Optimization & Stochastic Gradient Descent

Bibek Poudel

Sections

- Optimization
- Gradient Descent
- Problems with Gradient Descent
- Stochastic Gradient Descent and variants
- Recap

Optimization

Optimization

- “Doing most with the least”
- “Find most effective or favorable values”
- E.g., minimize cost, maximize profit

Optimization

- Statistics, Machine Learning, Data Science → Solving optimization
- Mathematically:

"maximize or minimize a function by systematically choosing input values from an allowed set while fulfilling constraints, if any"

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Optimization (Toy example)

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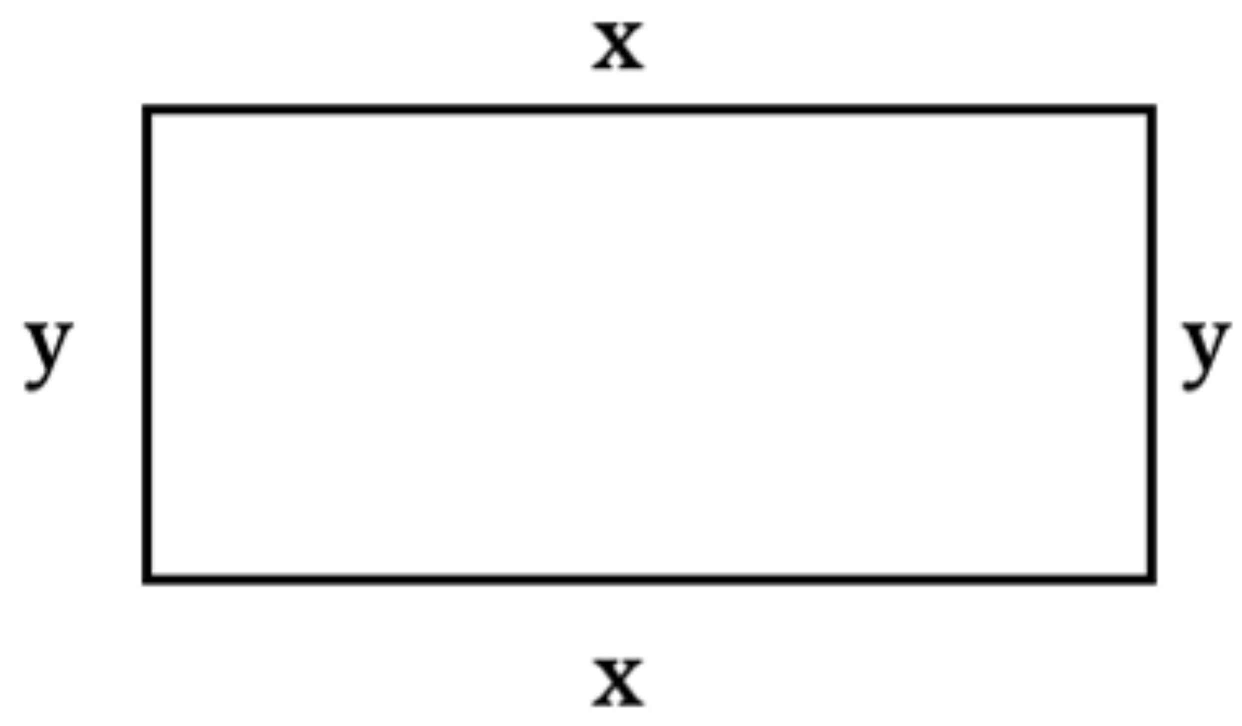
Find the length and breadth of a rectangle whose area is 100, keeping the perimeter as small as possible.



Optimization (Toy example)

- Objective Function
- Constraint

Find the length and breadth of a rectangle whose area is 100, keeping the perimeter as small as possible.

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Find the length and breadth of a rectangle whose area is 100, keeping the perimeter as small as possible.

Minimize: 2(x+y)
Subject to: x.y =100

Goal: Find the best fit of x and y
Solution: x=10 , y=10

Optimization

- Hand crafting a solution may not always be feasible
- A high dimensional problem may not be intuitive

Gradient Descent

Gradient Descent

- First order iterative algorithm to find a local minimum of a differentiable function.

Gradient Descent

- First order iterative algorithm to find a local minimum of a differentiable function.
- Key words:
  - First order
  - Iterative
  - Local minimum
  - Differentiable

Gradient Descent (Worked out example)

