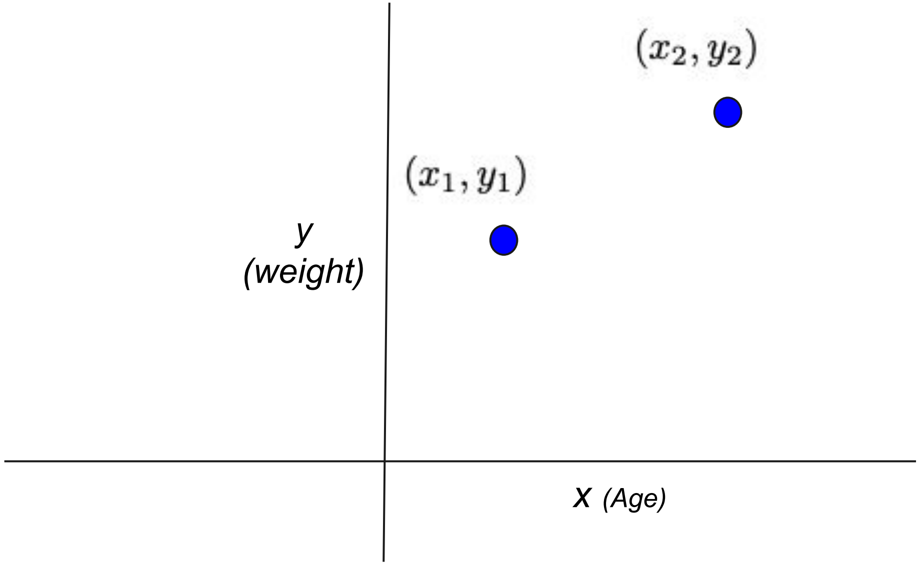
CIS 635 - Knowledge Discovery & Data Mining

ML Model training: Introduction to Gradient descent

What we'd like to accomplish today

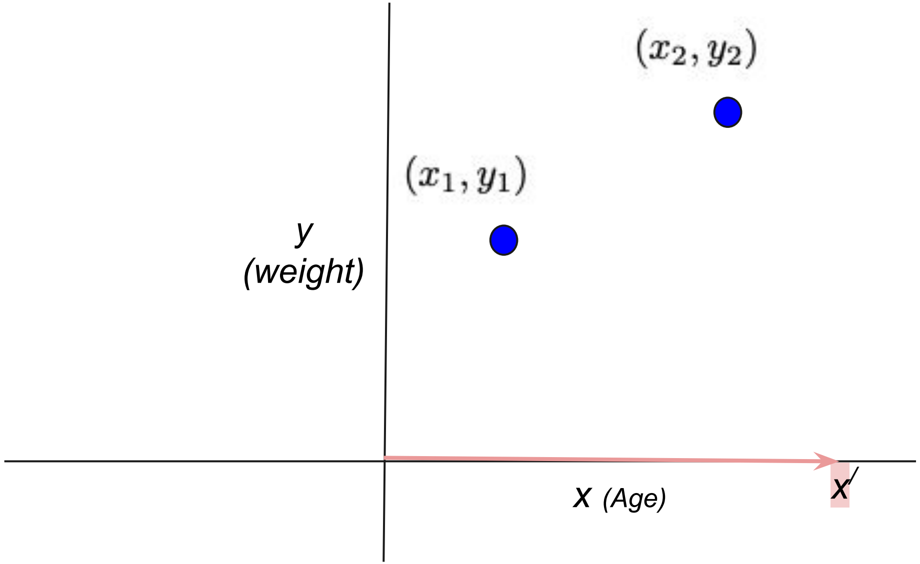
- Model training using Gradient descent
  - ➜ Refreshing some high school maths: **linear equation**
  - ➜ A simple two parameter **linear regression** model
  - ➜ The **Gradient descent algorithm**
- Hands on **Notebook implementation**
- QA

