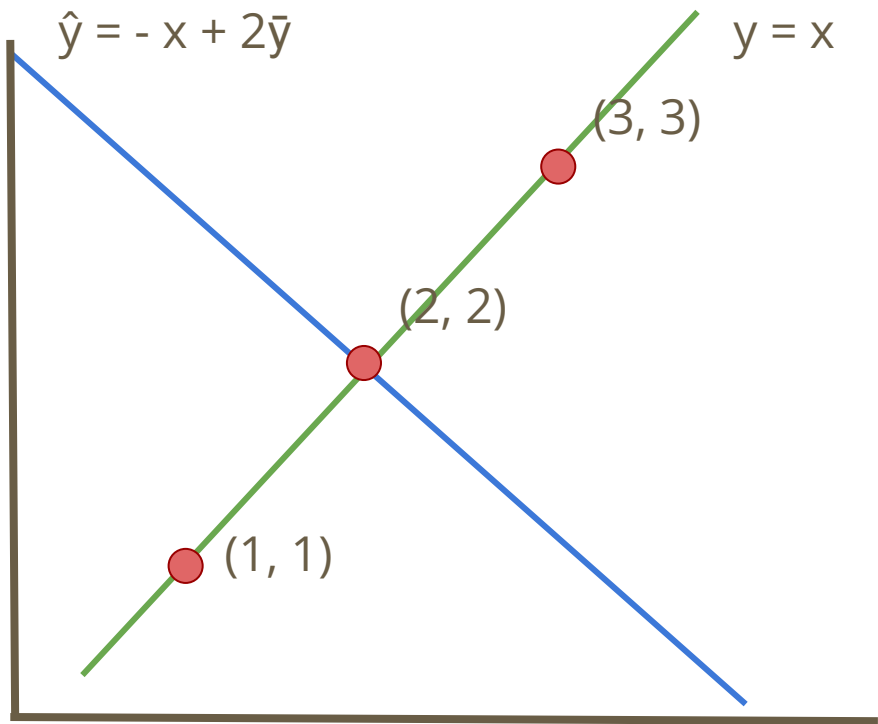
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$$\begin{aligned} (\hat{y} - \bar{y})^2 &= (-x + 2\bar{y} - \bar{y})^2 \\ &= (-x + \bar{y})^2 \\ &= (-(y - \bar{y}))^2 \\ &= (y - \bar{y})^2 \end{aligned}$$

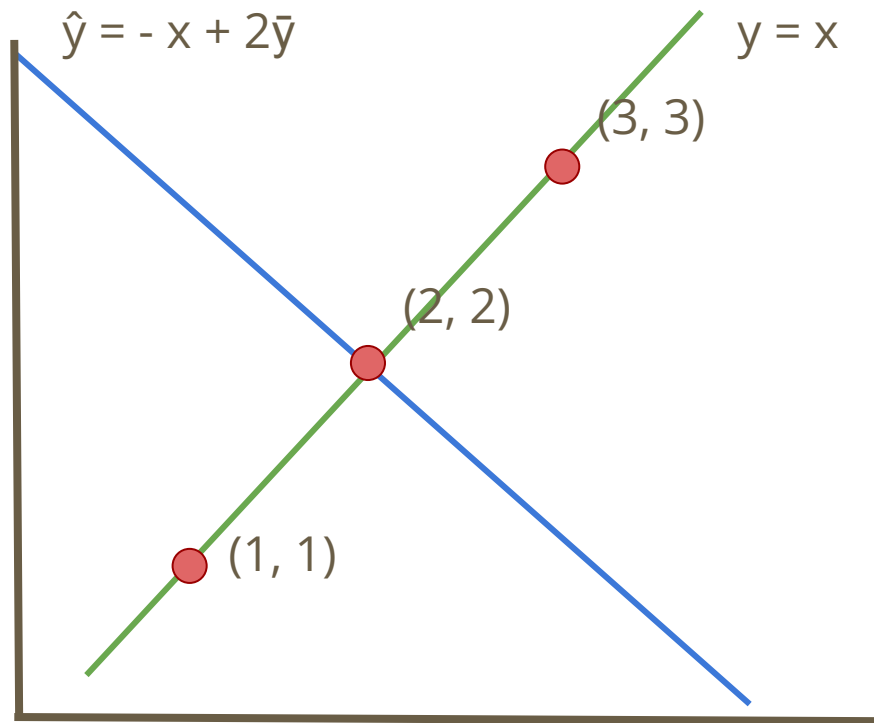
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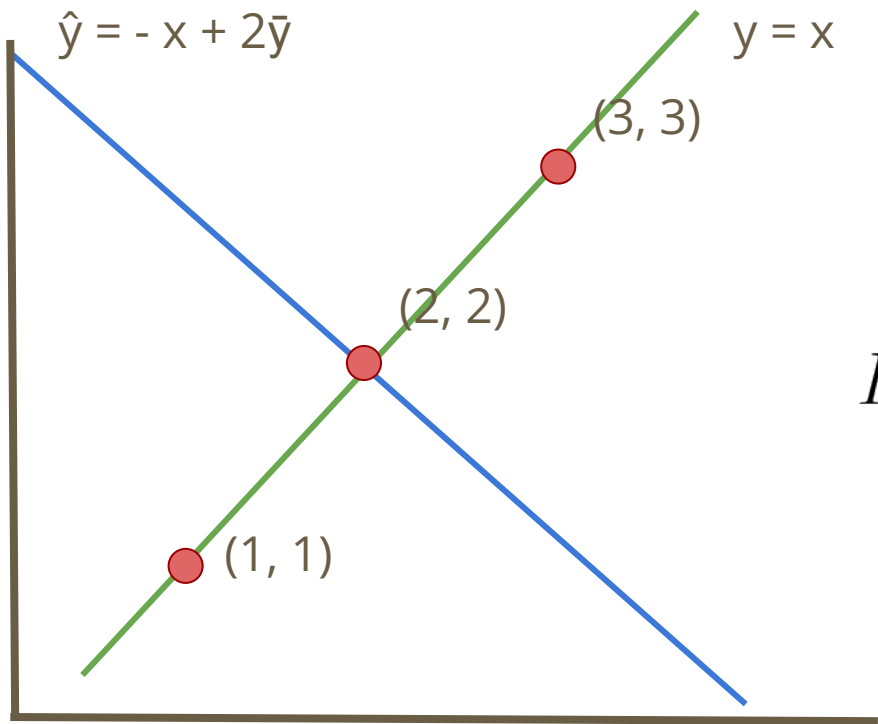
$$R^2 = 1$$