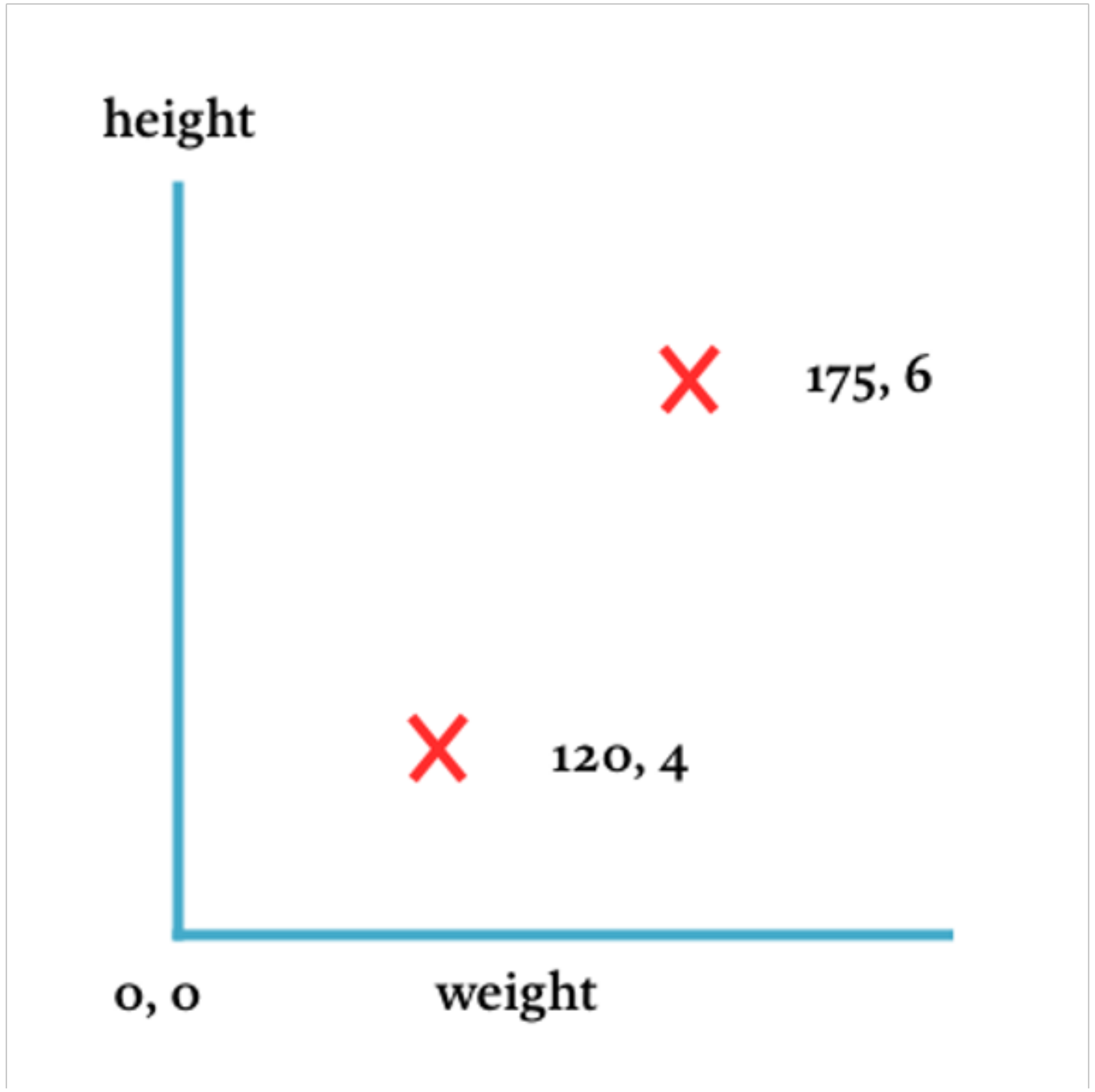
Gradient Descent (Worked out example)

- Data (feature, target)
- Goal

weight (lb.)	height (ft.)
120	4
175	6

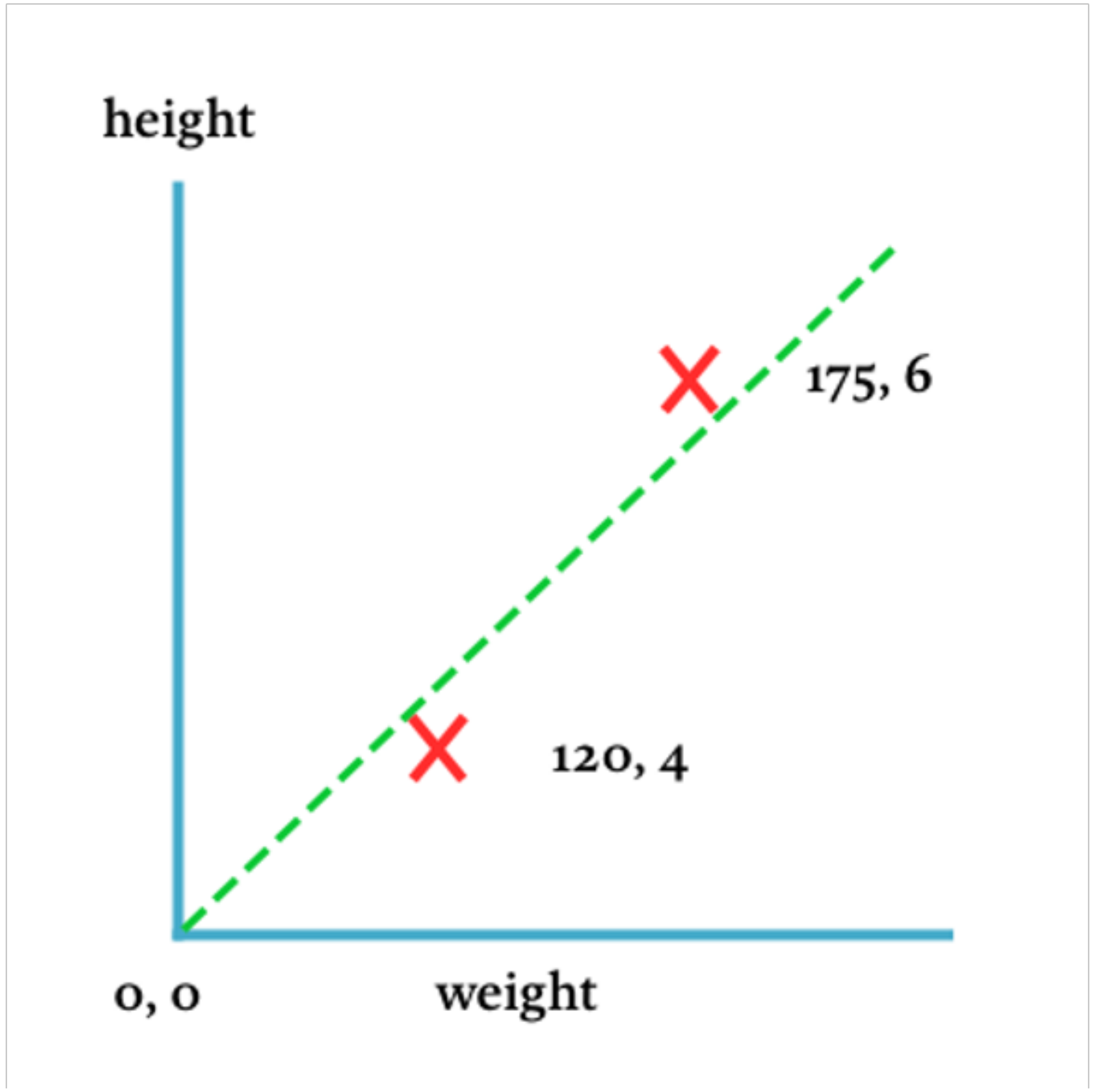
Gradient Descent (Worked out example)

