Introduction to Gradient Descent

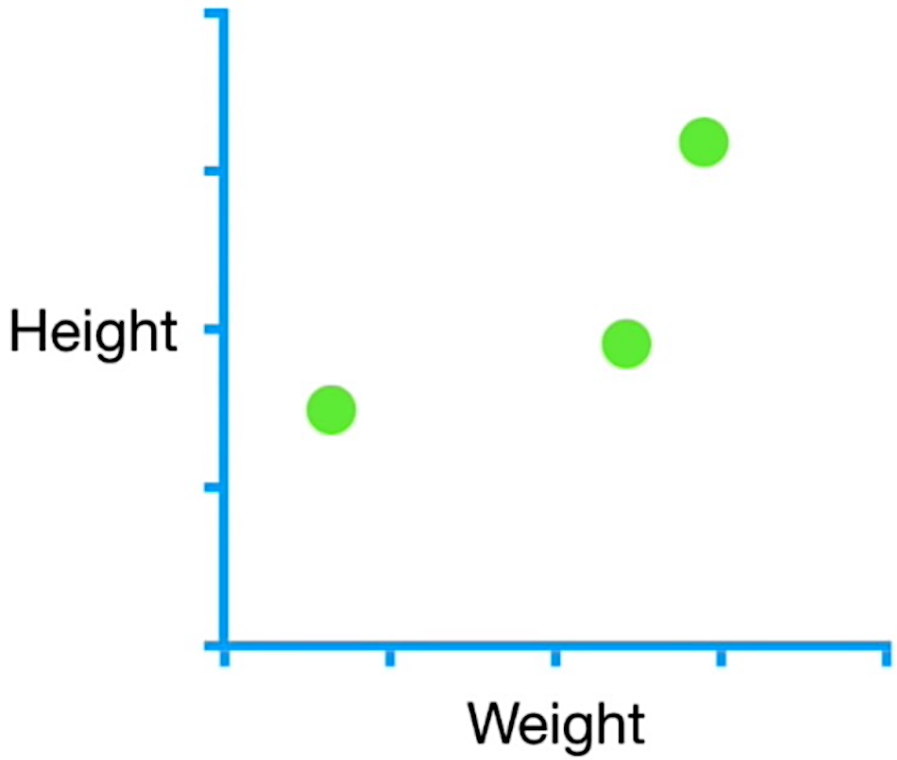
By Alan Grunberg

(with graphs adapted from Le Wagon and StatQuest)

Linear regression with 2 features:
finding the line **Y = mX + b** that best fits the relationship

m = slope
b = intercept

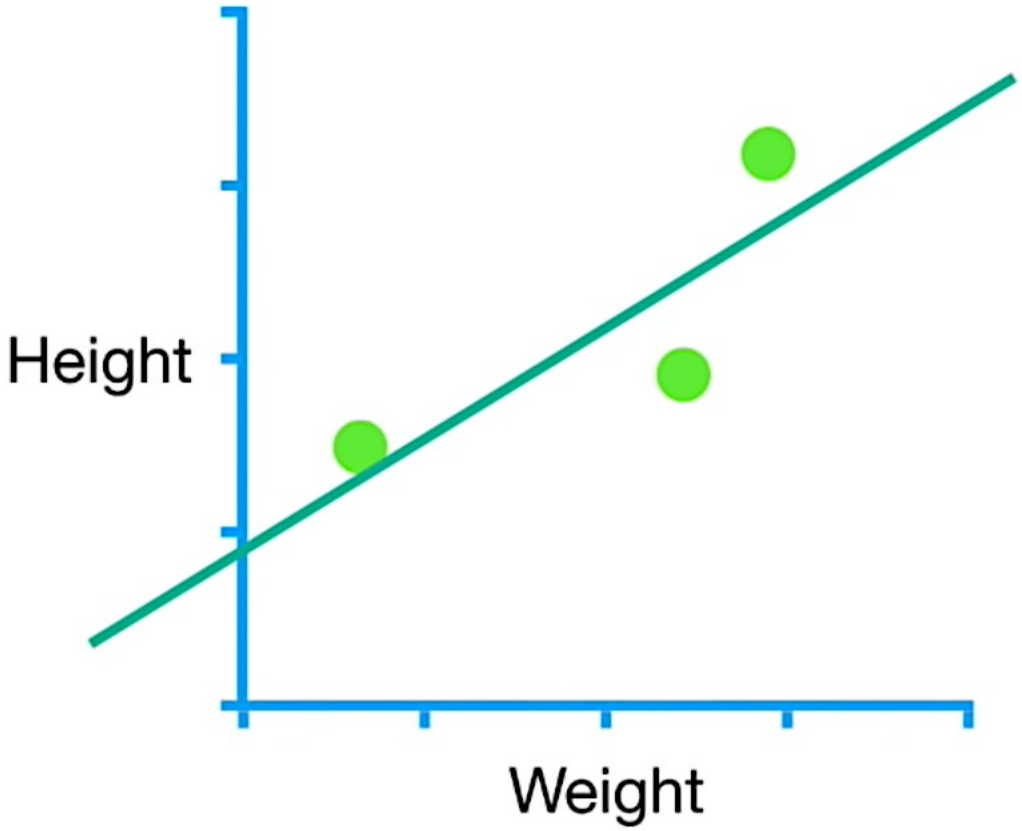
	weight	height
0	0.7	1.5
1	2.4	1.8
2	2.8	3.2



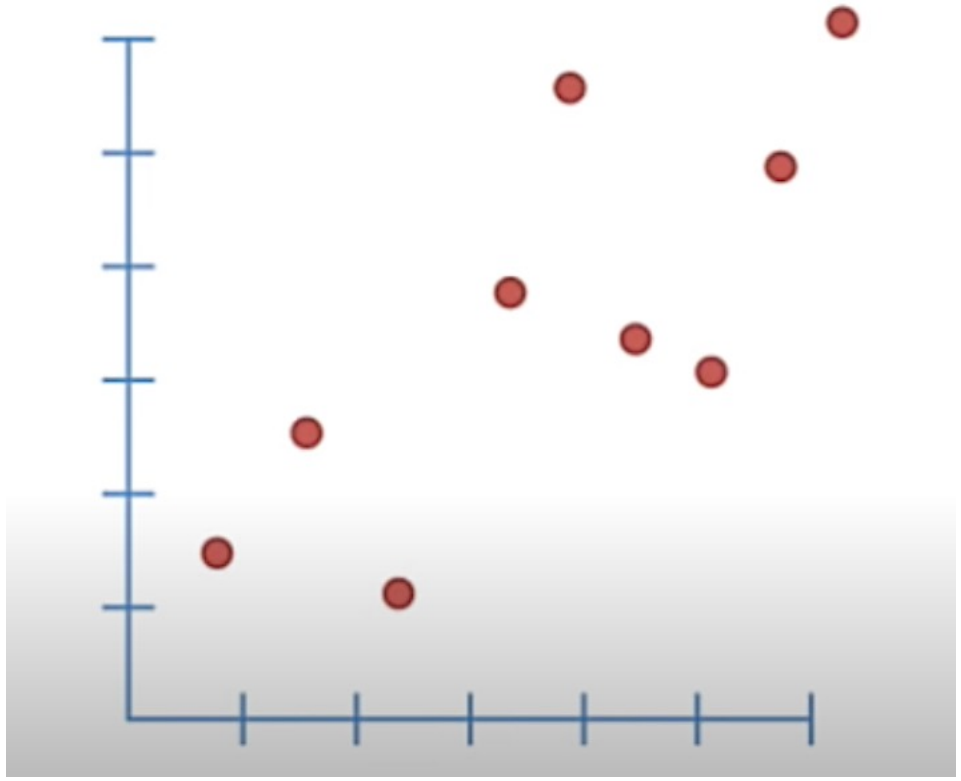
easy to eyeball (and to calculate) when just a few data points

parameters:
intercept = .943
slope = .622

(Y = .622X + .942)



But what about when there are more data points?



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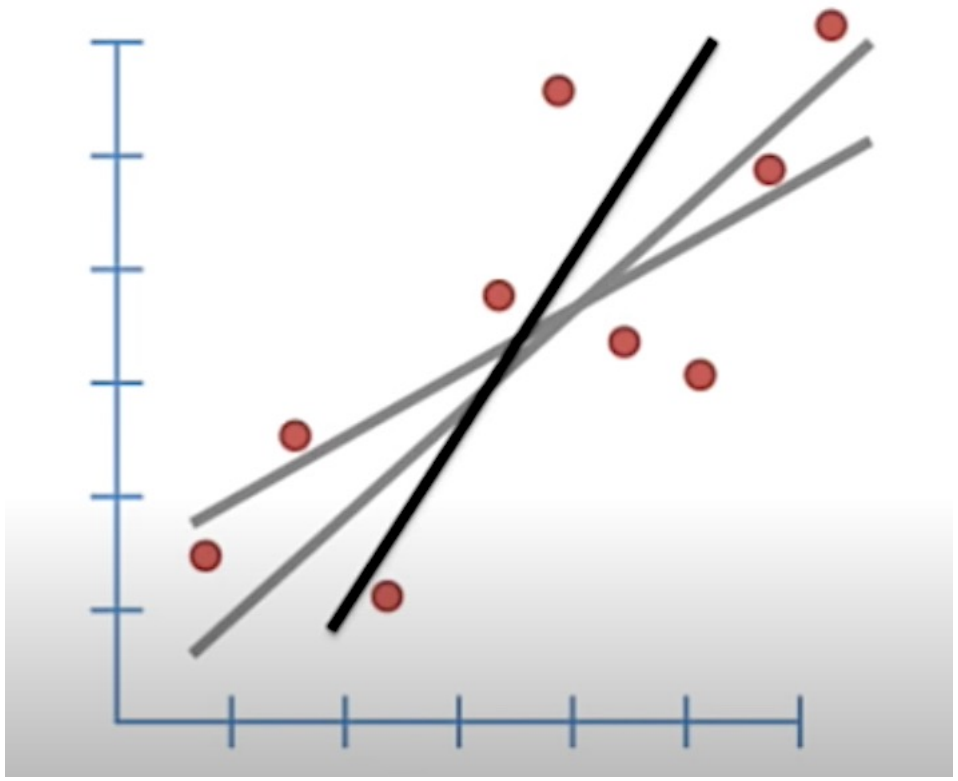
How do we know which line best fits the relationship?

And how does the computer figure it out?