k-NN Regression



Given two known data points (x_1,y_1), and (x_2,y_2), and

k-NN Regression



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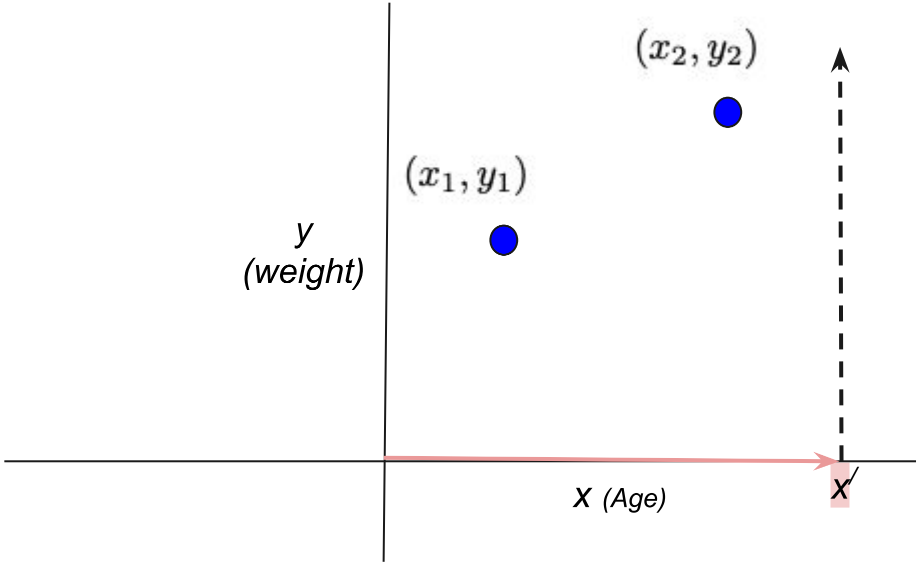
- for test input $x^{/}$, you have to predict $y(x^{/})$.
- I.e. you have to plot $(x^{/}, ?)$

k-NN Regression



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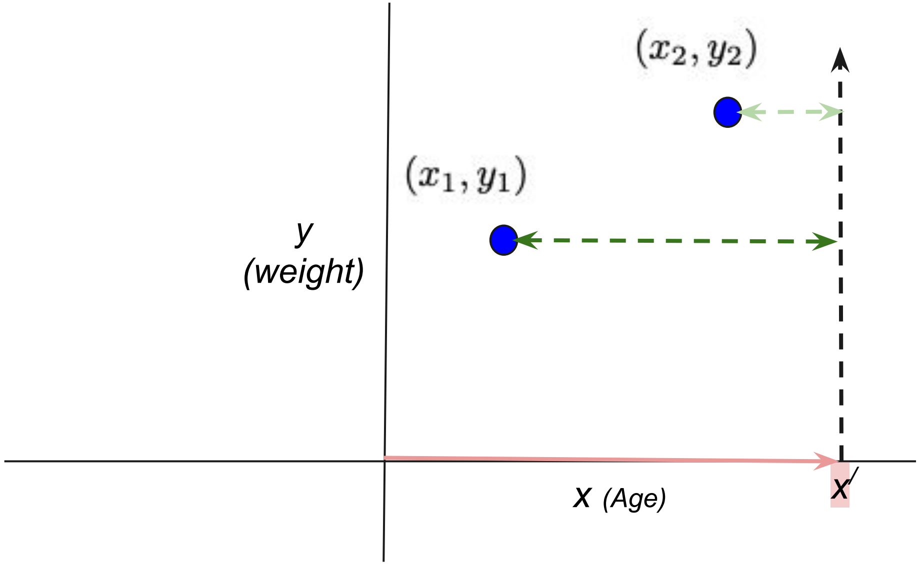
- To estimate the distances let's draw the vertical line

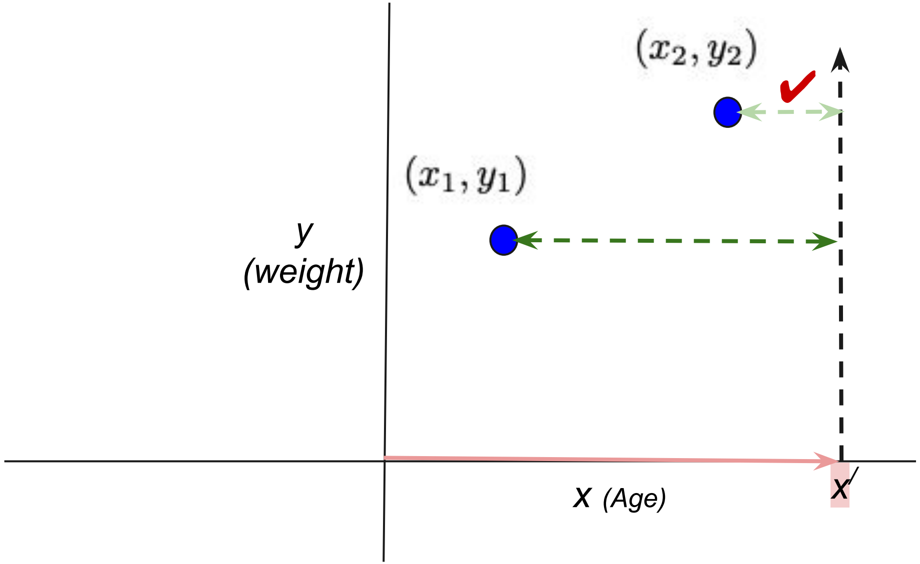
k-NN Regression



Given two known data points (x_1,y_1), and (x_2,y_2), and

- for test input x', you have to predict $y(x')$.
- I.e. you have to plot $(x', ?)$
- To estimate the distances let's draw the vertical line
- Horizontal dotted lines show the point distances (L1)

