DATA MINING 2 Gradient Descent

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Contains edited slides from StatQuest



Gradient Descent

- GD is a very effective and widely usable mathematical technique to find the best parameters in many and various tasks such as
- Linear Regression
- Logistic Regression
- Neural Networks
- ..

GD for Linear Regression















Predicted Height = intercept + 0.64 × **Weight**



The first thing we do is pick a random value for the **Intercept**.





































Sum of squared residuals = $1.1^2 + 0.4^2 + 1.3^2 = 3.1$





















A slow and painful method for finding the minimal Sum of the Squared Residuals is to plug and chug a bunch more values for the Intercept.












...and increases the number of calculations closer to the optimal value.

































```
Sum of squared residuals = (1.4 - (intercept + 0.64 \times 0.5))^2
```

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+ (1.9 - (intercept + 0.64 × 2.3))<sup>2</sup>
+ (3.2 - (intercept + 0.64 × 2.9))<sup>2</sup>
```

So let's take the derivative of the Sum of the Squared Residuals with respect to the Intercept.



Sum of squared residuals = $(1.4 - (intercept + 0.64 \times 0.5))^2$

+ (1.9 - (intercept + 0.64 × 2.3))²

+ (3.2 - (intercept + 0.64 × 2.9))²

 $\frac{d}{d \text{ intercept}}$ Sum of squared residuals =













 $\frac{d}{d \text{ intercept}}$ Sum of squared residuals = $-2(\mathbf{1.4} - (\text{intercept} + 0.64 \times \mathbf{0.5}))$

+ -2(**1.9** - (intercept + 0.64 × **2.3**))

 $+ -2(3.2 - (intercept + 0.64 \times 2.9))$













$$\frac{d}{d \text{ intercept}} \text{ Sum of squared residuals} = -2(1.4 - (intercept + 0.64 \times 0.5)) + -2(1.9 - (intercept + 0.64 \times 2.3)) + -2(3.2 - (intercept + 0.64 \times 2.9))$$

This makes **Gradient Descent** very useful when it is not possible to solve for where the derivative = **0**, and this is why **Gradient Descent** can be used in so many different situations.




$$\frac{d}{d \text{ intercept}} \text{ Sum of squared residuals} = -2(1.4 - (0 + 0.64 \times 0.5)) + -2(1.9 - (0 + 0.64 \times 2.3))) + -2(3.2 - (0 + 0.64 \times 2.9))$$
So we plug 0 into the derivative...





...and we get -5.7.



















$$\frac{d}{d \text{ intercept}} \text{ Sum of squared residuals} = -2(\mathbf{1.4} - (0 + 0.64 \times \mathbf{0.5})) + -2(\mathbf{1.9} - (0 + 0.64 \times \mathbf{2.3})) + -2(\mathbf{3.2} - (0 + 0.64 \times \mathbf{2.9})) = -5.7$$

So the size of the step should be related to the slope, since it tells us if we should take a baby step or a big step, but we need to make sure the big step is not too big.





$$\frac{d}{d \text{ intercept}} \text{ Sum of squared residuals} = -2(1.4 - (0 + 0.64 \times 0.5)) + -2(1.9 - (0 + 0.64 \times 2.3)) + -2(3.2 - (0 + 0.64 \times 2.9)) = -5.7$$

$$\text{Step Size} = -5.7 \times 0.1$$

$$\text{ 1}$$
....by a small number called The Learning Rate.





























After 6 steps, the **Gradient Descent** estimate for the **Intercept** is **0.95**.



Gradient Descent stops when the Step Size is Very Close To 0.

Step Size = Slope × Learning Rate





In practice, the **Minimum Step Size** = 0.001 or smaller.

Step Size = Slope × Learning Rate



That said, **Gradient Descent** also includes a limit on the number of steps it will take before giving up.












+ (**1.9** - (intercept + slope × **2.3**))² + (**3.2** - (intercept + slope × **2.9**))²