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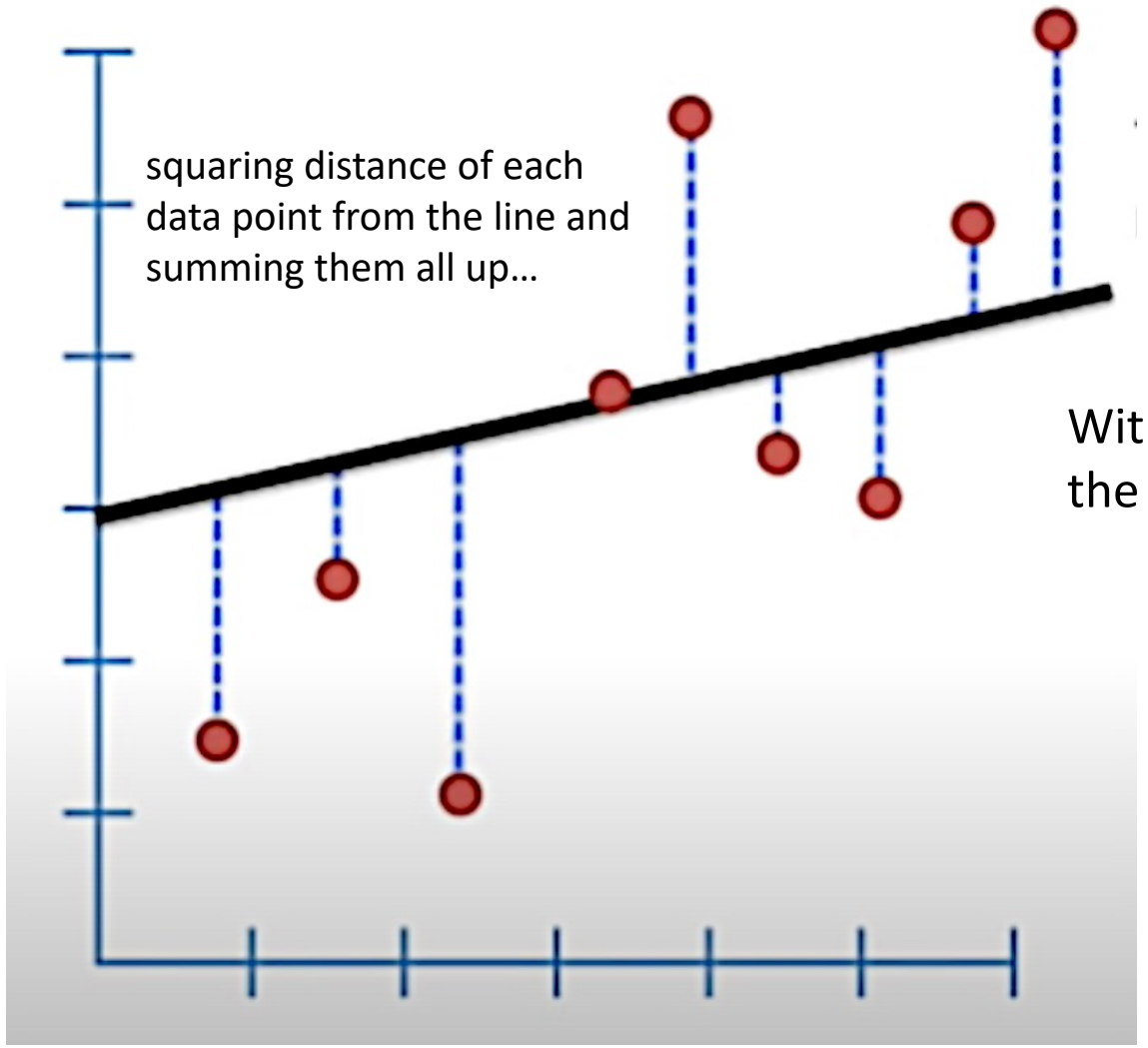
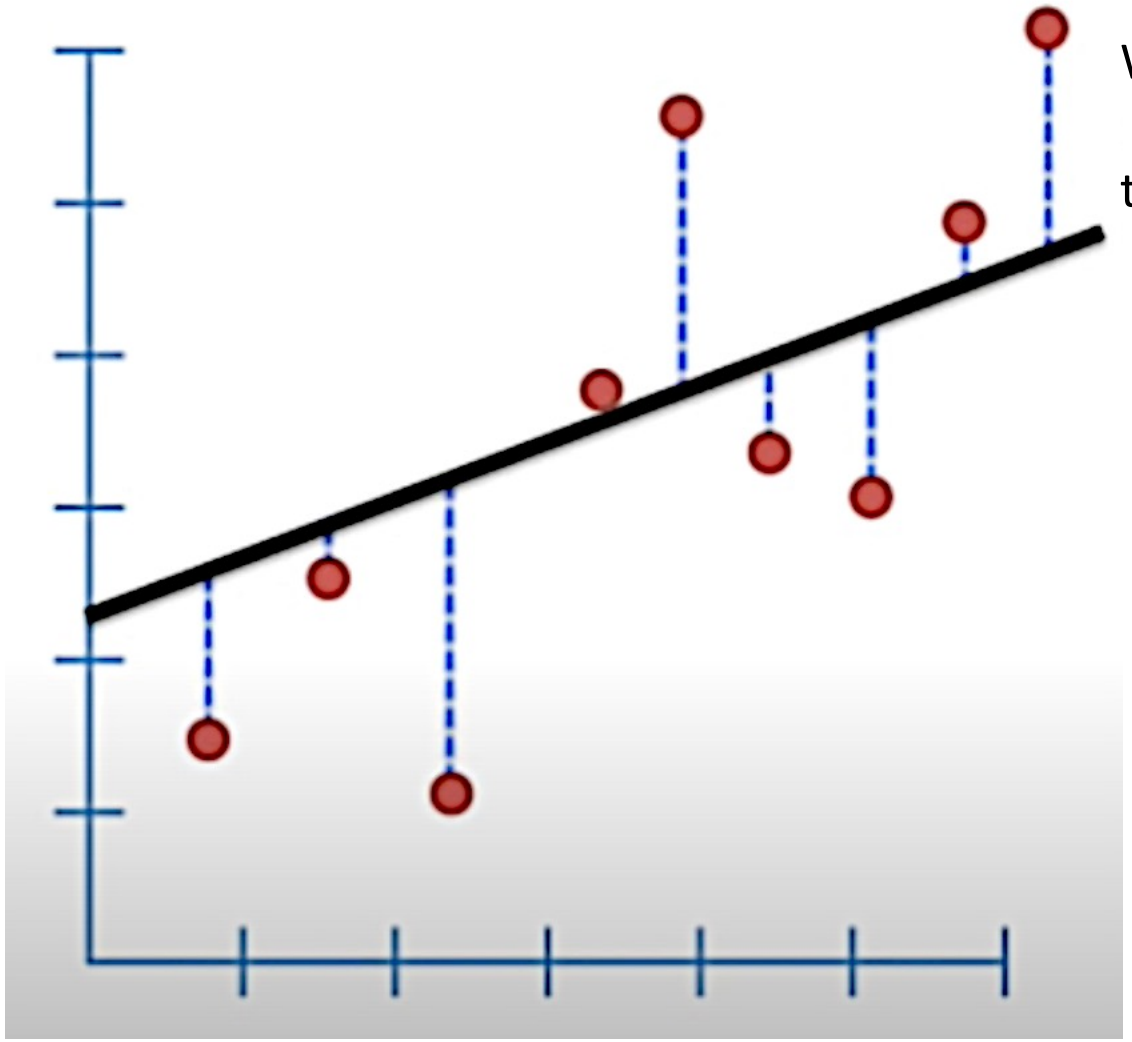
The answer lies in calculating **sum of squared residuals**



With this line,
the sum of squared residuals = 18.72



With this line,
(different slope and intercept)
the sum of squared residuals = 14.05

lower is better!

we want to find the line that gives us the **least sum of squared residuals**.

This is called
minimizing the loss function

There is an exact **analytic solution**…

$$X^T X = \begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ x_1 & x_2 & x_3 & \dots & x_n \end{bmatrix} x \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ . \\ . \\ . \\ 1 & x_n \end{bmatrix} = \begin{bmatrix} N & \sum X_i \\ \sum X_i & \sum X_i^2 \end{bmatrix}$$

$$X^T \vec{y} = \begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ x_1 & x_2 & x_3 & \dots & x_n \end{bmatrix} x \begin{bmatrix} y_1 \\ y_2 \\ . \\ . \\ . \\ y_n \end{bmatrix} = \begin{bmatrix} \sum y \\ \sum X_i y_i \end{bmatrix}$$

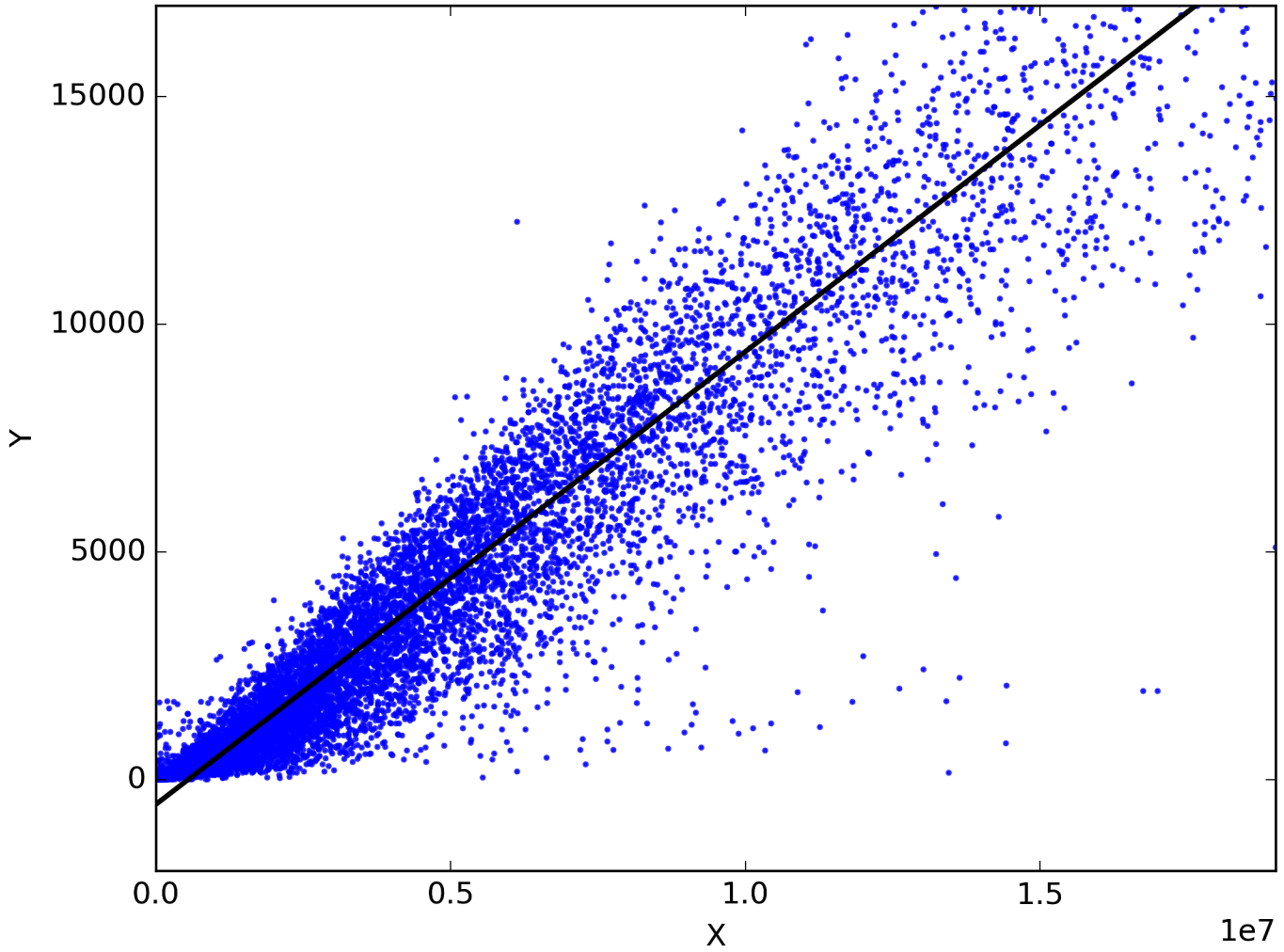
$$\vec{\beta} = (X^T X)^{-1} X^T \vec{y}$$

$$\begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} N & \sum X_i \\ \sum X_i & \sum x_i^2 \end{bmatrix}^{-1} \begin{bmatrix} \sum y \\ \sum X_i y_i \end{bmatrix}$$