k-NN Regression



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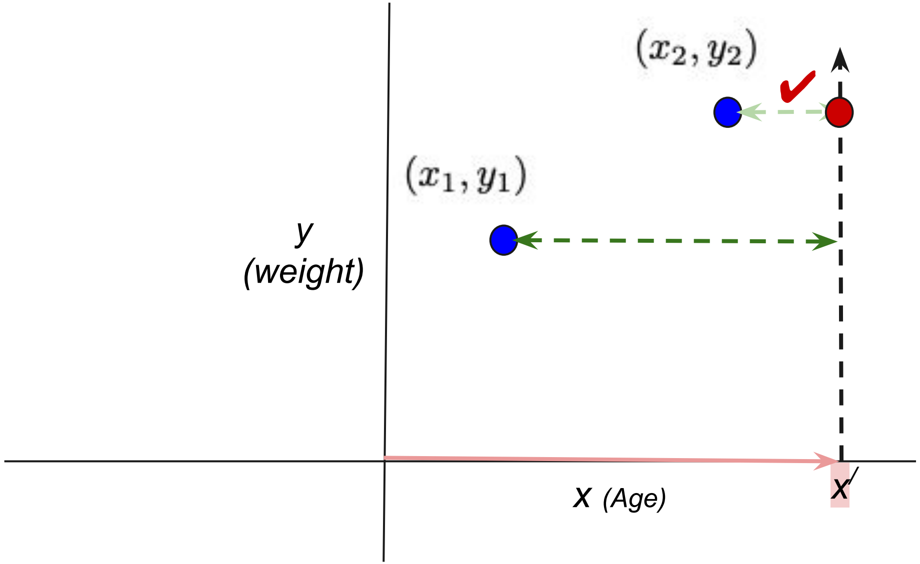
k-NN Regression



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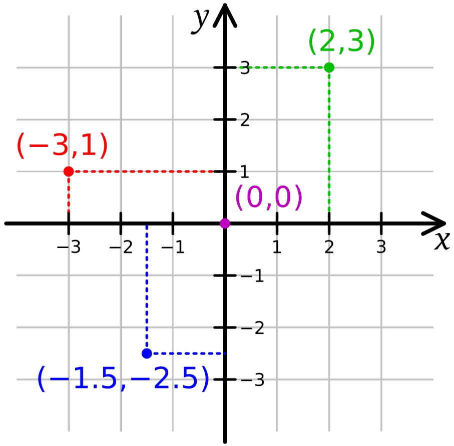
- I.e. you have to plot $(x^{/}, ?)$
- To estimate the distances let's draw the vertical line
- Horizontal dotted lines show the point distances (L1)
- We find the lighter green on is the closest one [k(1)-NN]
- We propagate the associated label(s), i.e.

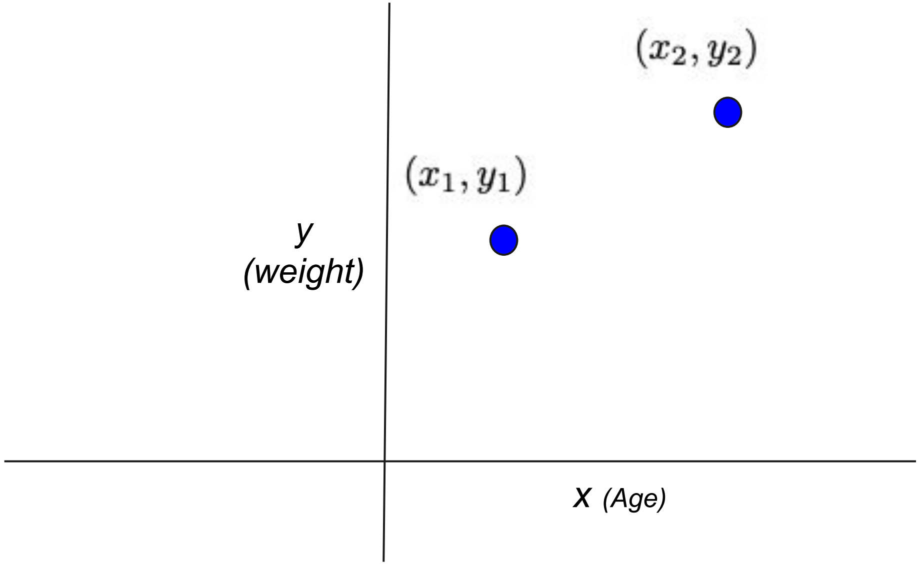
  $y(x^{/}) = y_2$
- If we have more data points we may go for a higher k, and take the average

Recall, we said k-NN is non parametric

- K-nearest neighbors (k-NN)
  - Supervised learning
  - **Non parametric**
- Based on what data (features are available) and on distance measures.