Why this new formula is standard

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

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

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



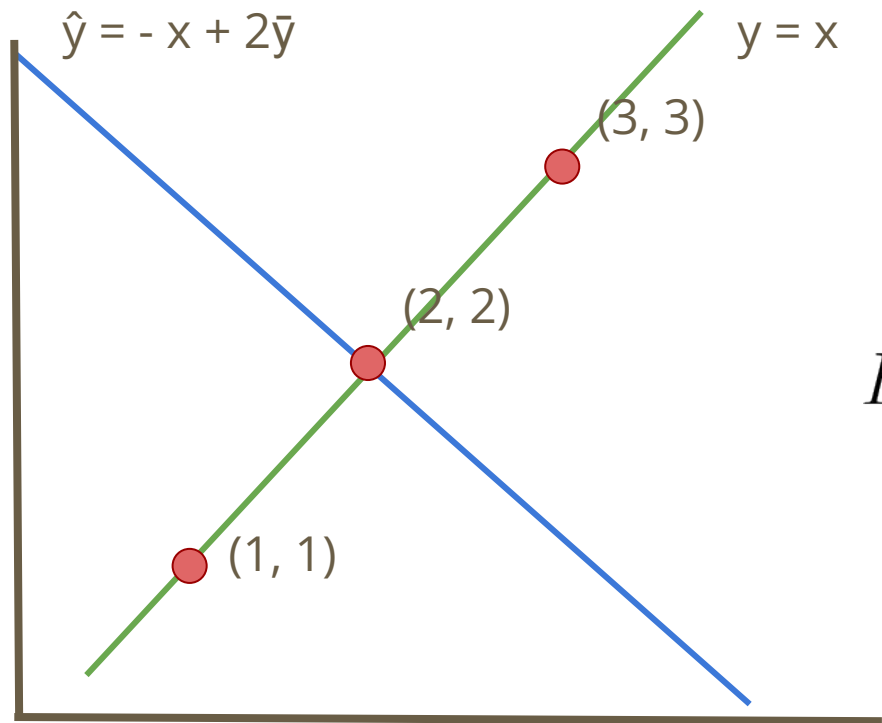
$$R^2 = 1 - \frac{RSS}{TSS}$$

Why this new formula is standard

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

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

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



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

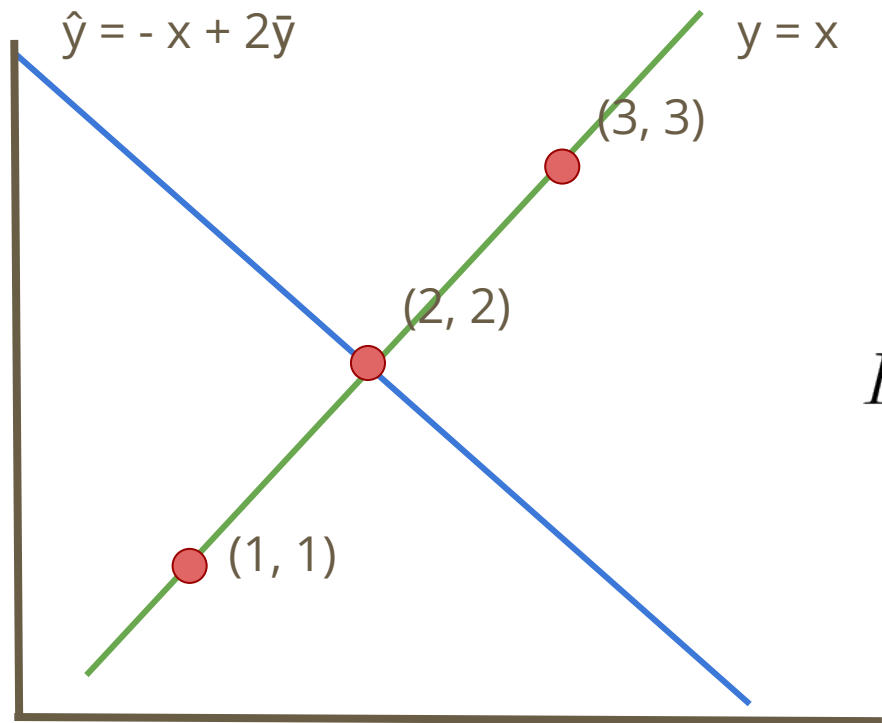
$$R^2 = 1 - \frac{RSS}{TSS}$$

Why this new formula is standard

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

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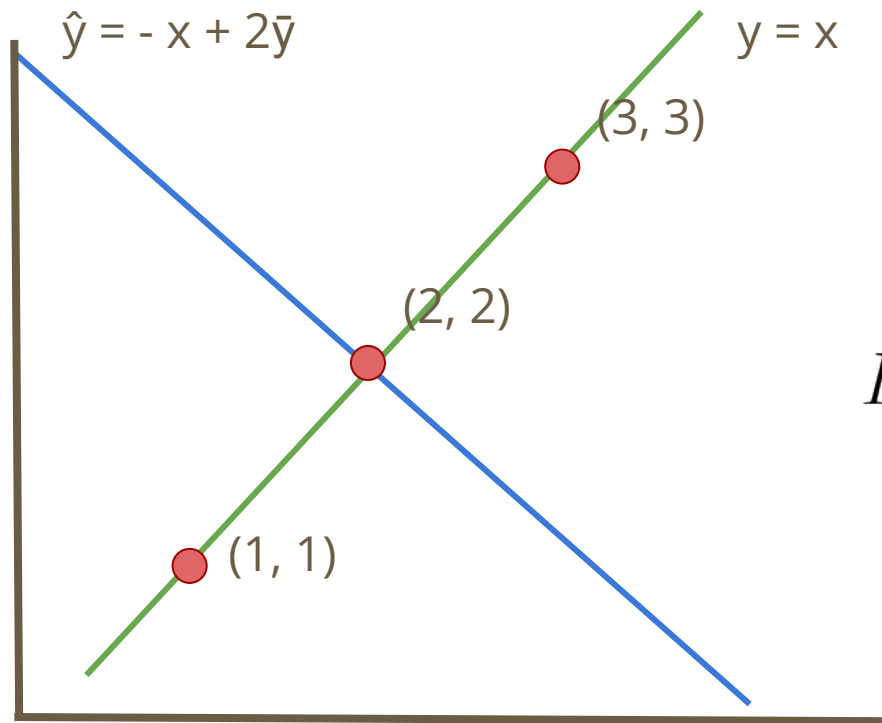
$$R^2 = 1 - 4$$