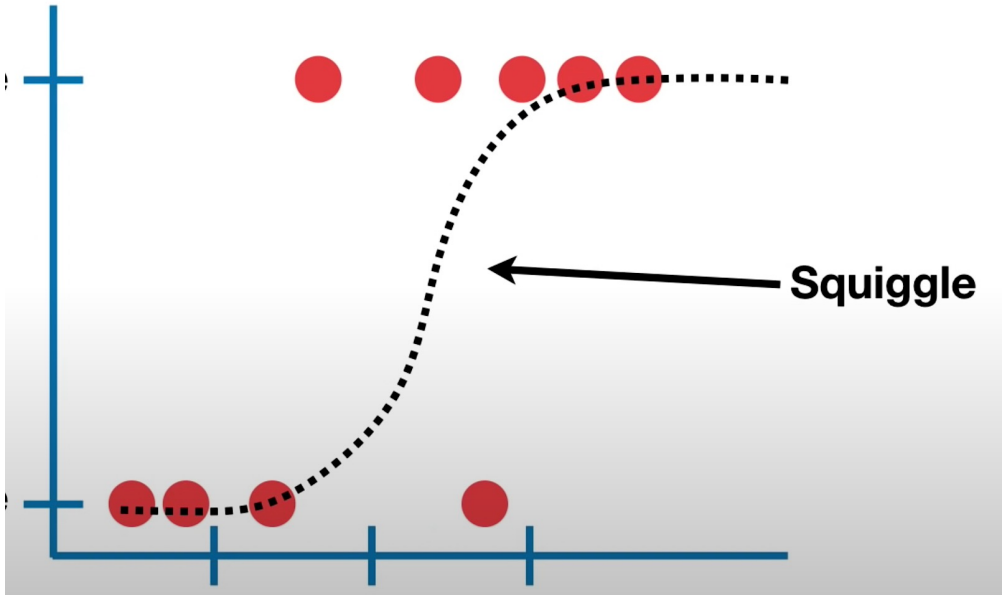
But it's complicated even for the computer and takes a ton of computing resources!

Plus, it only works for simple linear regressions

it’s very slow and computationally expensive
when there are lots of data points



And can’t be applied directly to other types of regression like logistic regression (can’t identify squiggle of best fit!)



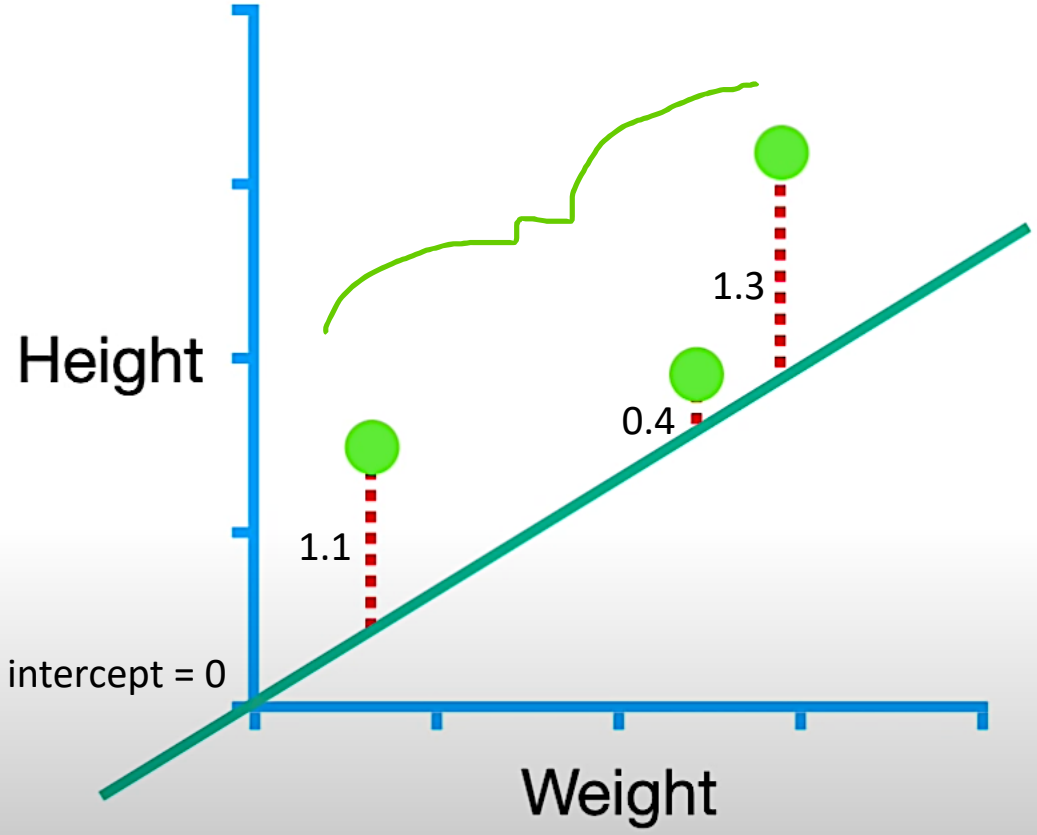
(process of repeated reviewing and testing)

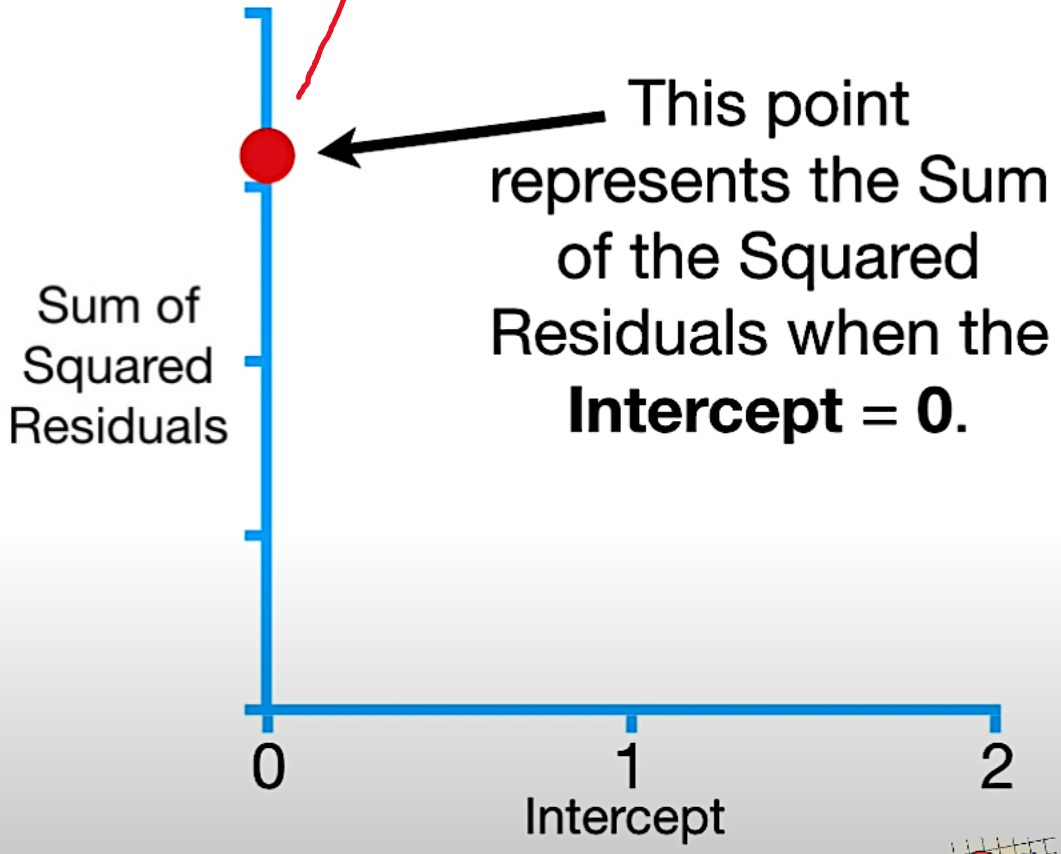
Luckily, there's an **iterative solution** that can estimate the optimal parameters, while using way less computer resources, and work in way more situations...

Gradient Descent

Let's start with 3 datapoints and a line with intercept 0

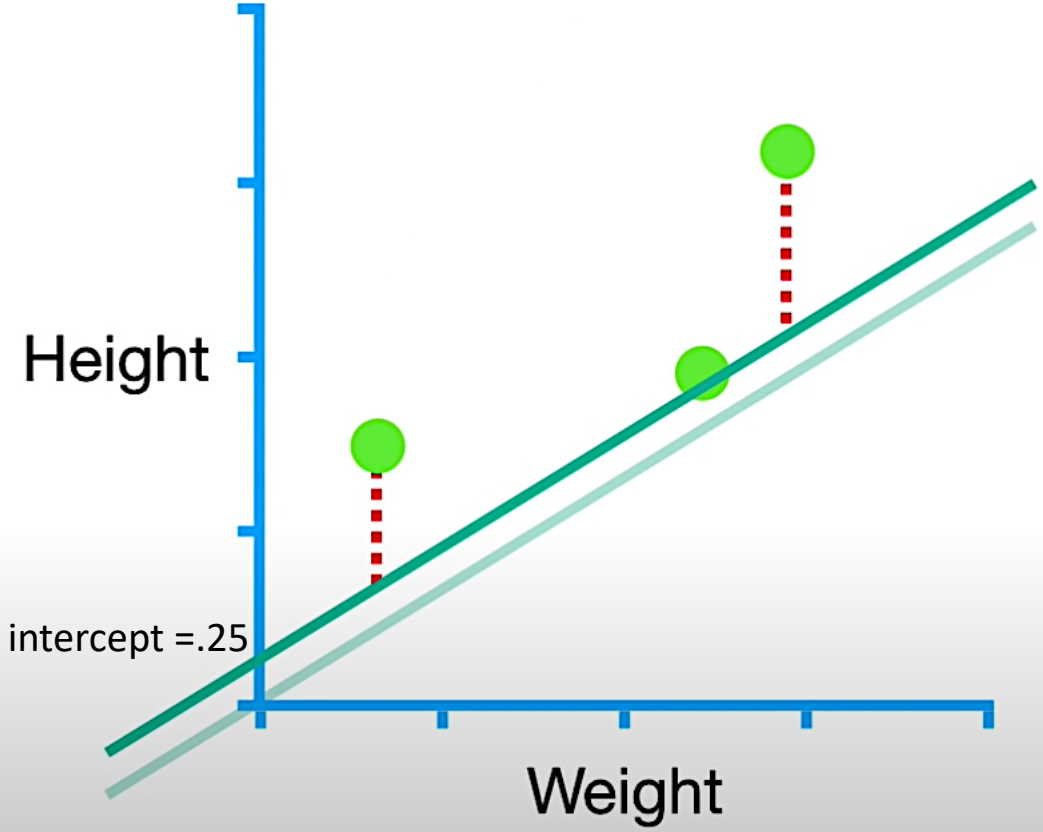
$$\text{Sum of squared residuals} = 1.1^2 + 0.4^2 + 1.3^2 = 3.1$$