- Data plot



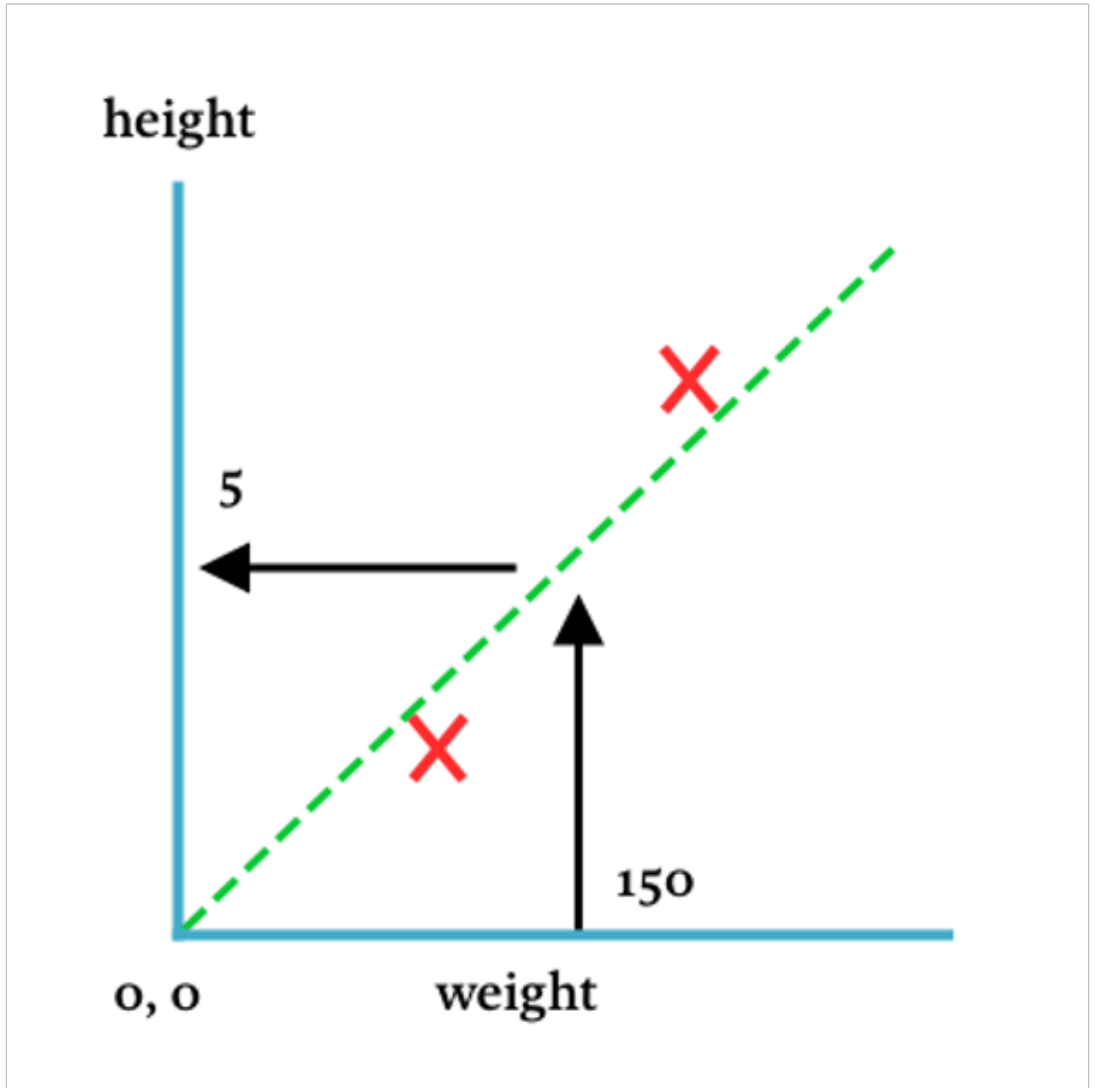
Gradient Descent (Worked out example)

- Fitted model



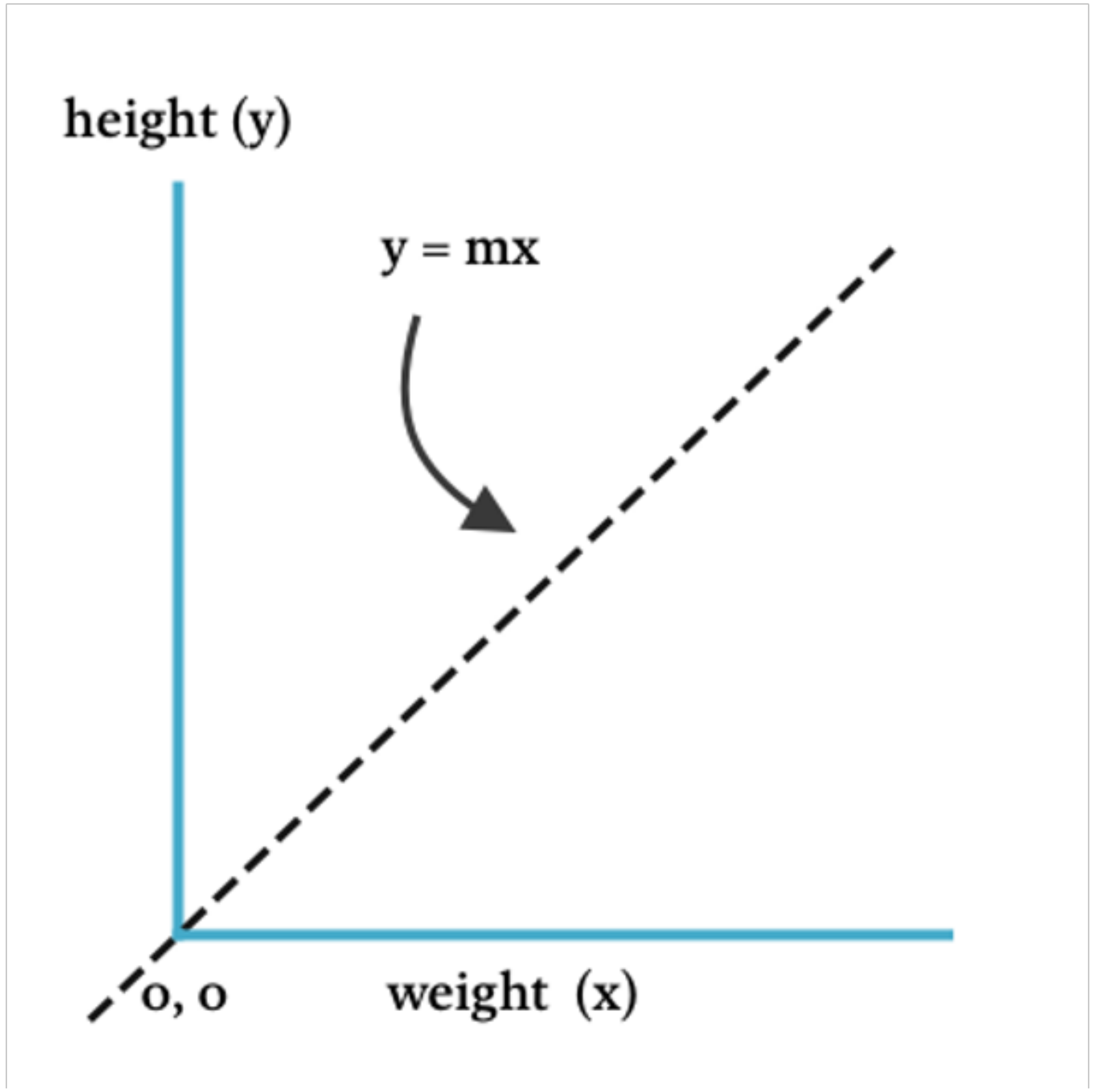
Gradient Descent (Worked out example)