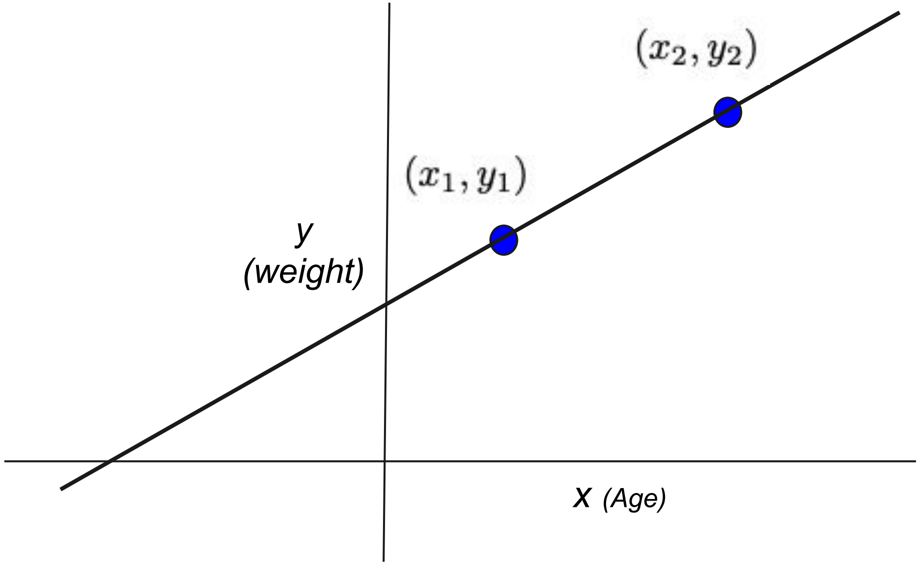


Linear equation, a quick review



Given two data points

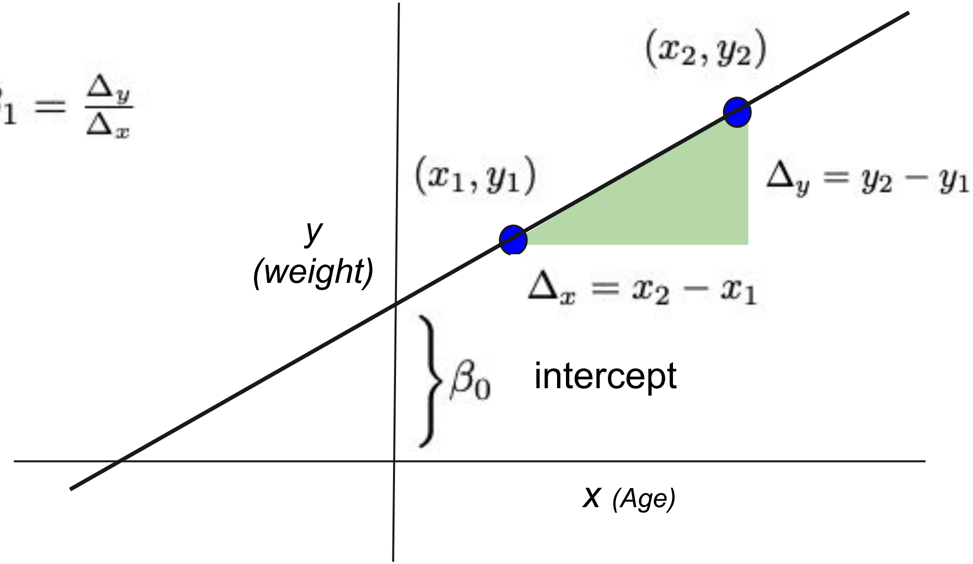
Linear equation, a quick review



We can fit a linear equation

Linear equation to a linear function, a quick review

slope $\beta_1 = \frac{\Delta_y}{\Delta_x}$



- This linear equation can be used to explain the relationship between the two axes ***x*** (independent variable) vs ***y*** (dependent variable) - as

$$y = \beta_0 + \beta_1 x$$

- A simple model with parameters: **slope**, and **intercept**

- For any given x', this model can predict $y(x')$ using the above equation.