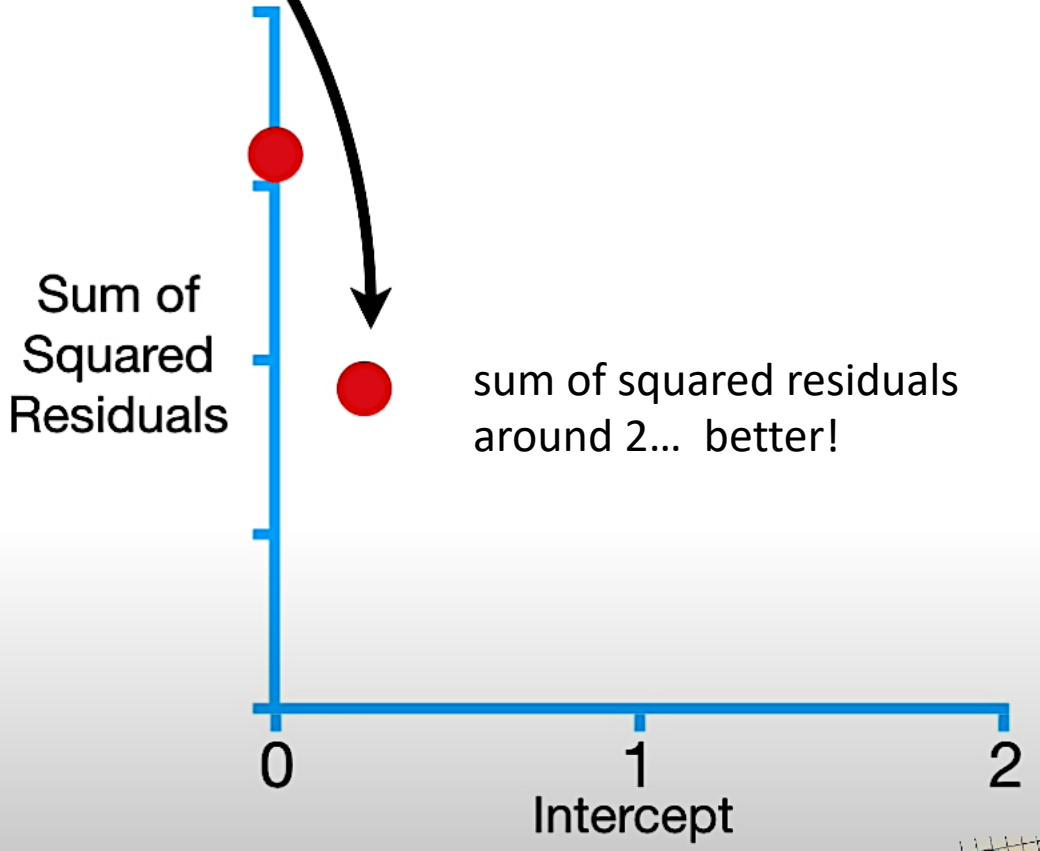




now let's change the intercept to .25

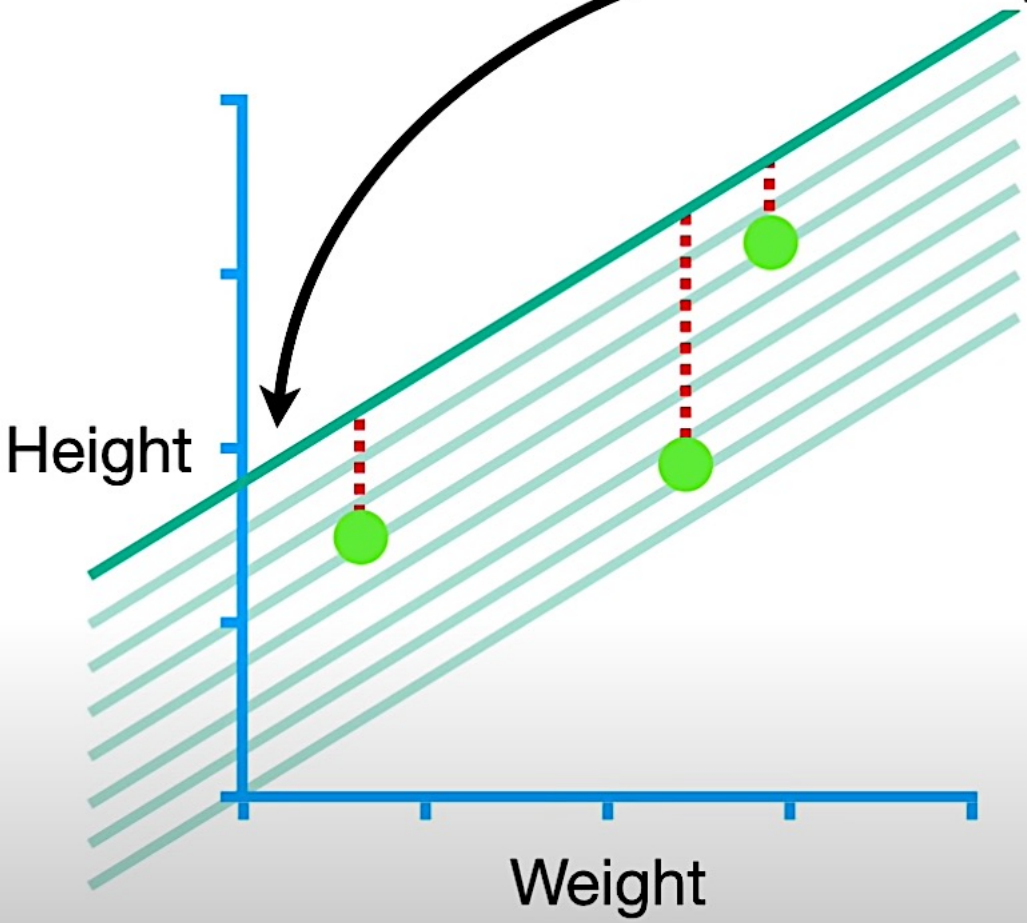
…then we would get this point on the graph.

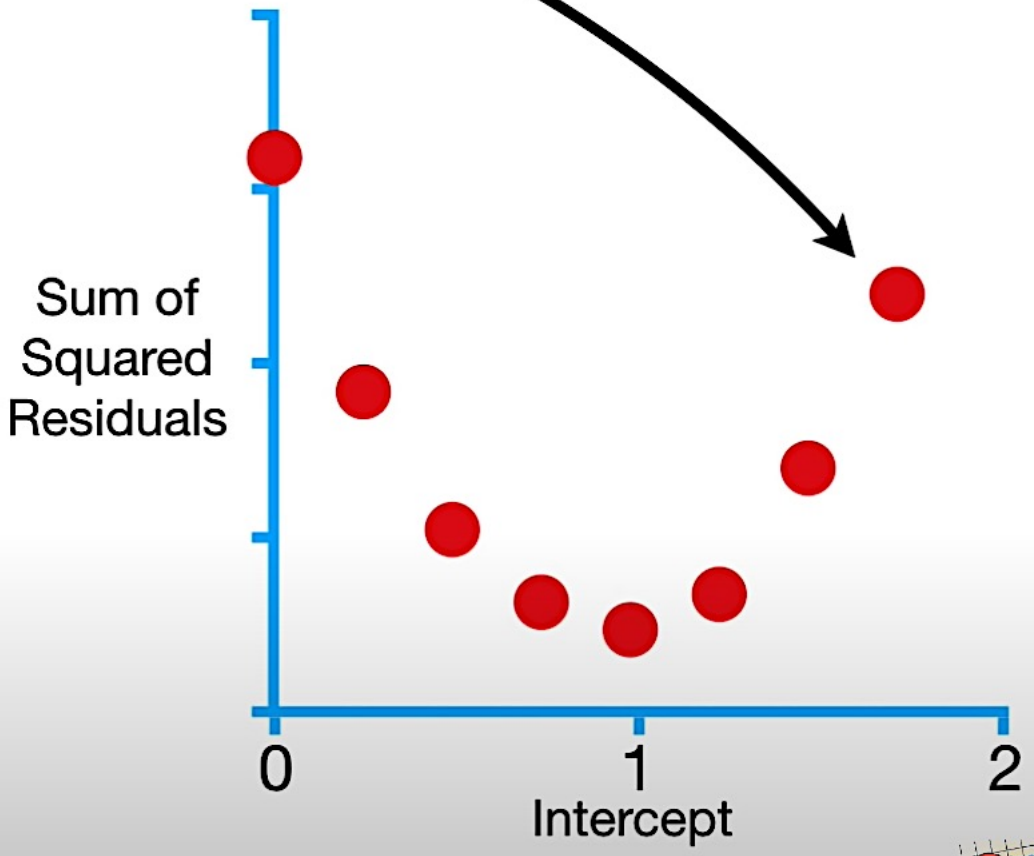




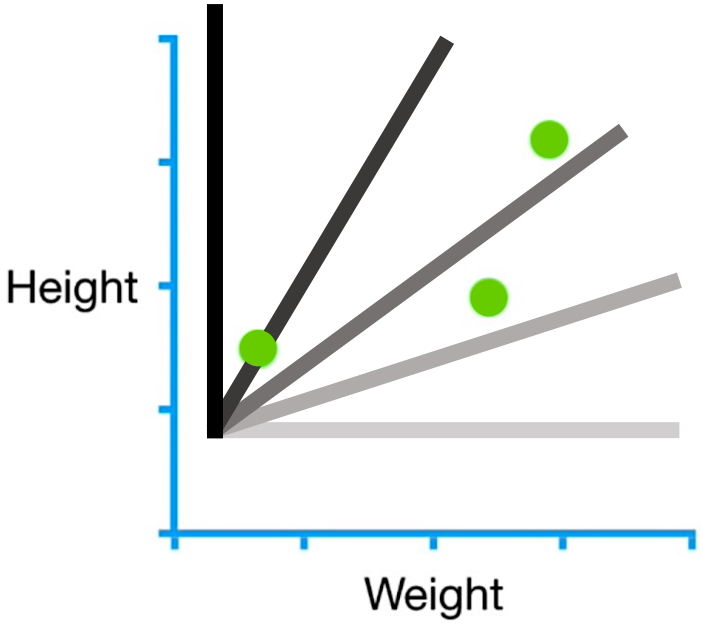
sum of squared residuals around 2… better!