Why this new formula is standard

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

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



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

$$R^2 = -3$$

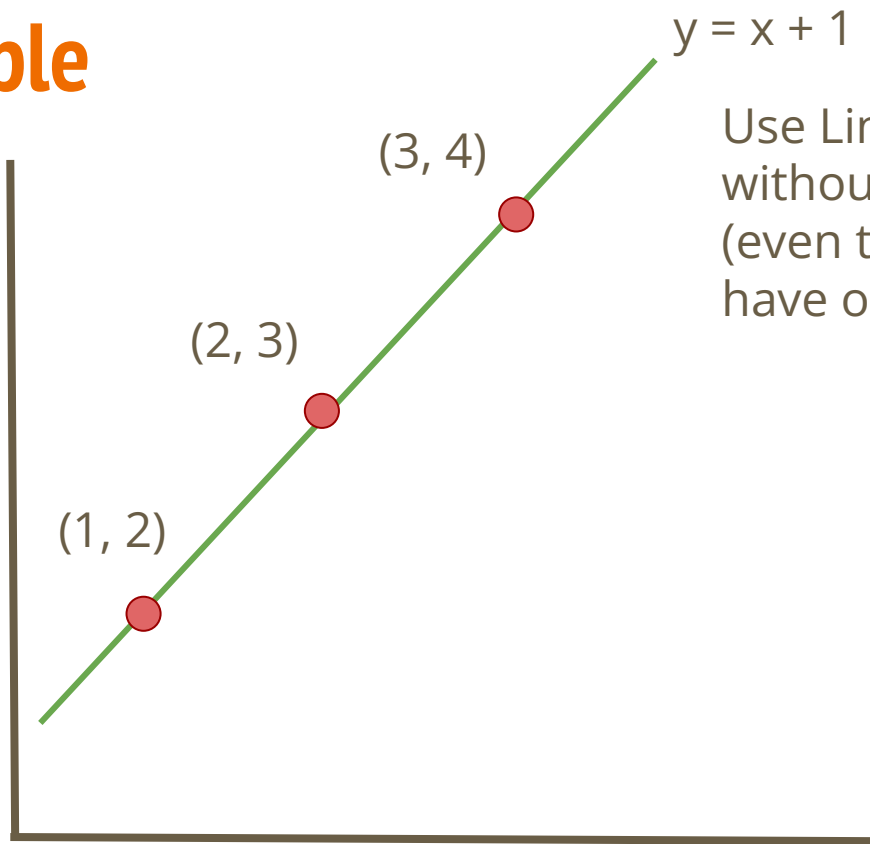
Another example

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

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

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

$$\bar{Y} = 3$$



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

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

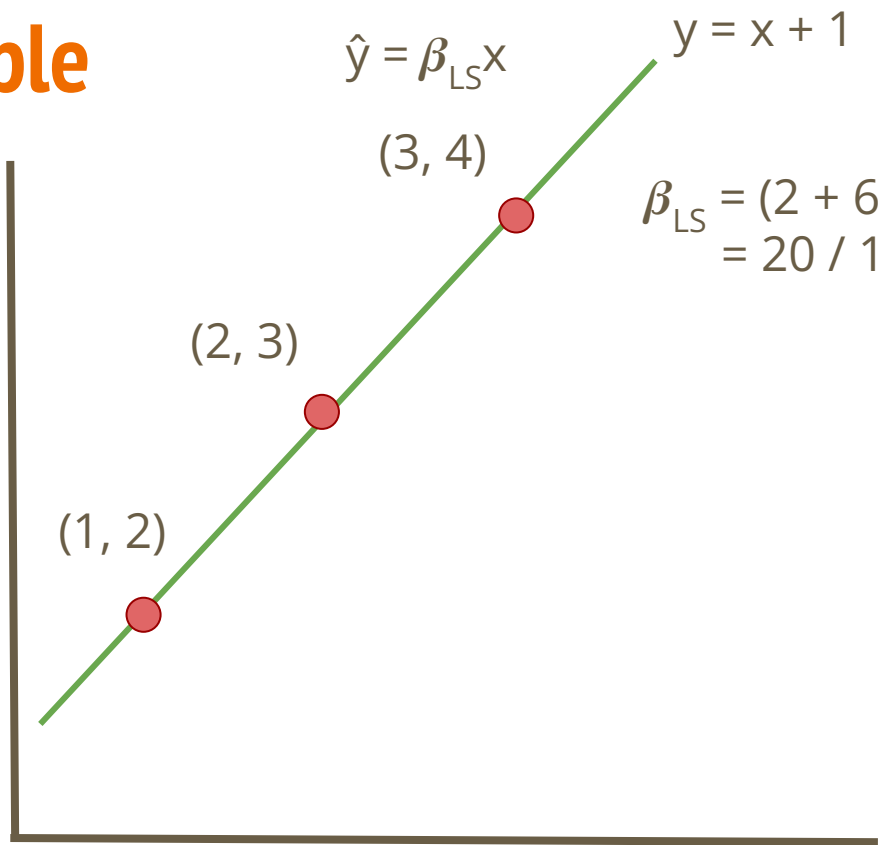
Another example

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