Linear equation to a linear function, a quick review

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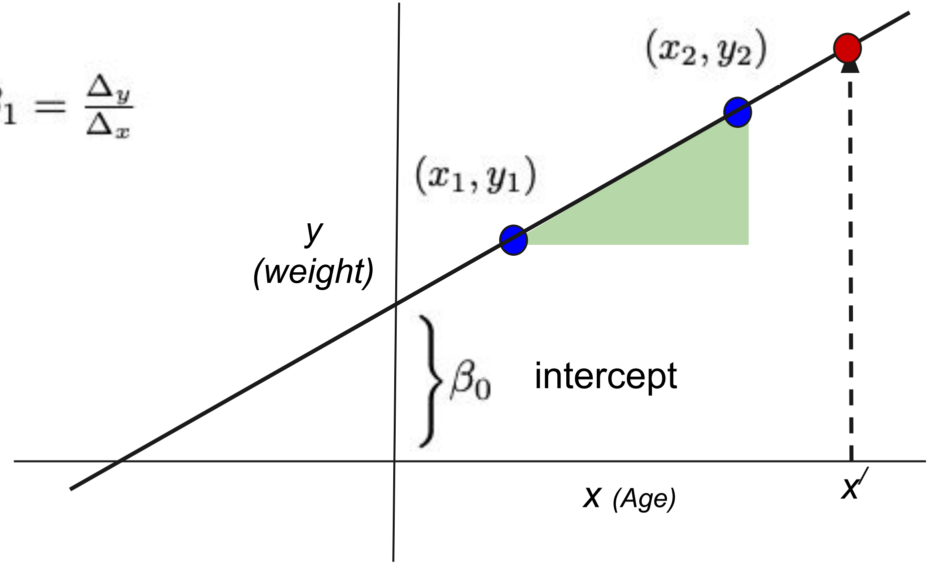

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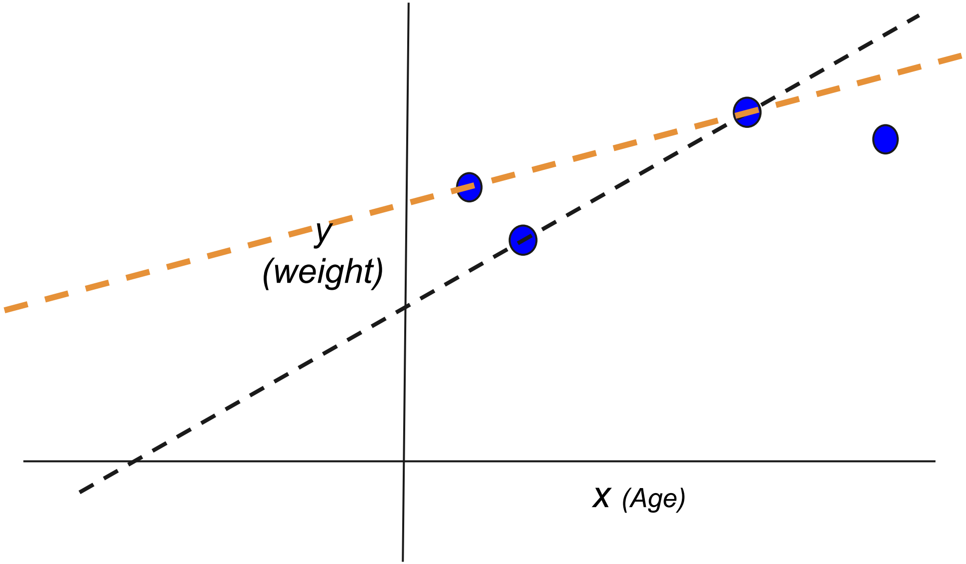
Fitting a Linear function, a quick review