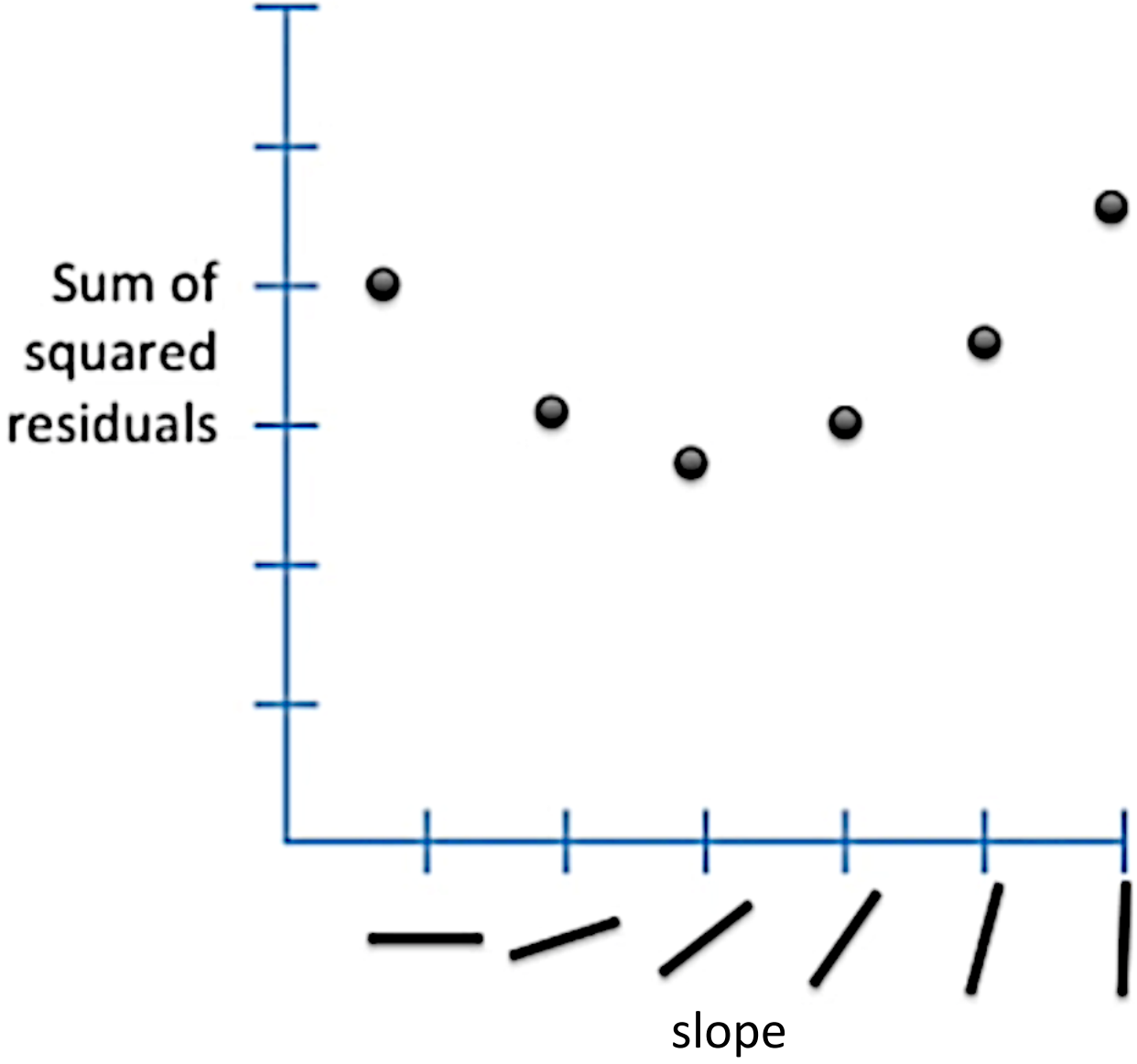
And for increasing values for the **Intercept**, we get these points.



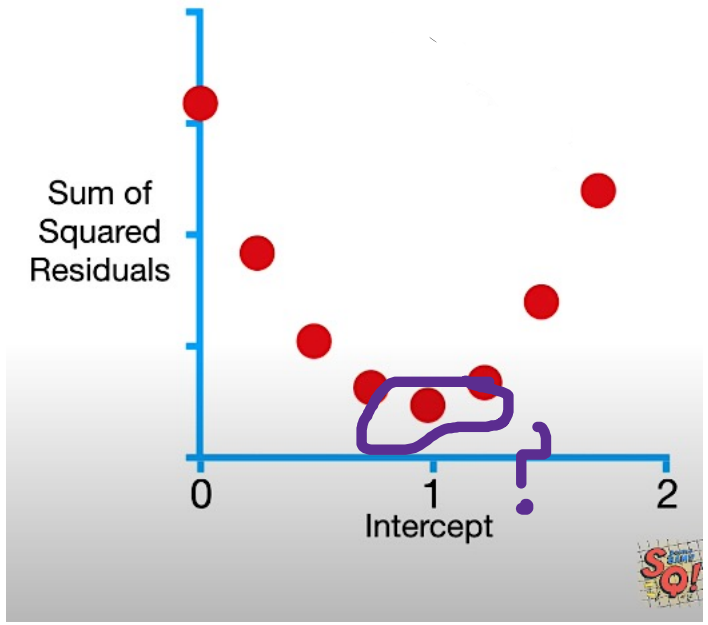


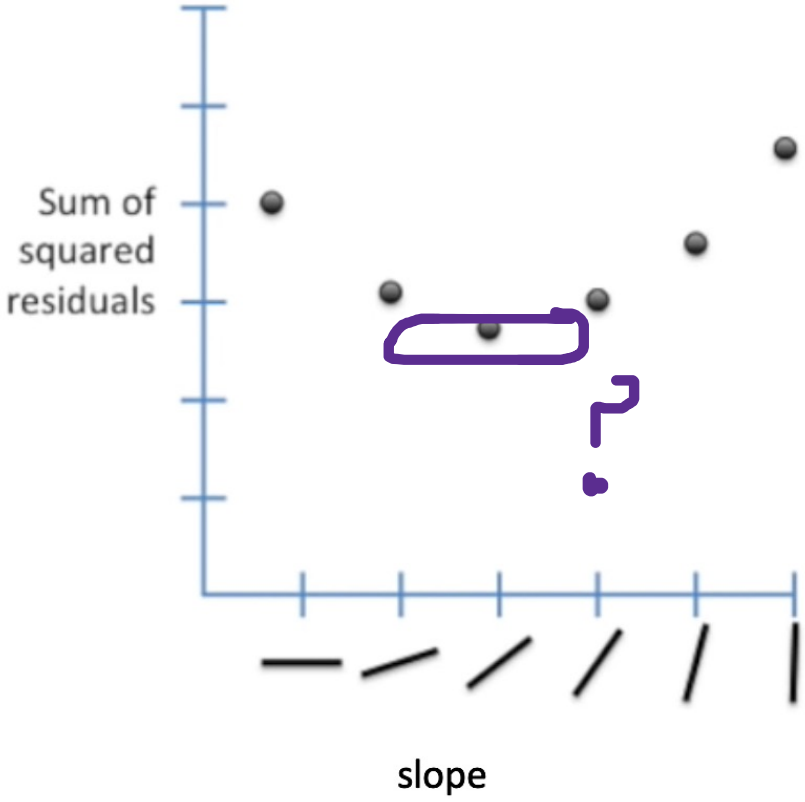
Starting with a slope of 0, adjusting the slope bit by bit and plotting the Sum of Squared Residuals for each angle we try, we see a similar pattern…





Remember, we are looking for the Least Sum of Squared Residuals,
so the optimal intercept and slope values must be at the bottom of each curve.