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$$\bar{Y} = 3$$



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

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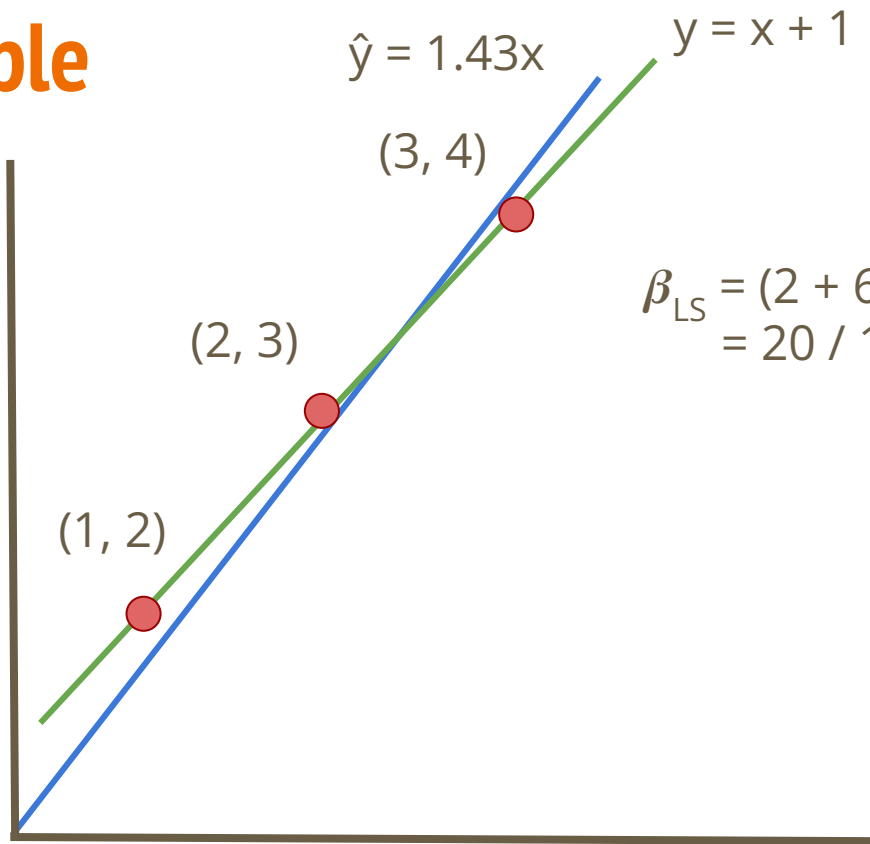
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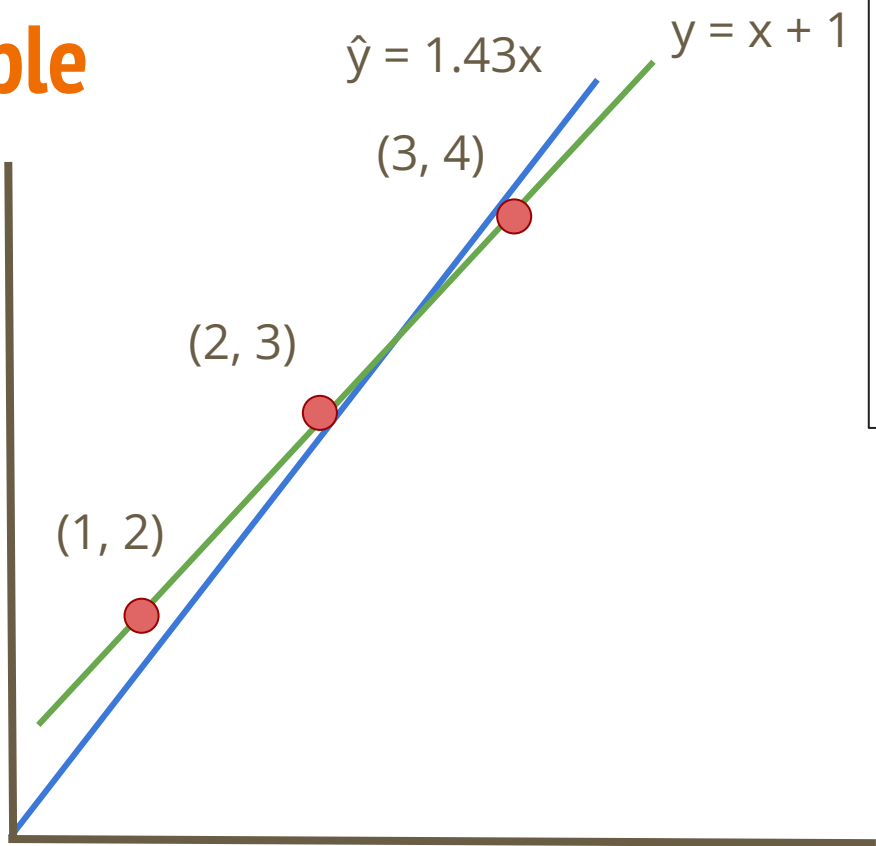
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$$\begin{aligned} ESS &= (1.43 - 3)^2 + \\ &\quad (2.86 - 3)^2 + (4.29 \\ &\quad - 3)^2 \\ &= 4.1 \end{aligned}$$

$$\begin{aligned} TSS &= 1^2 + 0^2 + 1^2 \\ &= 2 \end{aligned}$$

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

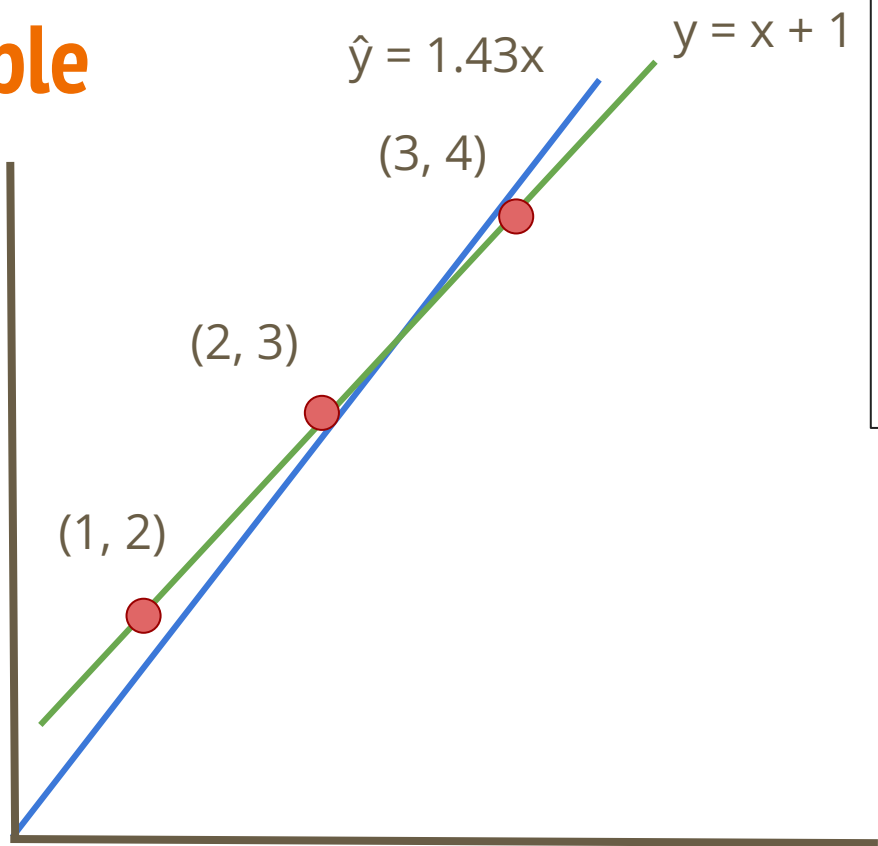
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$$R^2 = 2$$