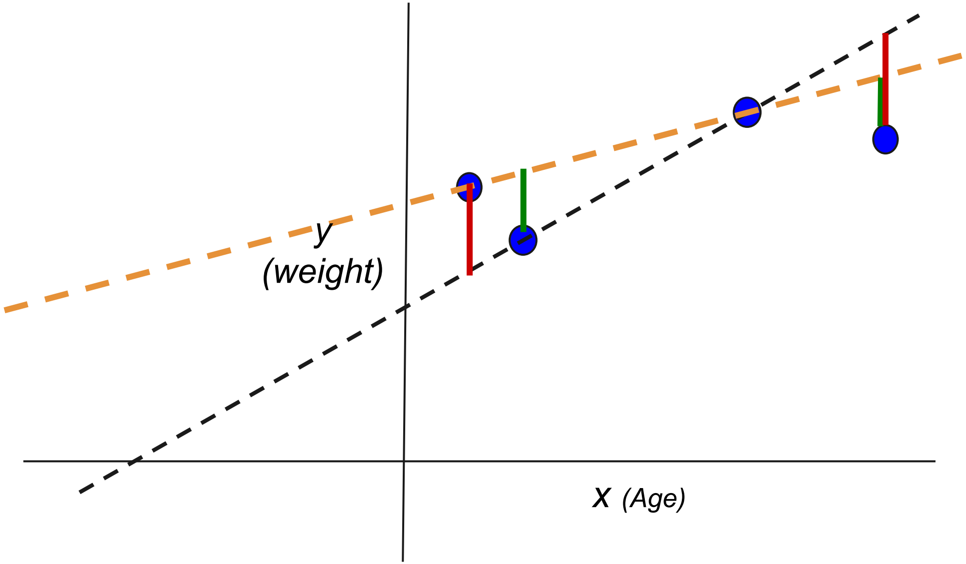
- Example of linear relationship: age vs weight of a person, marketing expense vs sales
- > 2 data points are unlikely fit perfectly on a straight line, which a straight line (2 param model) cannot fit
- We need some approximations
- Let's examine the two models for the 4 data points on the left

model β_0, β_1

model: β_0, β_1

- Both model perfectly fits 2 points each
- Orange (visual screening) model seems to be a better fit, but why?

Fitting a Linear function/function, a quick review



Based on Error is higher than **Error**

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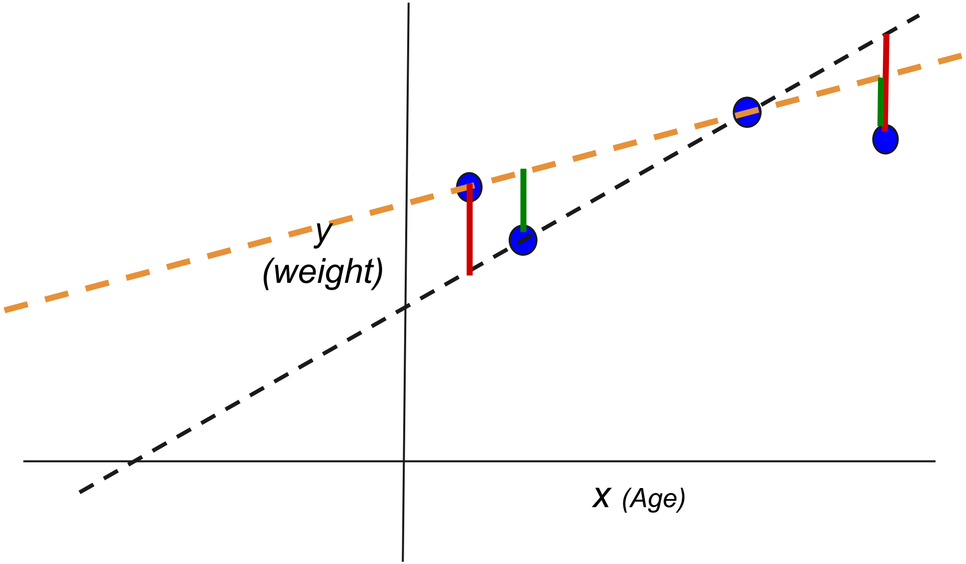
Fitting a linear function/model