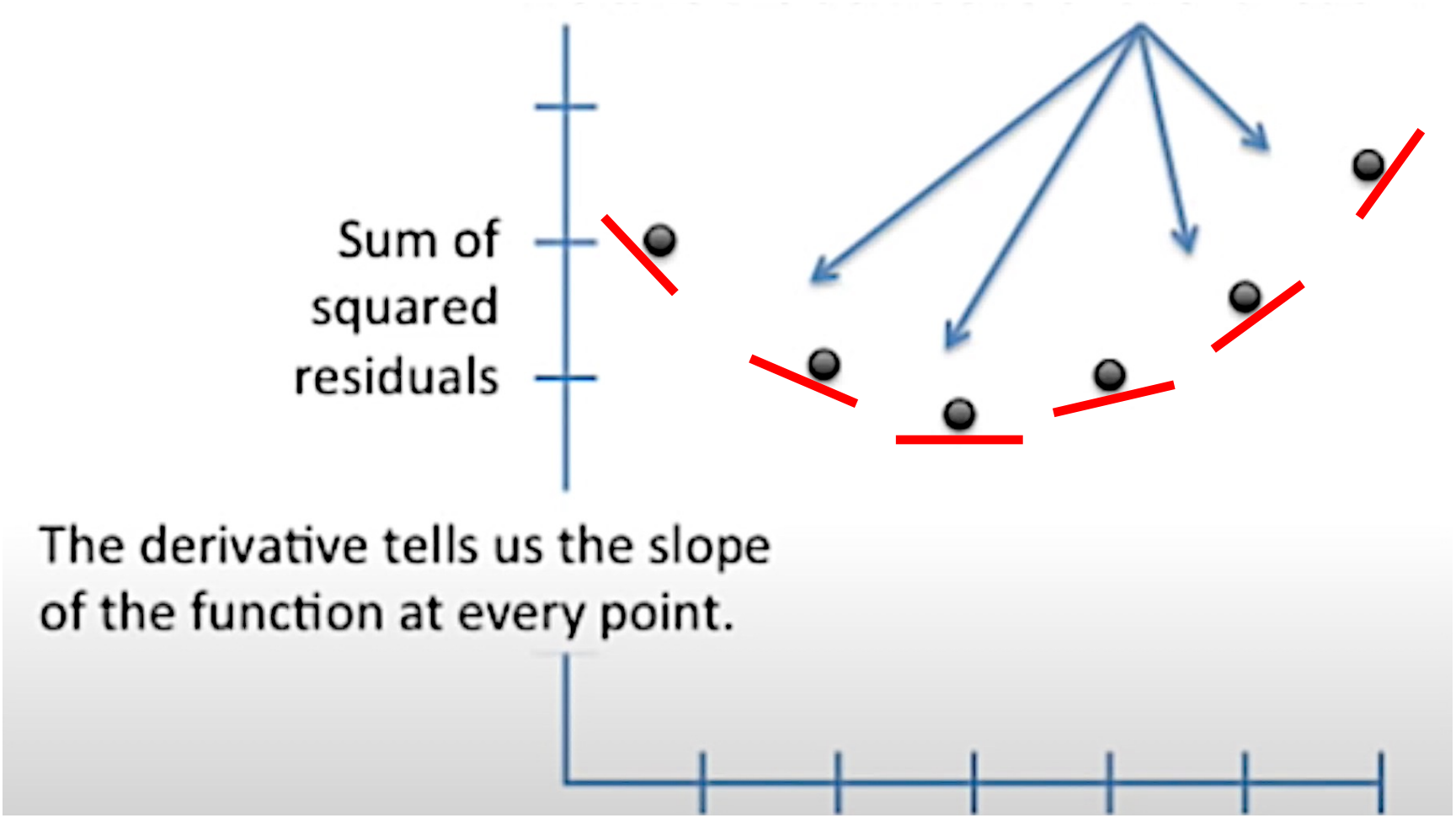


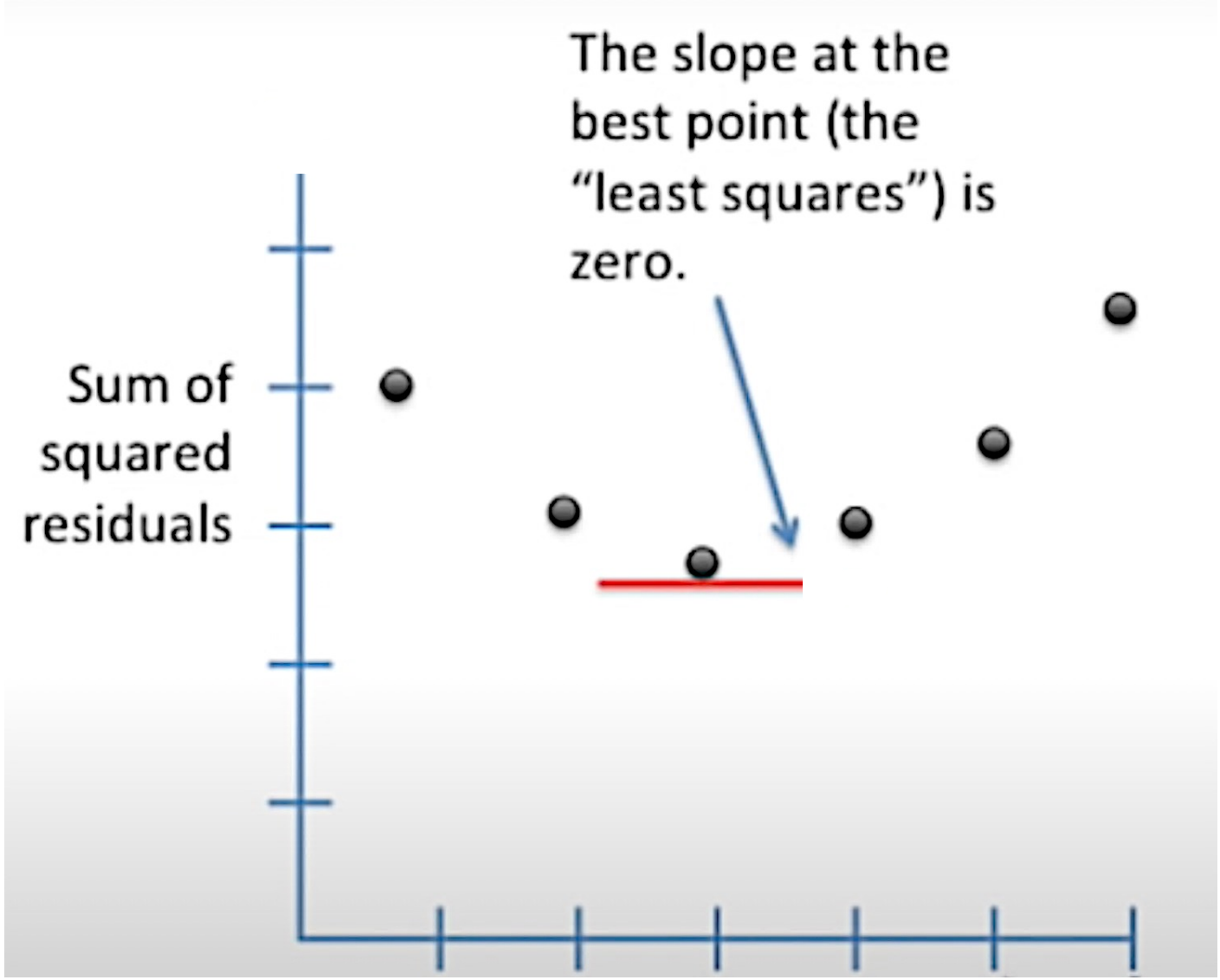
But in both cases, how do we know that we found the bottom of the curve?
What if the values we chose somewhat randomly missed the absolute bottom?

Gradient Descent is smart! It doesn’t just guess random numbers hoping to find the least sum of squares by chance.

It adjusts its guess on each iteration based on…

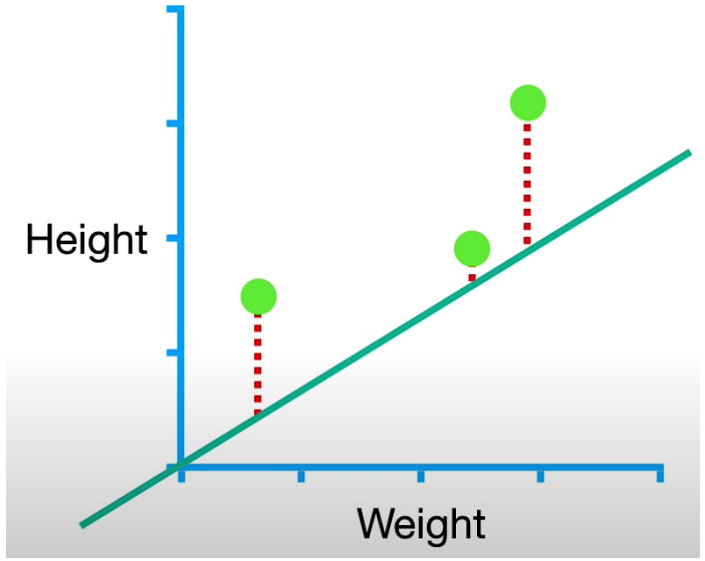
The Derivative

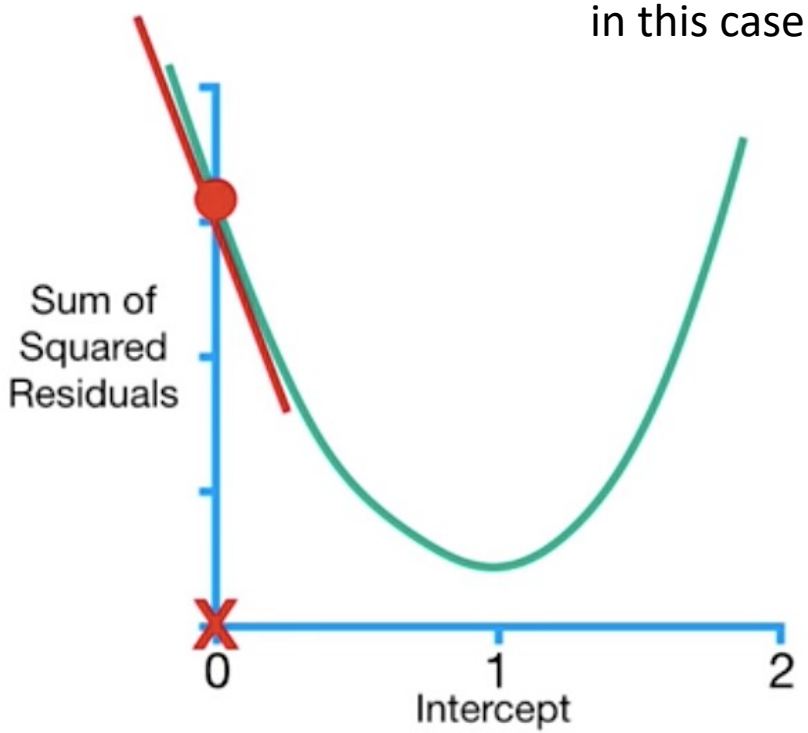

Sum of
squared
residuals
The derivative tells us the slope
of the function at every point.


The slope at the best point (the "least squares") is zero.
Sum of squared residuals

One Dimensional Gradient Descent

(looking for the optimal value for one parameter, in this case the intercept)



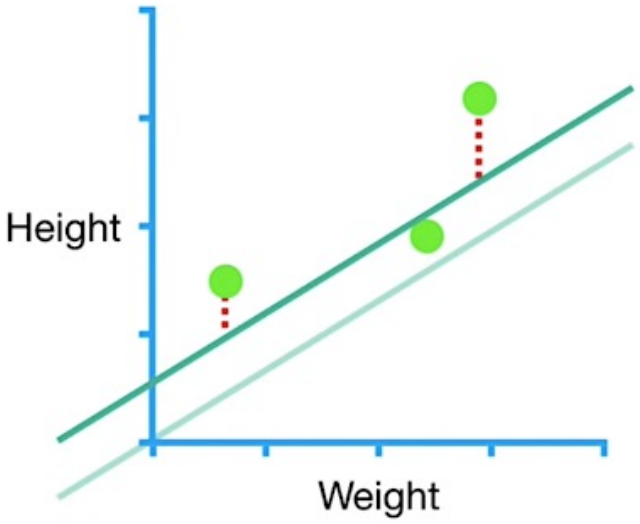


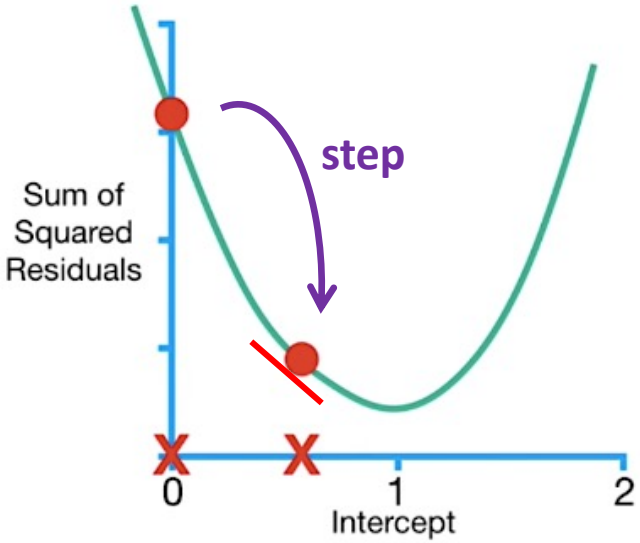
- choose random initial value for the parameter,
(let's say intercept = 0 for this example)
and plot sum of squared residuals at that point

- calculate derivative (slope of the function) at that point:
-5

- calculate **step size**: derivative * learning rate (.1)
-5 x .1 = -.5

hyperparameter
(we choose this number ourselves.
higher learning rate = bigger steps,
lower learning rate = smaller steps)

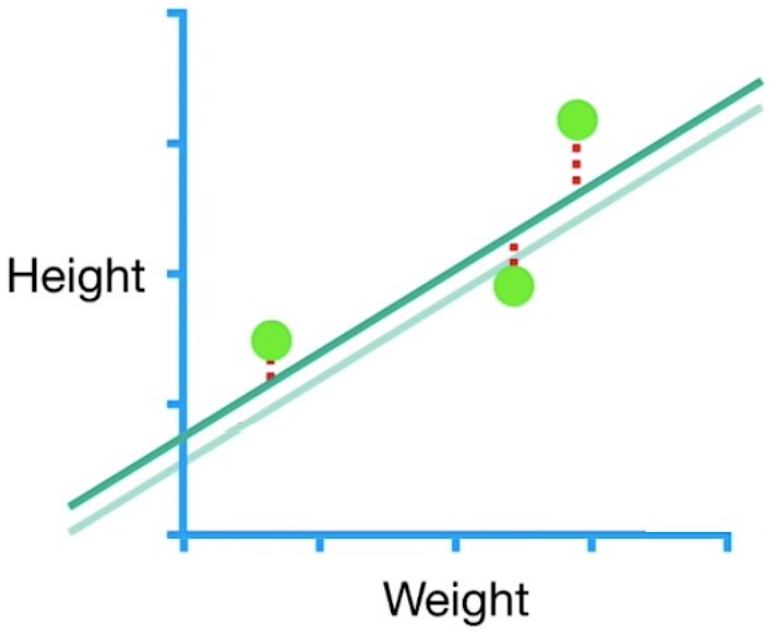


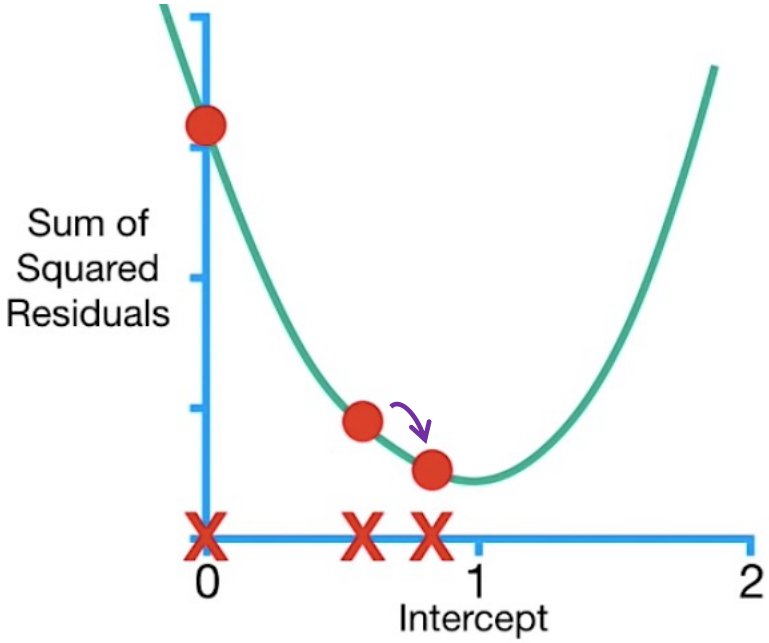


take a step!
opposite direction of the derivative,
so here we move .5 (**step size**) to the right
new intercept = .5