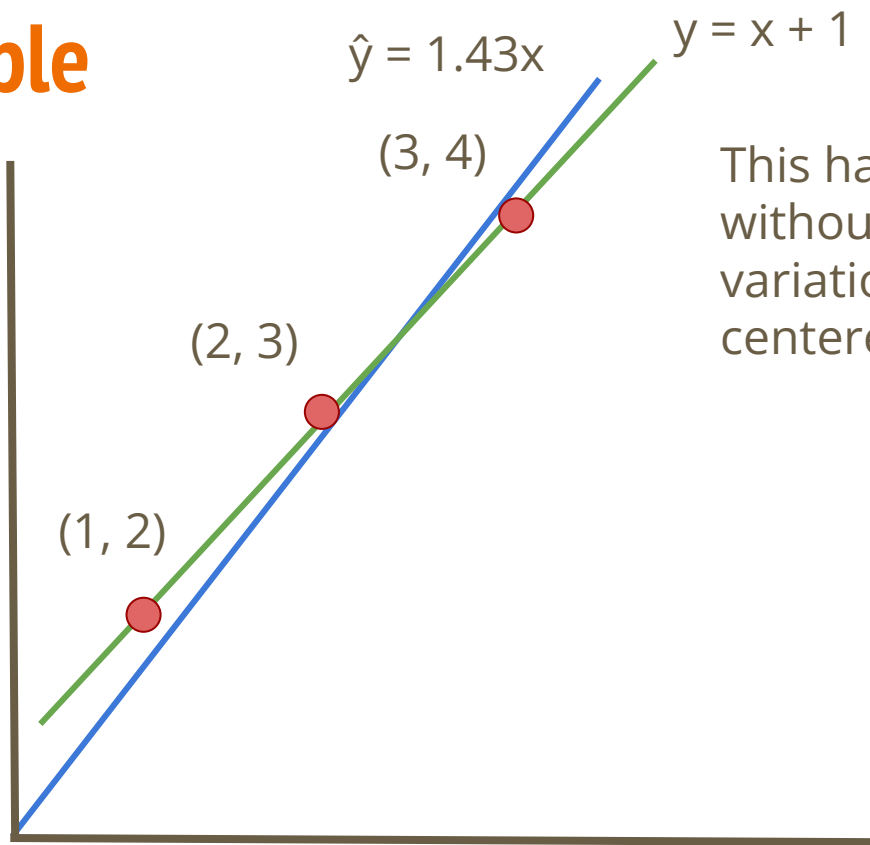
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$$ESS = \sum_i^n (\hat{y}_i - \bar{y})^2$$

$$\bar{Y} = 3$$



This happens because, without an intercept, variation of \hat{y} is not centered around \bar{Y}

$$R^2 = 2$$

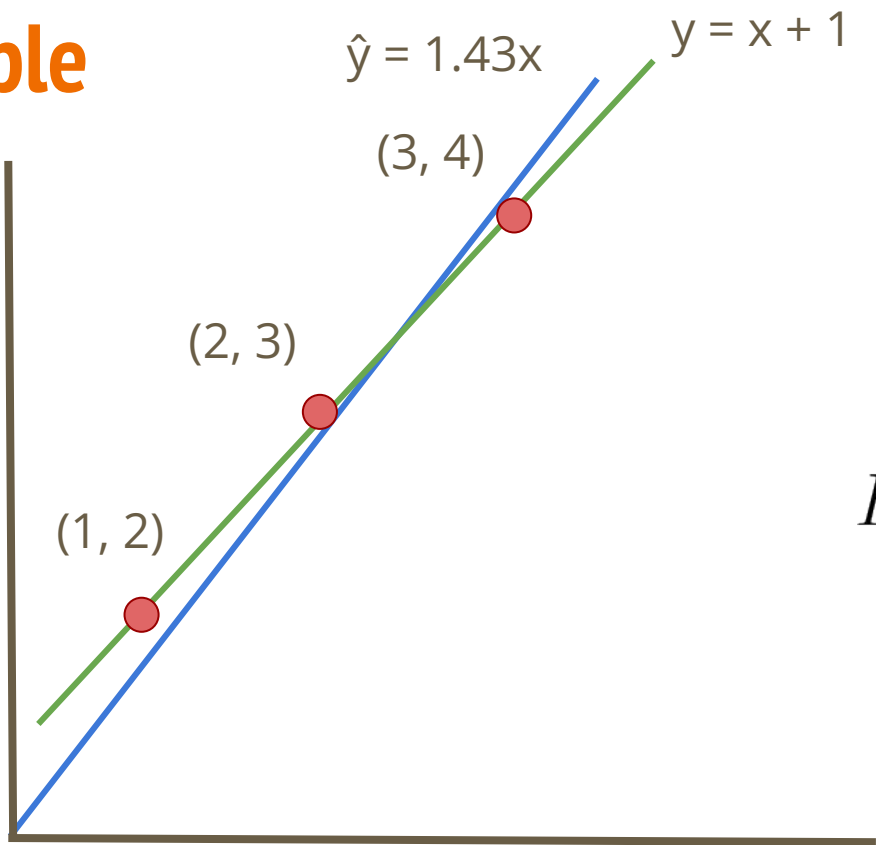
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$$R^2 = 1 - \frac{RSS}{TSS}$$