- Make inference



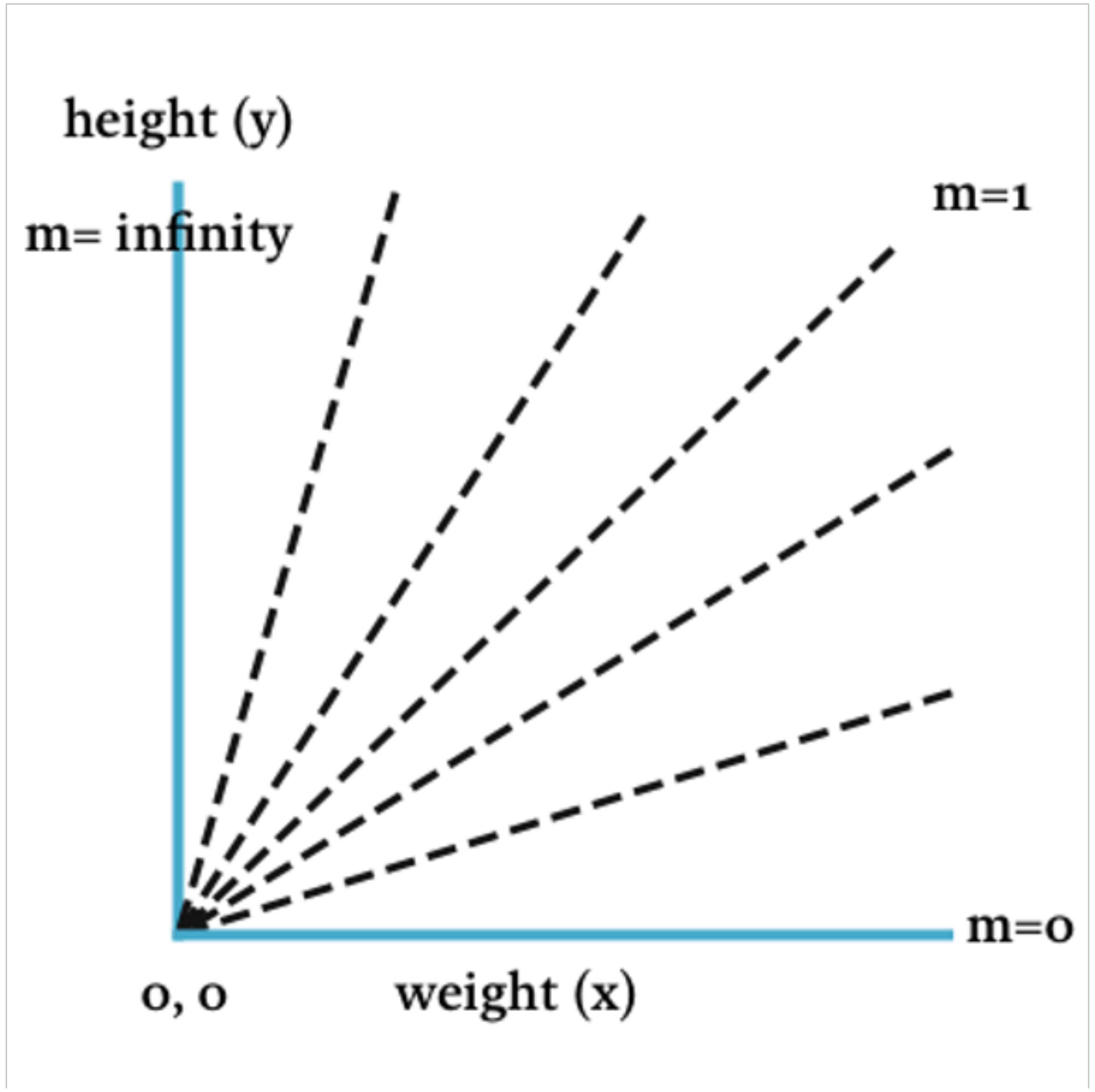
Gradient Descent (Worked out example)

- Linear model basics
  - Simplest equation of a line



Gradient Descent (Worked out example)

- Linear model basics
  - Parameter = slope (m)
  - Fit/ learn a model = find best ‘m’