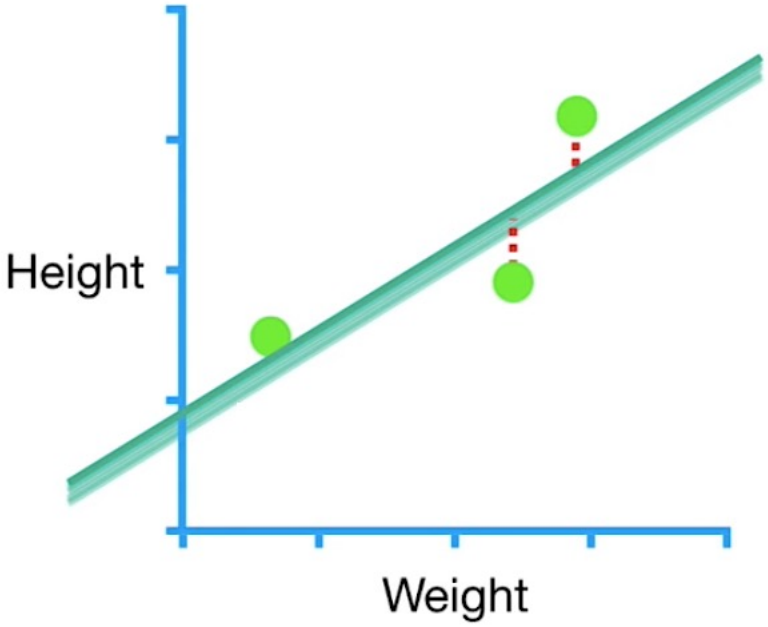
We just did 1 **epoch** (iteration).

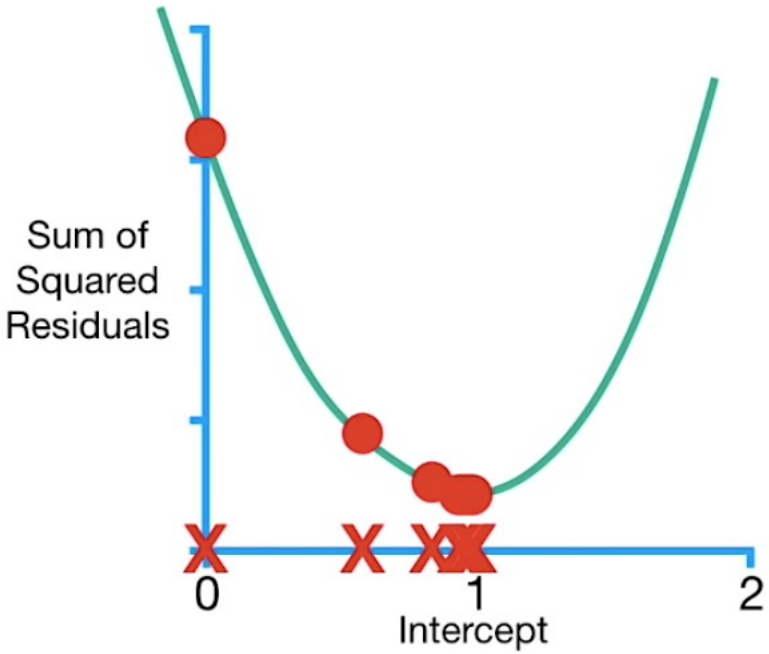
Now we repeat from our new intercept value .5:
calculate new derivative -> calculate new **step size** -> **take step**





As the **Loss** (sum of squared residuals) approaches its minimum, the derivative gets smaller, and so do the steps.





This makes Gradient Descent computationally efficient.
It does a few calculations far away from the minimum,
and more calculations as it approaches the minimum of the Loss Function.

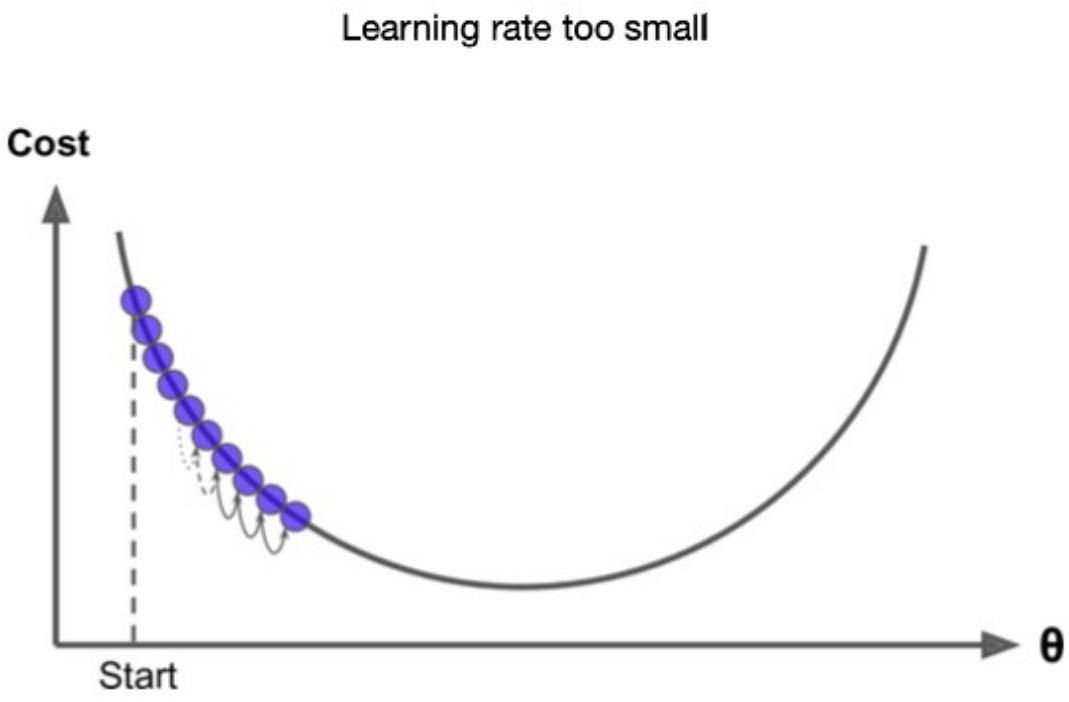
When does it stop?

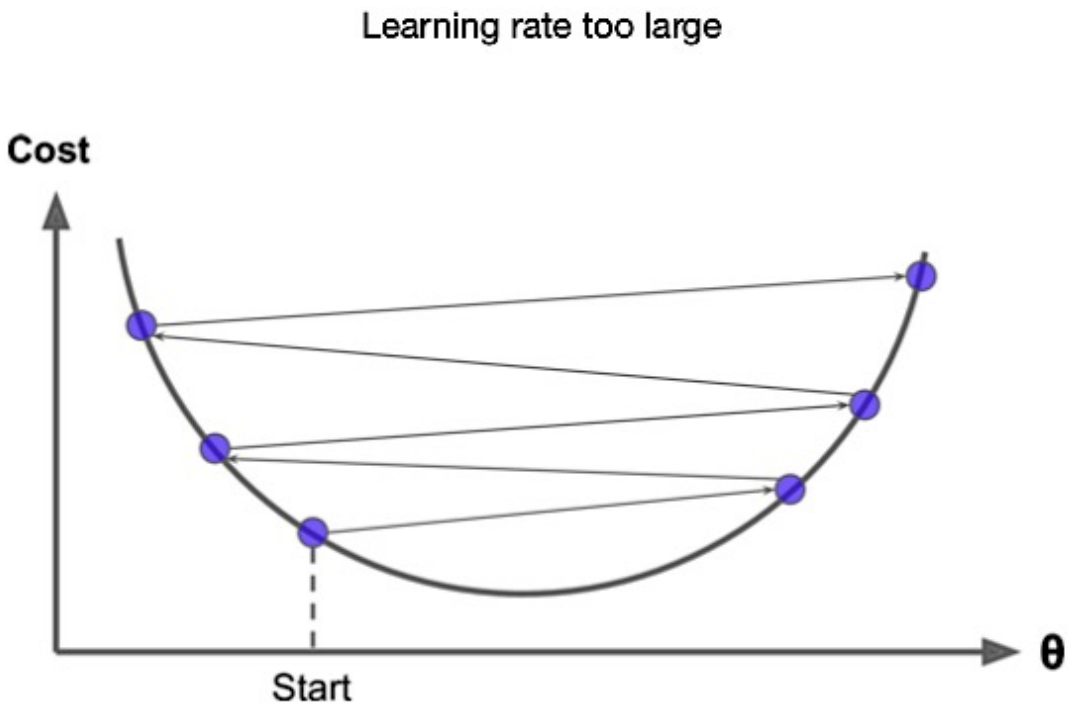
hyperparameter
(we get to choose!)

The Gradient Descent algorithm can have different **stopping criterions** :

- `Minimum Step Size` (e.g. 0.001). When the step size is smaller, the Gradient Descent has converged, and the corresponding intercept is the optimal value.
- `Maximum Number of steps` (e.g. 1000)

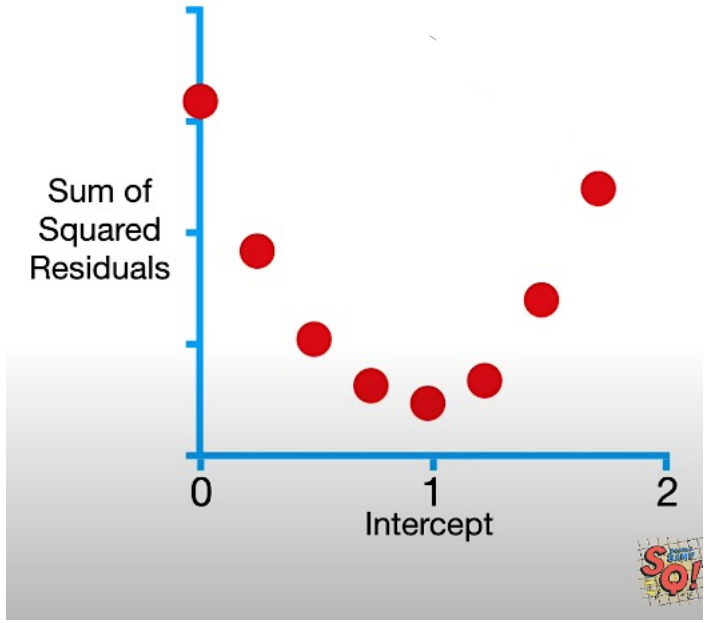
We must be careful choosing the learning rate, as it affects the step sizes.
too small or too large steps and gradient descent won't find the minimum of the loss function!