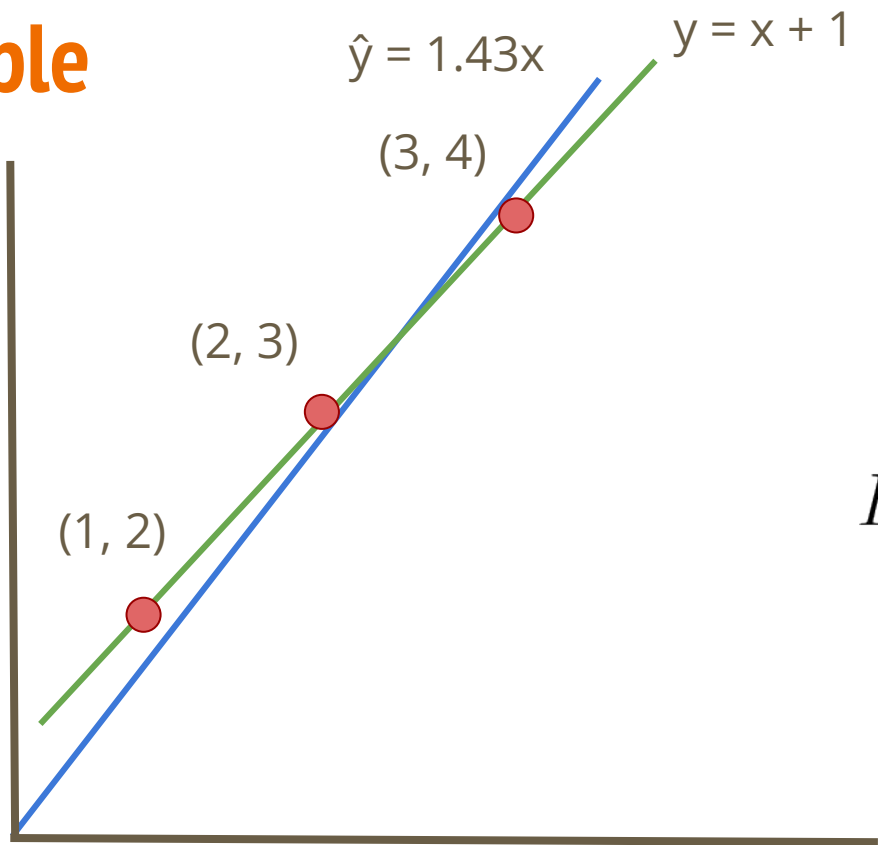
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$$\bar{Y} = 3$$



$$R^2 = .98$$

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?