Height Height Weight ...and just like before, we'll take the derivative with respect to the Intercept...

+ (**1.9** - (intercept + slope × **2.3**))² + (**3.2** - (intercept + slope × **2.9**))²



+ (1.9 - (intercept + slope × 2.3))²

+ (3.2 - (intercept + slope × 2.9))²

We'll start by taking the derivative with respect to the intercept. $\frac{d}{d \text{ intercept}}$ Sum of squared residuals =

+ (1.9 - (intercept + slope × 2.3))²

+ (3.2 - (intercept + slope × 2.9))²

Just like before, we take the derivative of each part...

$$\frac{d}{d \text{ intercept}}$$
 Sum of squared residuals =
$$\frac{d}{d \text{ intercept}} (\mathbf{1.4} - (\text{intercept} + \text{slope} \times \mathbf{0.5}))^2$$

+ (1.9 - (intercept + slope × 2.3))²

+ (**3.2** - (intercept + slope × **2.9**))²

Just like before, we take the derivative of each part...

$$\frac{d}{d \text{ intercept}} \text{ Sum of squared residuals} = \frac{d}{d \text{ intercept}} (1.4 - (\text{intercept} + \text{slope} \times 0.5))^2 + \frac{d}{d \text{ intercept}} (1.9 - (\text{intercept} + \text{slope} \times 2.3))^2 + \frac{d}{d \text{ intercept}} (3.2 - (\text{intercept} + \text{slope} \times 2.9))^2$$



GD for *m*, *b*



+ -2(**1.9** - (intercept + slope × **2.3**))² + -2(**3.2** - (intercept + slope × **2.9**))²



+ (1.9 - (intercept + slope × 2.3))²

+ (3.2 - (intercept + slope × 2.9))²

Now let's take the derivative of the Sum of the Squared Residuals with respect to the **Slope**. $\frac{d}{d \ slope}$ Sum of squared residuals =

+ (1.9 - (intercept + slope × 2.3))²

+ (3.2 - (intercept + slope × 2.9))²

Just like before, we take the derivative of each part...

$$\frac{d}{d \ slope}$$
 Sum of squared residuals =
$$\frac{d}{d \ slope}$$
 (**1.4** - (intercept + slope × **0.5**))²

+ (1.9 - (intercept + slope × 2.3))²

+ (**3.2** - (intercept + slope × **2.9**))²

Just like before, we take the derivative of each part...

$$\frac{d}{d \ slope} \text{ Sum of squared residuals} = \frac{d}{d \ slope} (1.4 - (intercept + slope \times 0.5)) + \frac{d}{d \ slope} (1.9 - (intercept + slope \times 2.3))^2 + \frac{d}{d \ slope} (3.2 - (intercept + slope \times 2.9))^2$$









 $\frac{d}{d \text{ intercept}}$ Sum of squared residuals = -2(**1.4** - (intercept + slope × **0.5**) + -2(**1.9** - (intercept + slope × **2.3**)) + -2(**3.2** - (intercept + slope × **2.9**))

> **NOTE:** When you have two or more derivatives of the same function, they are called a **Gradient**.

 $\frac{d}{d \text{ slope}}$ Sum of squared residuals = -2 × **0.5(1.4** - (intercept + slope × **0.5**))

+ -2 × 2.9(3.2 - (intercept + slope × 2.9))²

+ -2 × **2.3(1.9** - (intercept + slope × **2.3**))²

 $\frac{d}{d \text{ intercept}}$ Sum of squared residuals = -2(**1.4** - (intercept + slope × **0.5**) + -2(**1.9** - (intercept + slope × **2.3**)) + -2(**3.2** - (intercept + slope × **2.9**))

We will use this **Gradient** to **descend** to lowest point in the **Loss Function**, which, in this case, is the Sum of the Squared Residuals...

...thus, this is why this algorithm is called Gradient Descent!



+ -2 × 2.9(3.2 - (intercept + slope × 2.9))²

+ -2 × 2.3(1.9 - (intercept + slope × 2.3))²

```
\frac{d}{d \text{ intercept}}Sum of squared residuals =
-2(1.4 - (intercept + slope × 0.5)
+ -2(1.9 - (intercept + slope × 2.3))
+ -2(3.2 - (intercept + slope × 2.9))
```

Just like before, we will start by picking a random number for the Intercept. In this case we'll set the Intercept = 0...

...and we'll pick a random number for the **Slope**. In this case we'll set the **Slope** = **1**.