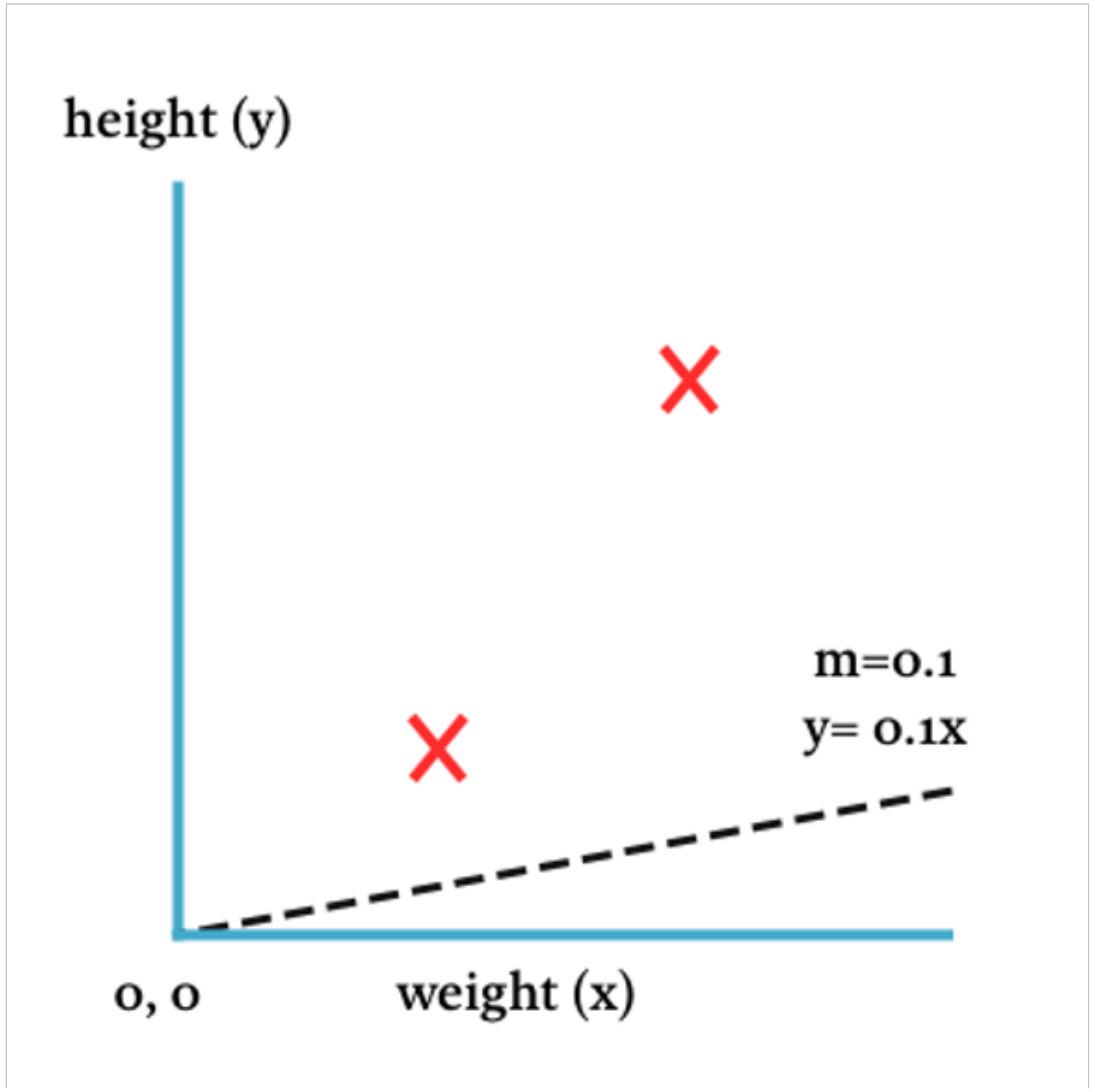


Gradient Descent (Worked out example)

- Start

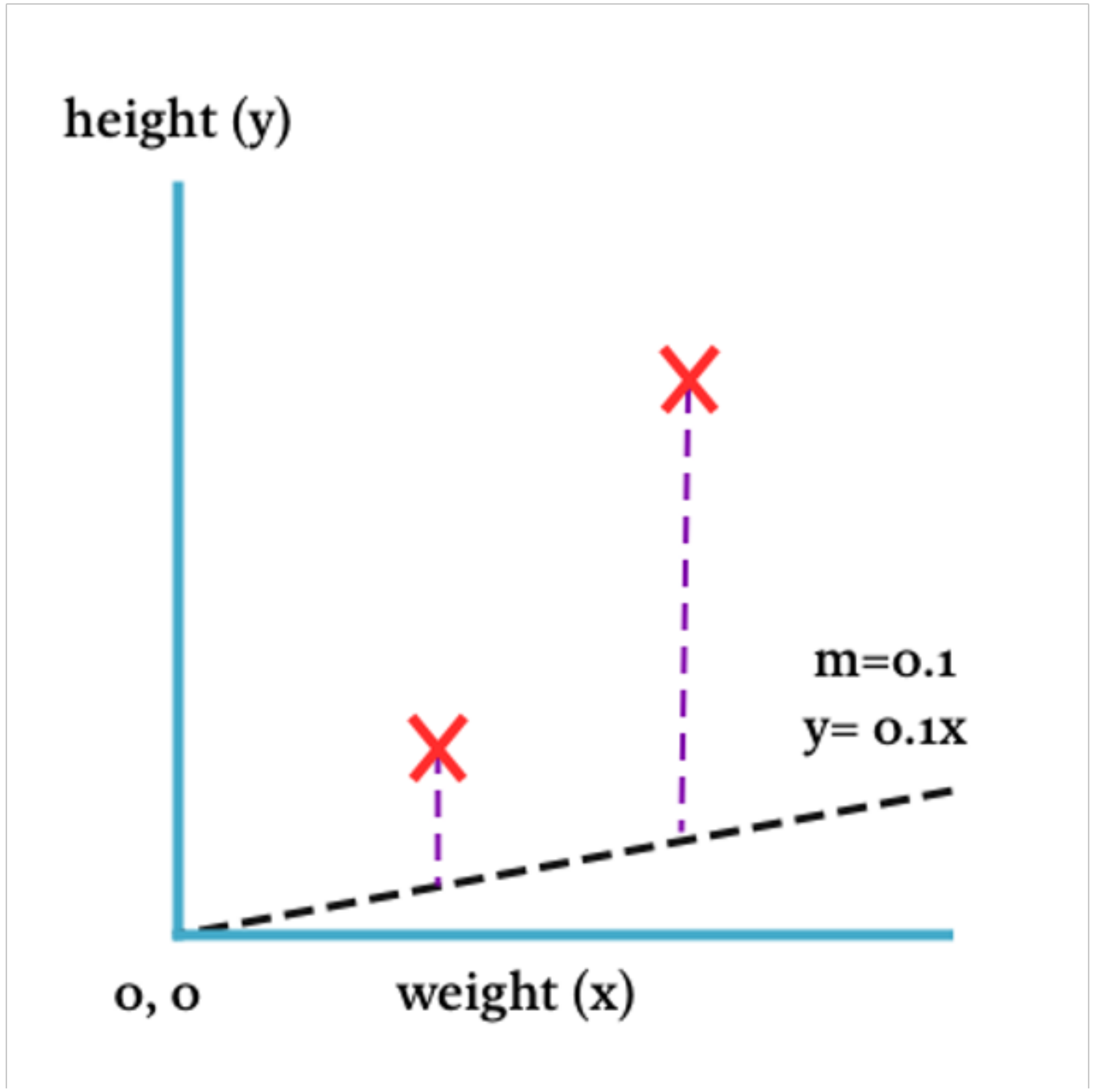
Gradient Descent (Worked out example)