Evaluating our Regression Model

```

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```

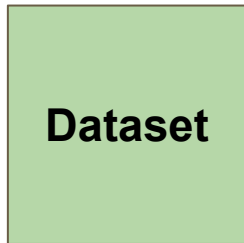
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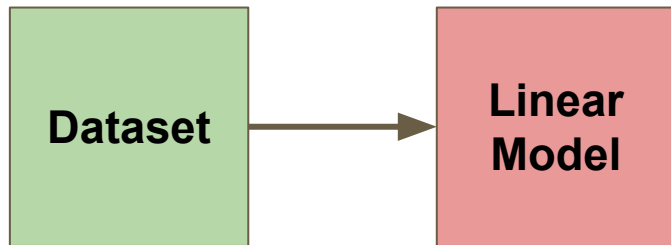
=====
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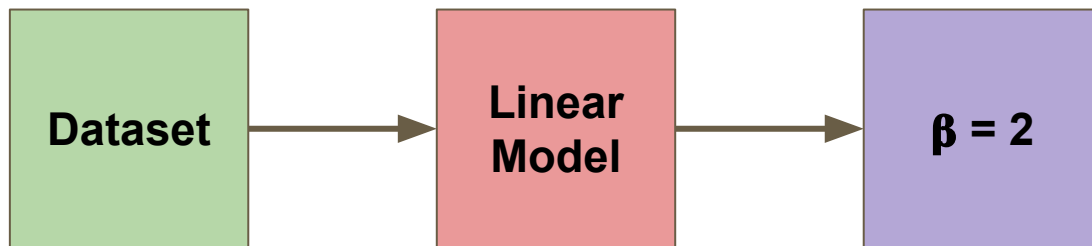
Hypothesis Testing



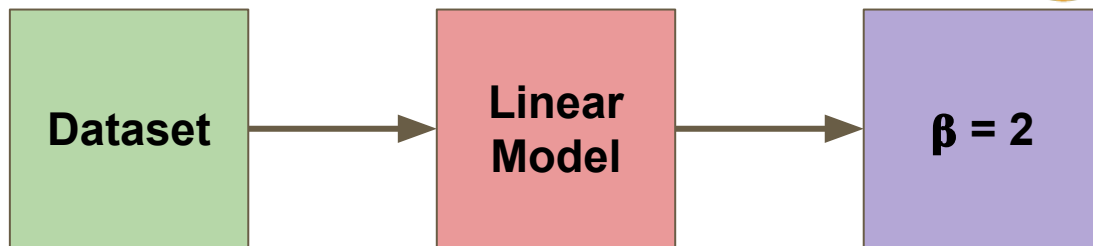
Hypothesis Testing



Hypothesis Testing



Hypothesis Testing



Could the
real beta
be 5?

H H H H H H H H



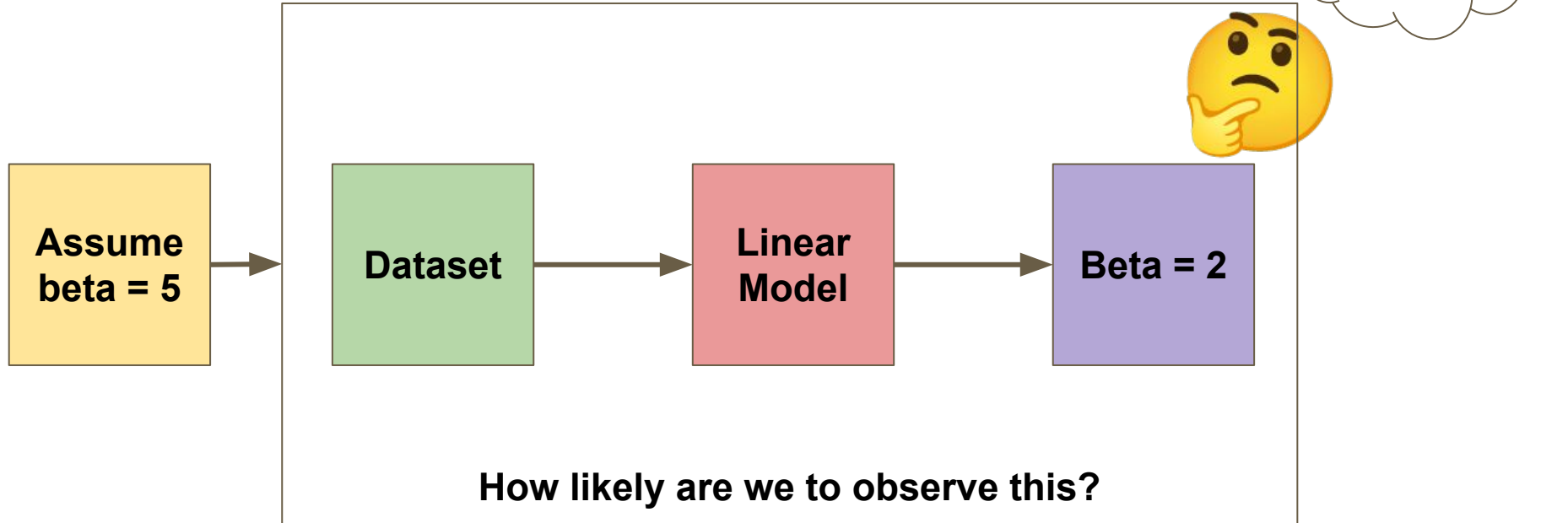
The coin is
probably
not fair

H T H H T H T T

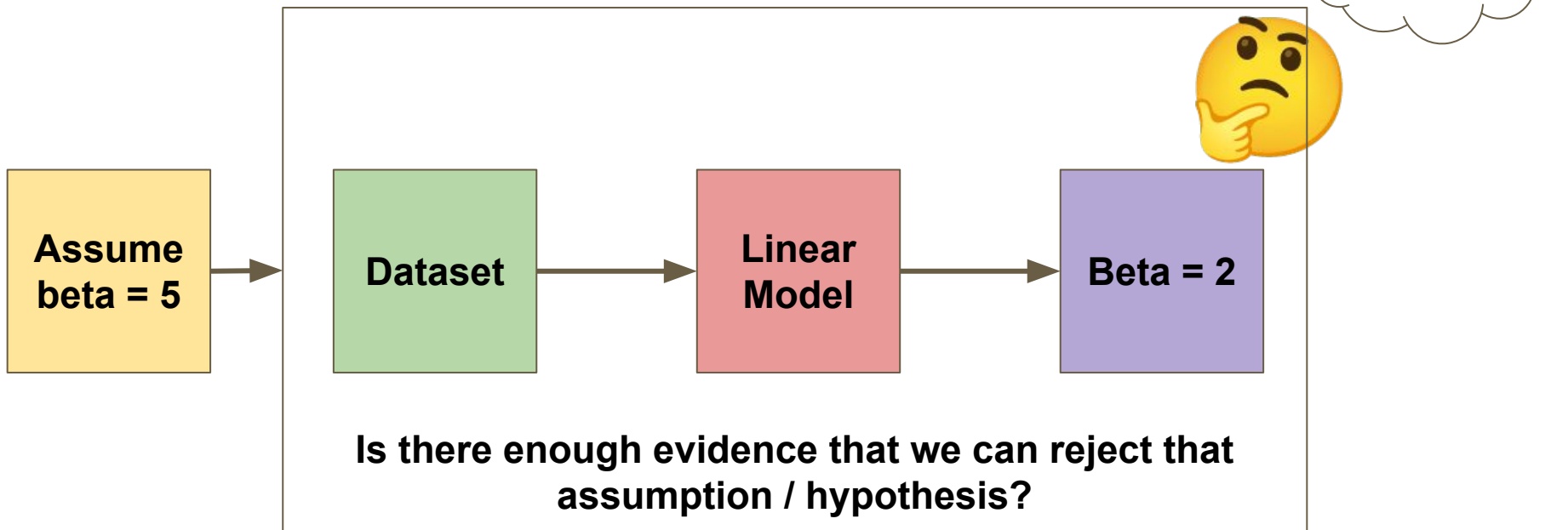


The coin
could be
fair

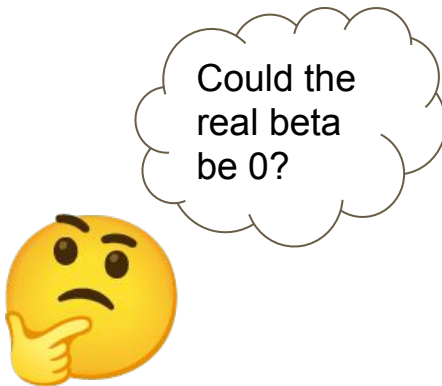
Hypothesis Testing



Hypothesis Testing



worksheet



Hypothesis Testing

Each parameter of an independent variable \mathbf{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 \mathbf{y} (i.e. if the interval includes 0 or if the p-value is too large)

Hypothesis Test

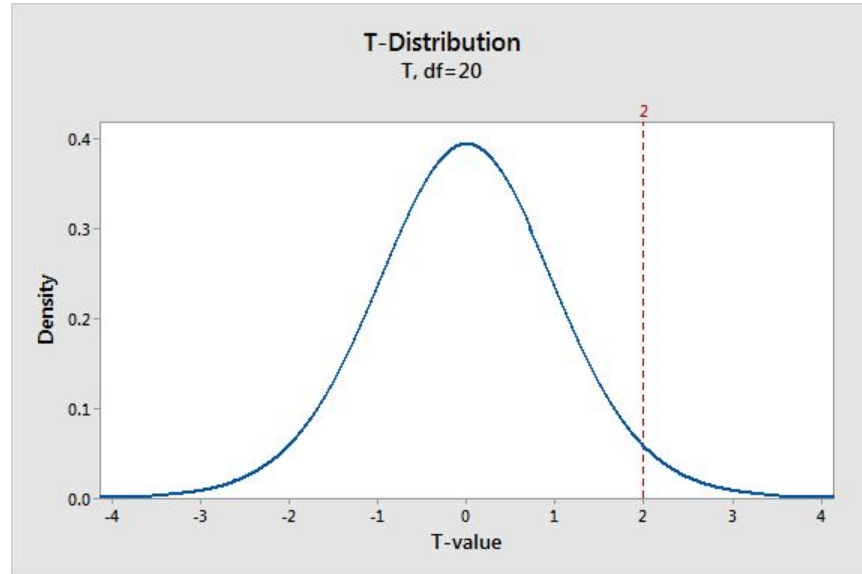
We want to know if there is evidence to reject the hypothesis $H_0 : \beta = 0$ (i.e. that there is no linear relation between X and Y) using the information from $\hat{\beta}$.

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?

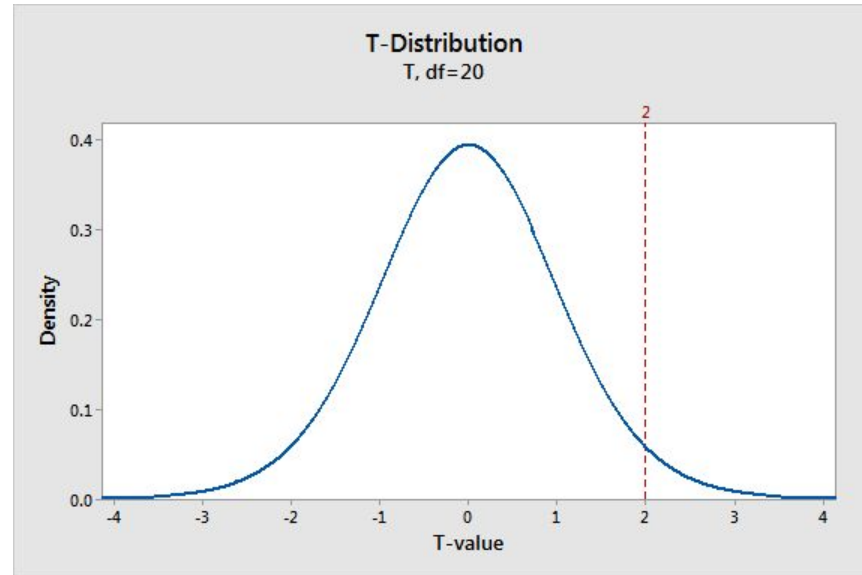
Hypothesis Test