```
\frac{d}{d \ slope}Sum of squared residuals =
-2 × 0.5(1.4 - (intercept + slope × 0.5))
+ -2 × 2.9(3.2 - (intercept + slope × 2.9))<sup>2</sup>
```

+ -2 × 2.3(1.9 - (intercept + slope × 2.3))²













```
\frac{d}{d \text{ intercept}} Sum of squared residuals =
-2(1.4 - (0 + 1 × 0.5) Step Size<sub>Intercept</sub> = -1.6 × 0.01 = -0.016
                 + -2(1.9 - (0 + 1 \times 2.3)) New Intercept = 0 - (-0.016) = 0.016
                 + -2(3.2 - (0 + 1 \times 2.9)) = -1.6
                                                                                  ... and we end up
                                                                               with a New Intercept
                                                                                 and a New Slope.
                                                      Step Size<sub>Slope</sub> = -0.8 × 0.01 = 0.008
\frac{d}{d \text{ slope}} Sum of squared residuals = -2 \times 0.5(1.4 - (0 + 1 \times 0.5))
                                                             New Slope = 1 - (-0.008) = 1.008
                 + -2 \times 2.9(3.2 - (0 + 1 \times 2.9))^2
                 + -2 \times 2.3(1.9 - (0 + 1 \times 2.3))^2 = -0.8
```

GD for *m*, *b*



GD for *m*, *b*















Weight



Weight





We now know how **Gradient Descent** optimizes two parameters, the **Slope** and **Intercept**.

GD for more parameters and variables



If we had more parameters, then we'd just take more derivatives and everything else stays the same.

Gradient Descent Recap

Step 1: Take the derivative of the **Loss Function** for each parameter in it. In fancy Machine Learning Lingo, take the **Gradient** of the **Loss Function**.
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Step 2: Pick random values for the parameters.

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Step 3: Plug the parameter values into the derivatives (ahem, the Gradient).

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Step 4: Calculate the Step Sizes: Step Size = Slope × Learning Rate

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Step 4: Calculate the Step Sizes: Step Size = Slope × Learning Rate

Step 5: Calculate the New Parameters:

New Parameter = Old Parameter - Step Size

Now go back to Step 3 and repeat until Step Size is very small, or you reach the Maximum Number of Steps.

Step 3: Plug the parameter values into the derivatives (ahem, the Gradient).

Step 4: Calculate the Step Sizes: Step Size = Slope × Learning Rate

Step 5: Calculate the New Parameters:

New Parameter = Old Parameter - Step Size

Stochastic Gradient Descent



Stochastic Gradient Descent



...but when you have millions of data points, it can take a long time.

Stochastic Gradient Descent



So there is a thing called **Stochastic Gradient Descent** that uses a randomly selected subset of the data at every step rather than the full dataset.

This reduces the time spent calculating the derivatives of the **Loss Function**.

GD Summary

- GD is an optimization algorithm.
- You can use GD to find minimum (or maximum, then it is called Gradient Ascent) of many different functions.
- GD does not really care what is the function that it minimizes, it just does what it was asked for.
- Using GD, you must know how tell if one value of the parameter of interest is "better" than the other.
- You must provide GD some function to minimize/maximize, and GD will deal with finding its optimum value.

References

- Lemaréchal, C. (2012). "Cauchy and the Gradient Method" (PDF). Doc Math Extra: 251–254.
- An overview of gradient descent optimization algorithms [pdf]