- Step 1: Random initialization
  - $m = 0.1$



Gradient Descent (Worked out example)

- Step 1: Random initialization
  - m = 0.1
  - Does not fit well



Gradient Descent (Worked out example)

- Need to improve current parameter value

Gradient Descent (Worked out example)

- Need to improve current parameter value
- But… Before we improve it

Gradient Descent (Worked out example)

- Need to improve current parameter value
- But… Before we improve it
- We need to measure how “good” it is

Gradient Descent (Worked out example)

- Step 2: Define a Loss/ Error/ Cost function
  - Loss = f (parameters)

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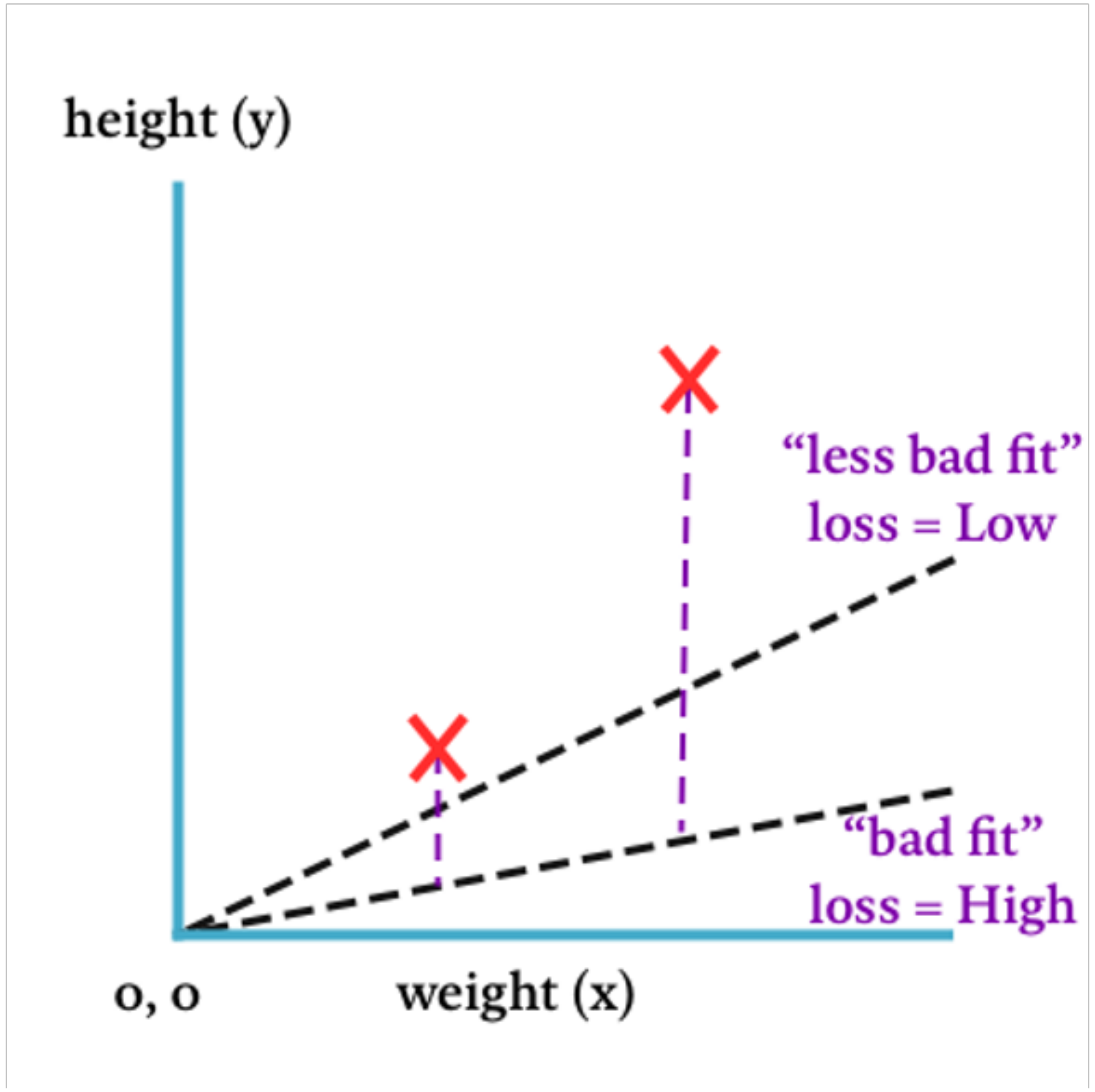
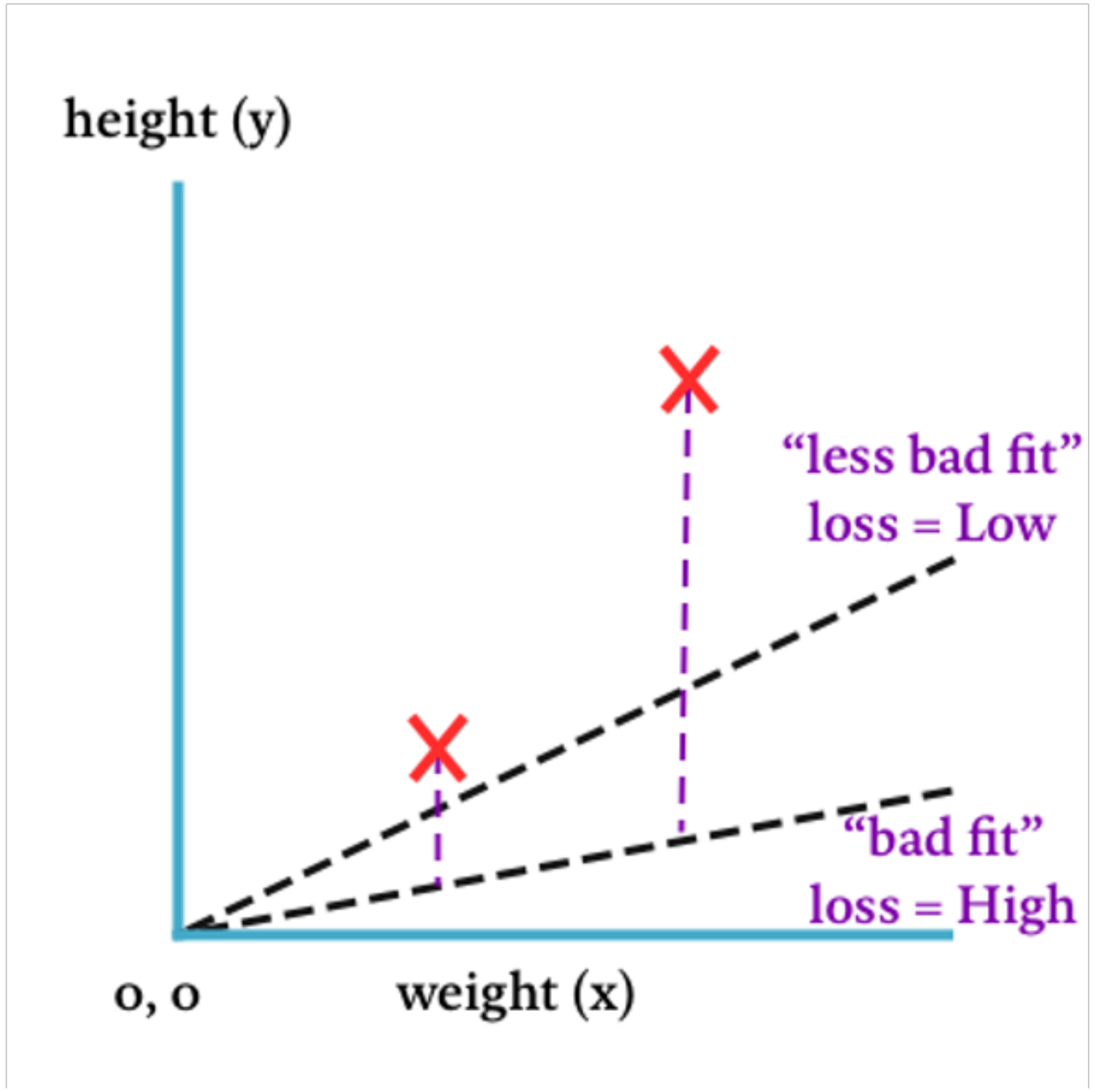