Model

$$\hat{y} = \beta_0 + \beta_1 x$$

$$\Theta = \{\beta_0, \beta_1\}$$

Fitting Error

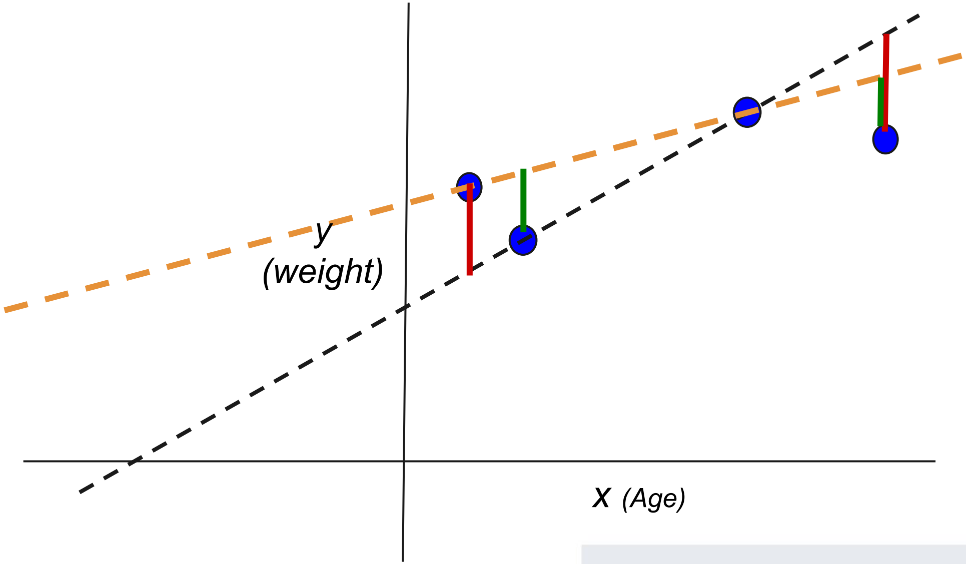
$$\epsilon = |\hat{y} - y|$$

Optimization/loss function

$$E_\Theta = \frac{1}{2}\sum_{i=1}^{N}(\hat{y}_i - y_i)^2$$

$$\Theta^* = \text{argmin}_\Theta\, E\{(x_i, y_i)\}_{i=1,\cdots,N}$$

Fitting a linear function/model



Ordinary Least Squares(OLS)

$$\hat{\beta} = (\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{y},$$

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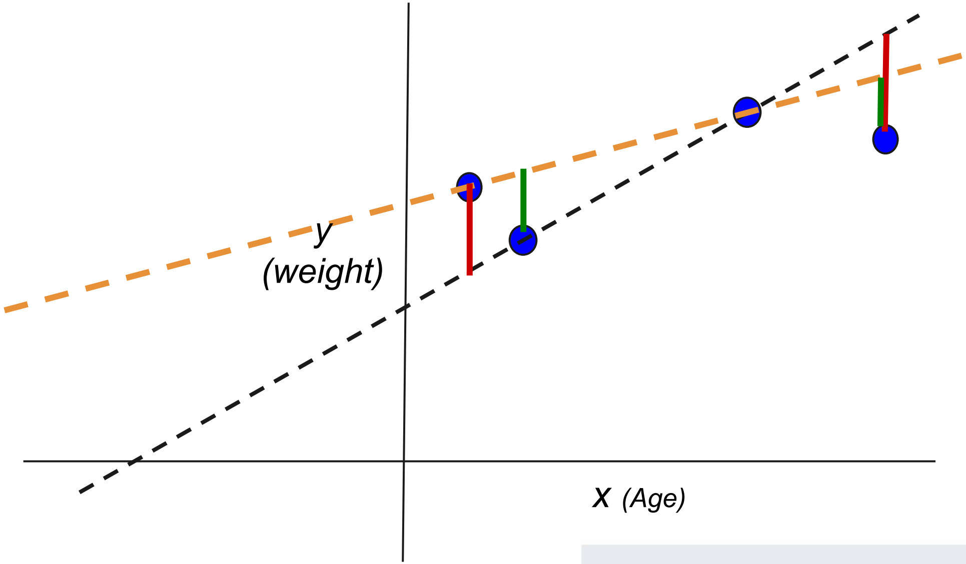

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Out of scope today

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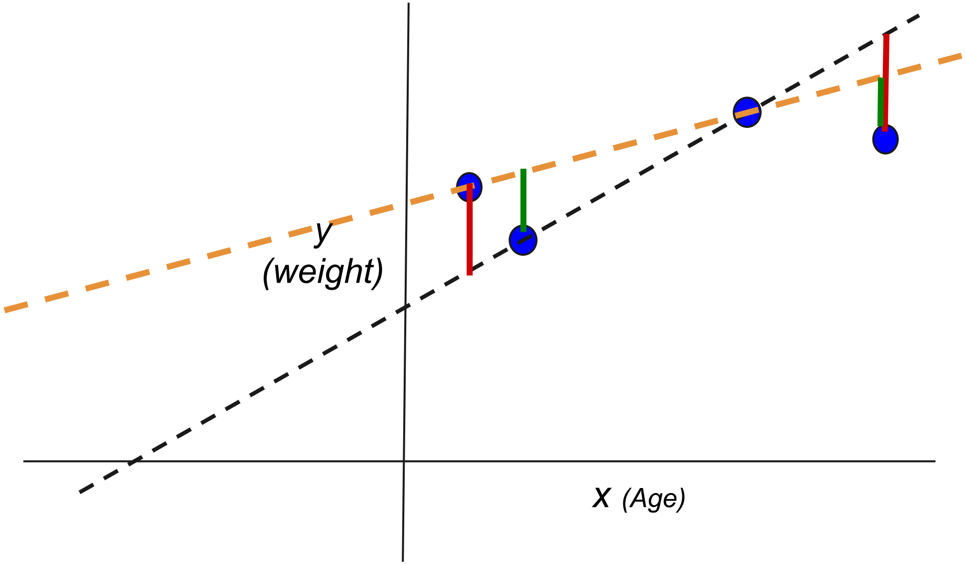
Gradient descent (- ascent)