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



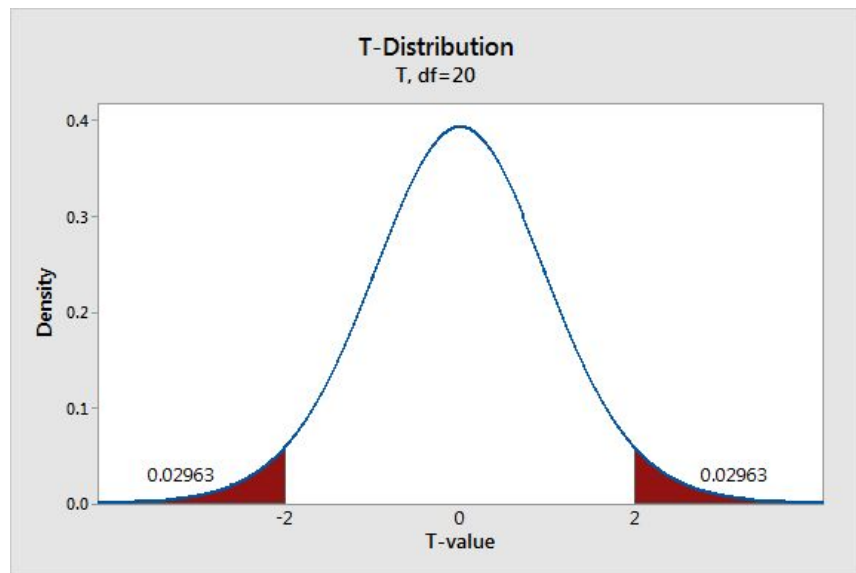
Hypothesis Test

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



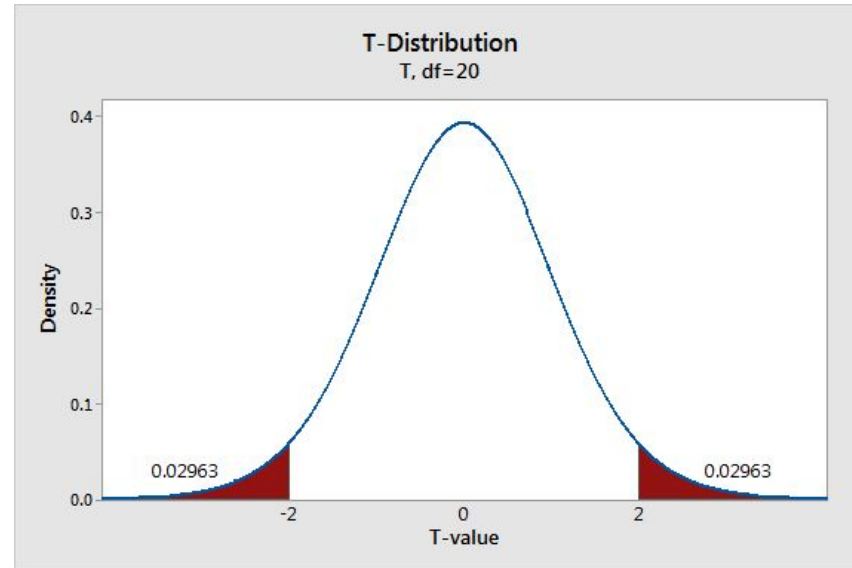
Hypothesis Test

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 H_0)



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 H_0 so we can reject the hypothesis H_0 . If not, then we lack the evidence to reject H_0 .

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Hypothesis Test

Which parameters should we not include in our linear model?

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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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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:

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

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 $\mathbf{Y}_i \sim \mathbf{N}(5, 25)$, for $1 \leq i \leq 100$ and $\mathbf{y}_i = \mu + \epsilon$ where $\epsilon \sim \mathbf{N}(0, 25)$. Then the Least Squares estimator of μ (μ_{LS}) is

the sample mean \bar{y}

What is the 95% confidence interval for μ_{LS} ?

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

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

Z-value for 95% Confidence Interval

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)