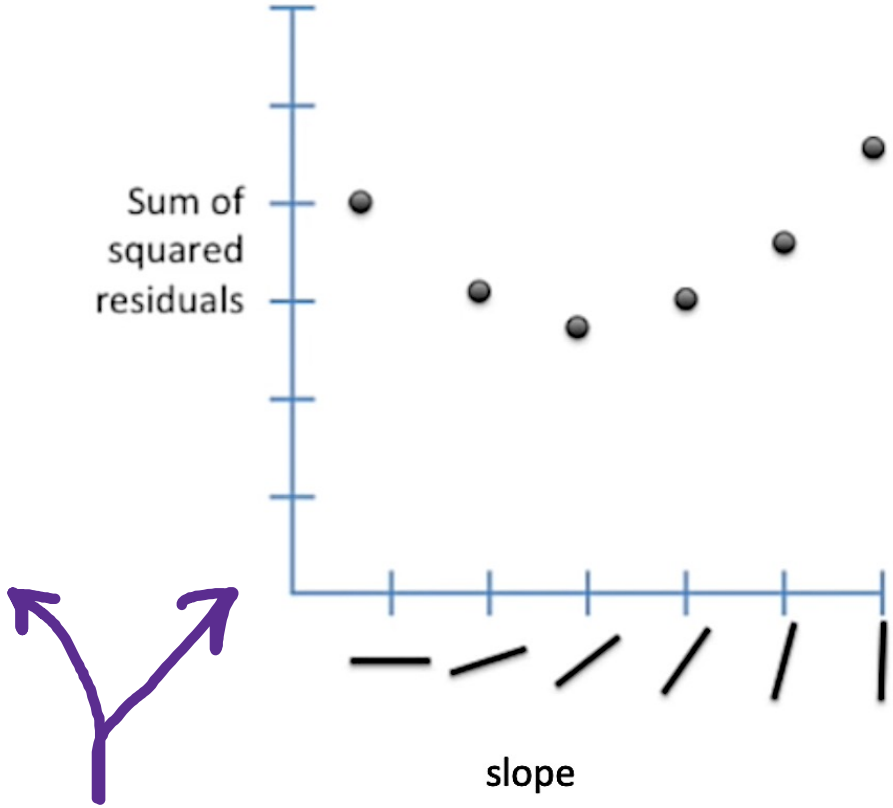




Credit: Hands-on-ML-with-Sklearn (2020)

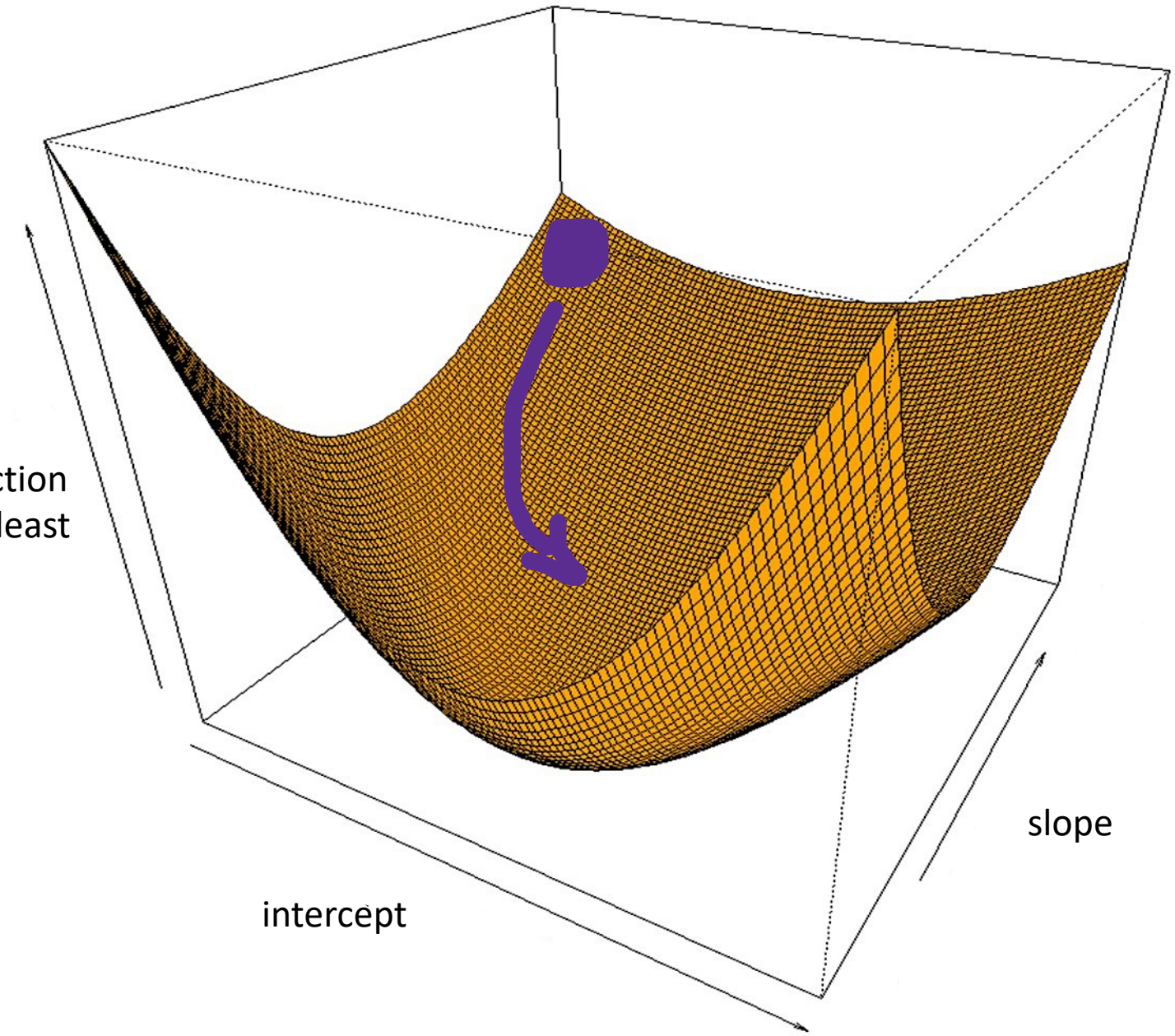
We've been talking on one-dimensional gradient descent,
looking for the optimal value for one parameter at a time…





But in reality, gradient descent looks for the optimal value for intercept and slope simultaneously!

This is called the
"**energy landscape**
of loss function"



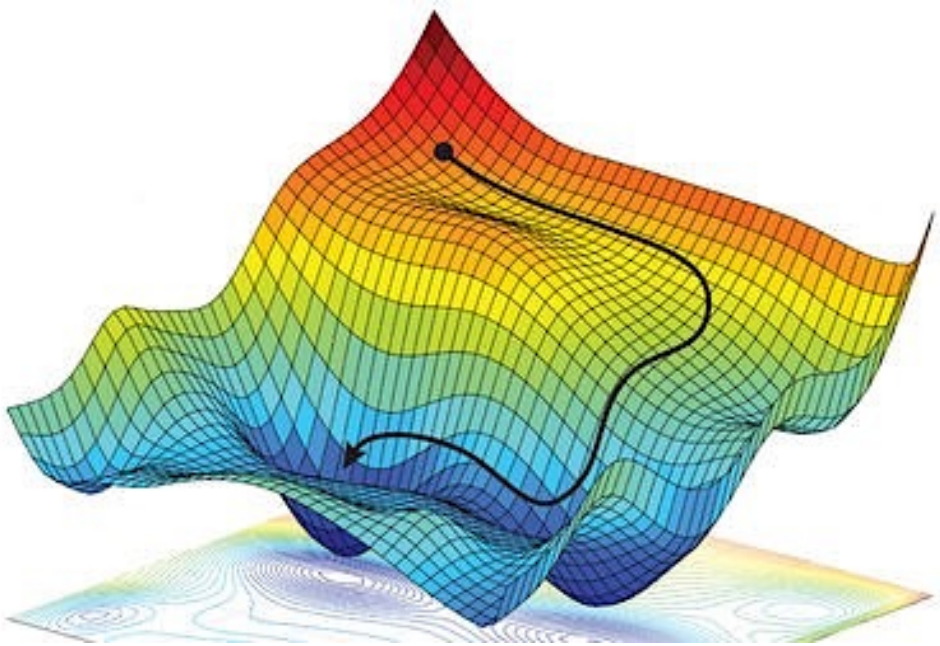
starting at a randomly chosen **slope** and **intercept**…

calculating derivatives of **both** at each epoch…

taking a step in the direction and step size set by the derivatives…

and repeat.

kind of like a ball rolling down the energy landscape until it slows down and stops at the bottom (**minimized loss function**)

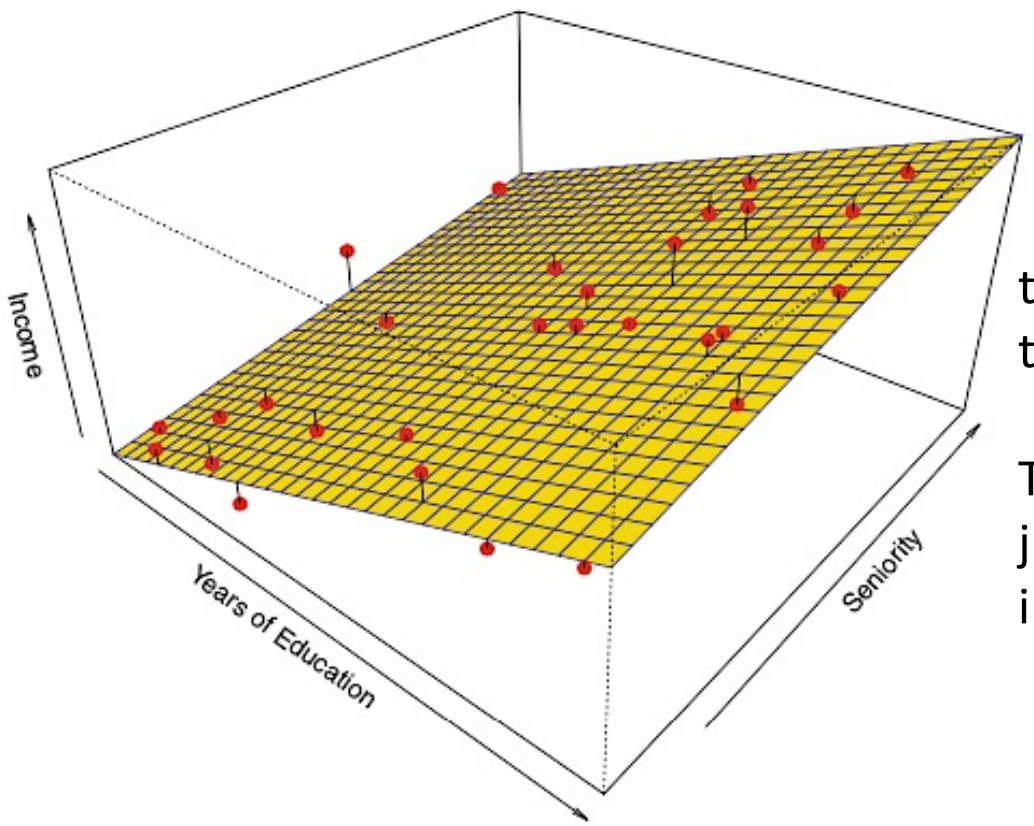


The energy landscape of the function isn't always so smooth and minimal loss isn't always so easy to find!

Some models/loss functions are much more complicated than simple linear regression/sum of squared residuals. They can have very complicated energy landscapes with 'pockets' the gradient descent could get 'stuck' in, preventing it from reaching the global (true) minimum.

We can try avoid this by adjusting the **learning rate** and **stopping criteria** hyperparameters.

what about a problem with 3 features?



then we're looking for a **plane of best fit** (instead of line of best fit) to minimize the loss function.

The loss function will still be sum of squared residuals, just calculated using the data points' distances from the plane instead of from a line.

The associated energy landscape of the loss function is in **4D**. We can't visualize it, but gradient descent still works the same to find its global minimum, calculating derivates and taking steps accordingly.

4, 5, 10, 100, 70000 features…
gradient descent will still work!

Thank You!