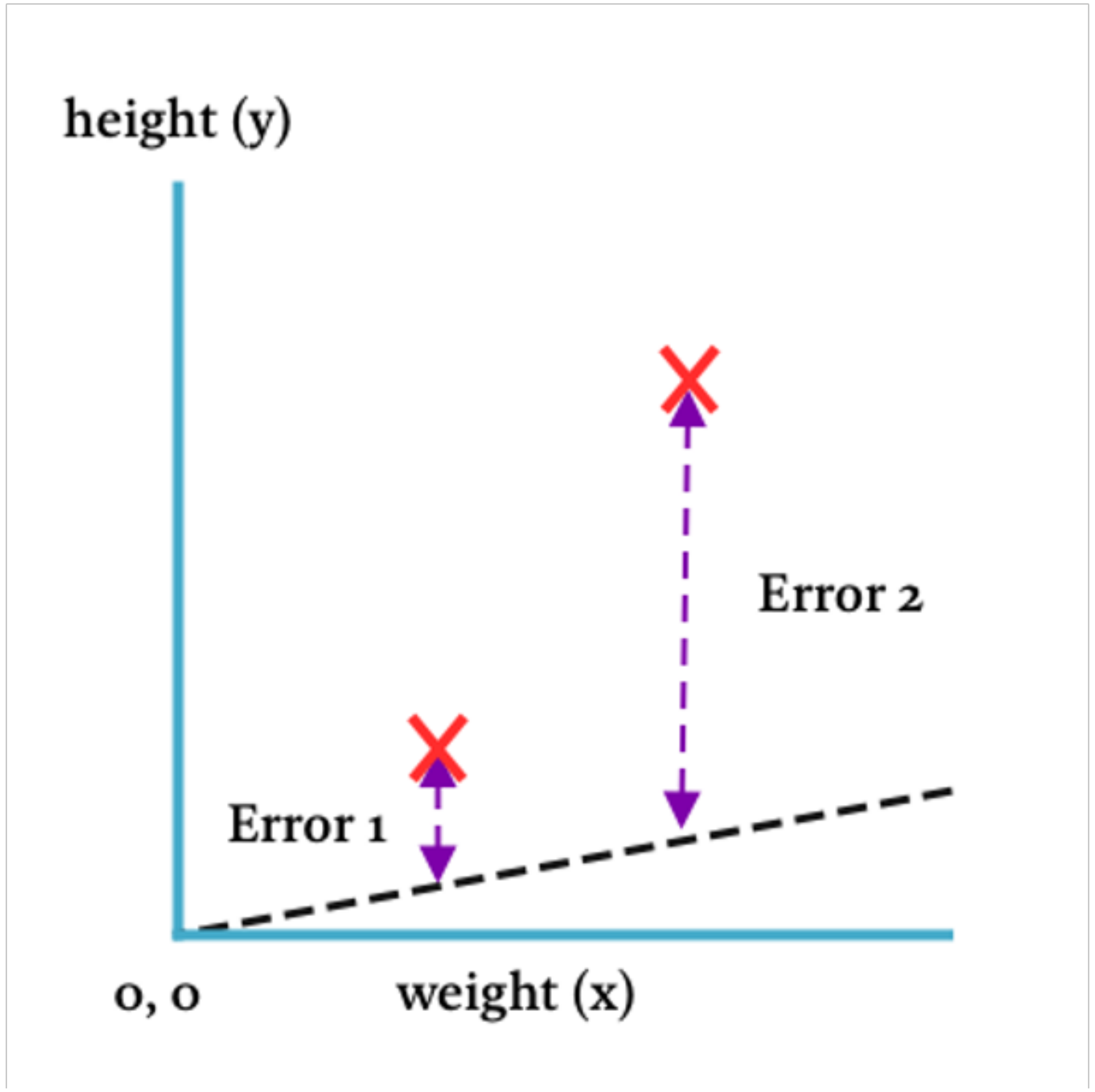
Gradient Descent (Worked out example)