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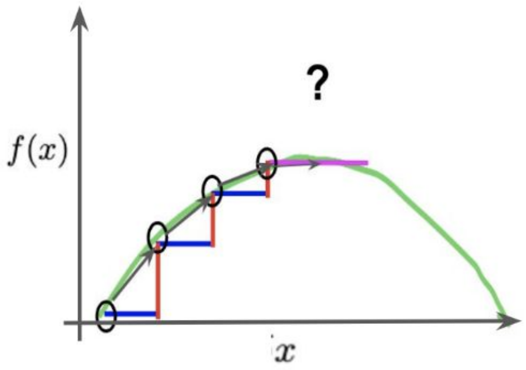
Gradient descent (- ascent)

- We have decided to build some stairs as we need to visit the top of a mountain frequently. We want
  - To produce **equal** width stairs (**step size**)
  - To make the stair corners **touch the periphery** of the mountain (maybe someday we want recreate the shape of the mountain)

- For such a **convex** function ***f(x)***, we will have varying height stairs, and at the **top of the mountain** stairs height will be **close to zero**, an indicator that we are at the top.
- Stair **height/width** is called the **gradient** of *f(x)*, the arrowhead denoting ts **direction (towards an increasing value)**.
- We have to choose the **step size** sensibly: larger step size may miss the peak while smaller step size will take too much efforts to reach to the top



$step\ size:\ \delta x$

$gradient:\ \frac{\delta}{\delta x} f(x)$

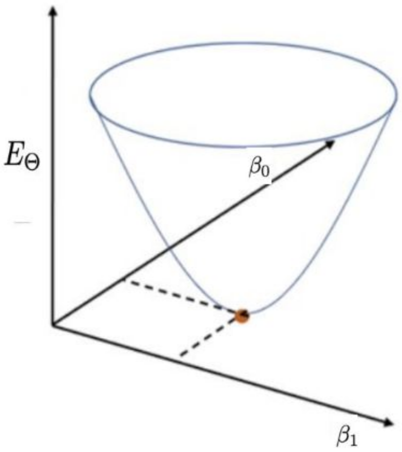
Gradient descent (- ascent)

1. Start with an initial ***(β_0, β_1)*** and a ***learning rate (L)*** , a scalar, which controls the gradient step.
2. For ***N*** training data points, estimate the **model loss**
3. Estimate the gradient (vector of partial derivatives): $\nabla E_\Theta = \left[\frac{\delta}{\delta\beta_0}(E_\Theta), \frac{\delta}{\delta\beta_1}(E_\Theta)\right]$
4. Update parameters

$$\beta_0 \leftarrow \beta_0 - L * \frac{\delta}{\delta\beta_0}(E_\Theta)$$

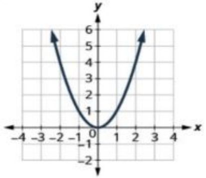
$$\beta_1 \leftarrow \beta_1 - L * \frac{\delta}{\delta\beta_1}(E_\Theta)$$

4. Go to step 2) and iterate until the model loss reaches a predefined **threshold** or a certain **number of iterations** are executed.



Objective function

$$\Theta^* = \text{argmin}_\Theta\, E\{(x_i, y_i)\}_{i=1,\cdots,N}$$



Partial derivatives

$$\frac{\delta}{\delta\beta_0}(E_\Theta) = \sum_{i=1}^{N}(\beta_0 + \beta_1 x_i - y_i)$$

$$\frac{\delta}{\delta\beta_1}(E_\Theta) = \sum_{i=1}^{N}(\beta_0 + \beta_1 x_i - y_i)x_i$$

Variants of gradient descent (- ascent)

- **Batch gradient descent**: Gradient based on chunk of data
- **Stochastic gradient descent**: chunk size is **1**

Notebook presentation

- Notebook github
  - ➜ Gradient descent training (Linear Regression)

What we have discussed today

- Model training using Gradient descent
  - ➜ Refreshing some high school maths: **linear equation**
  - ➜ A simple two parameter **linear regression** model
  - ➜ The **Gradient descent algorithm**
- Hands on **Notebook implementation**
- **QA …….**

GPT

I know one of your
tricks; get you soon!!

Our model today