- Step 2: Define a Loss/ Error/ Cost function
  - Loss = f (parameters)
  - Does any loss function work?



Gradient Descent (Worked out example)

- Step 2: Define a Loss/ Error/ Cost function
  - Regression → Mean Squared Error
  - $$\text{MSE} = \frac{(\text{Error } 1)^2 + (\text{Error } 2)^2}{2}$$



Gradient Descent (Worked out example)

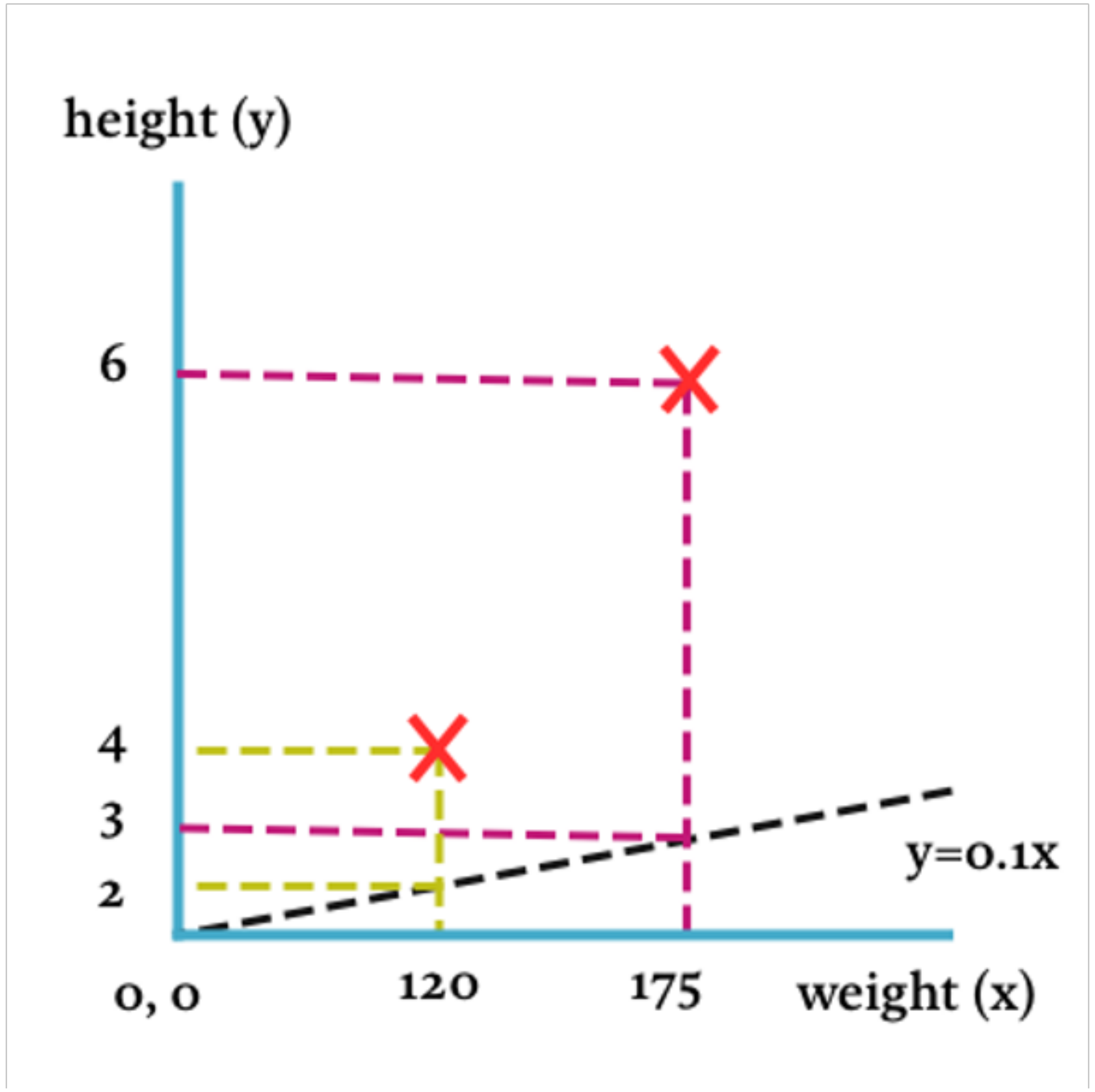
- Step 2: Define a Loss/ Error/ Cost function
  - MSE calculation

Error 1 = (4 - 2) = 2
Error 2 = (6 - 3) = 3

$$MSE = \frac{(Error\ 1)^2 + (Error\ 2)^2}{2}$$

$$MSE = \frac{(2)^2 + (3)^2}{2}$$

MSE = 6.5



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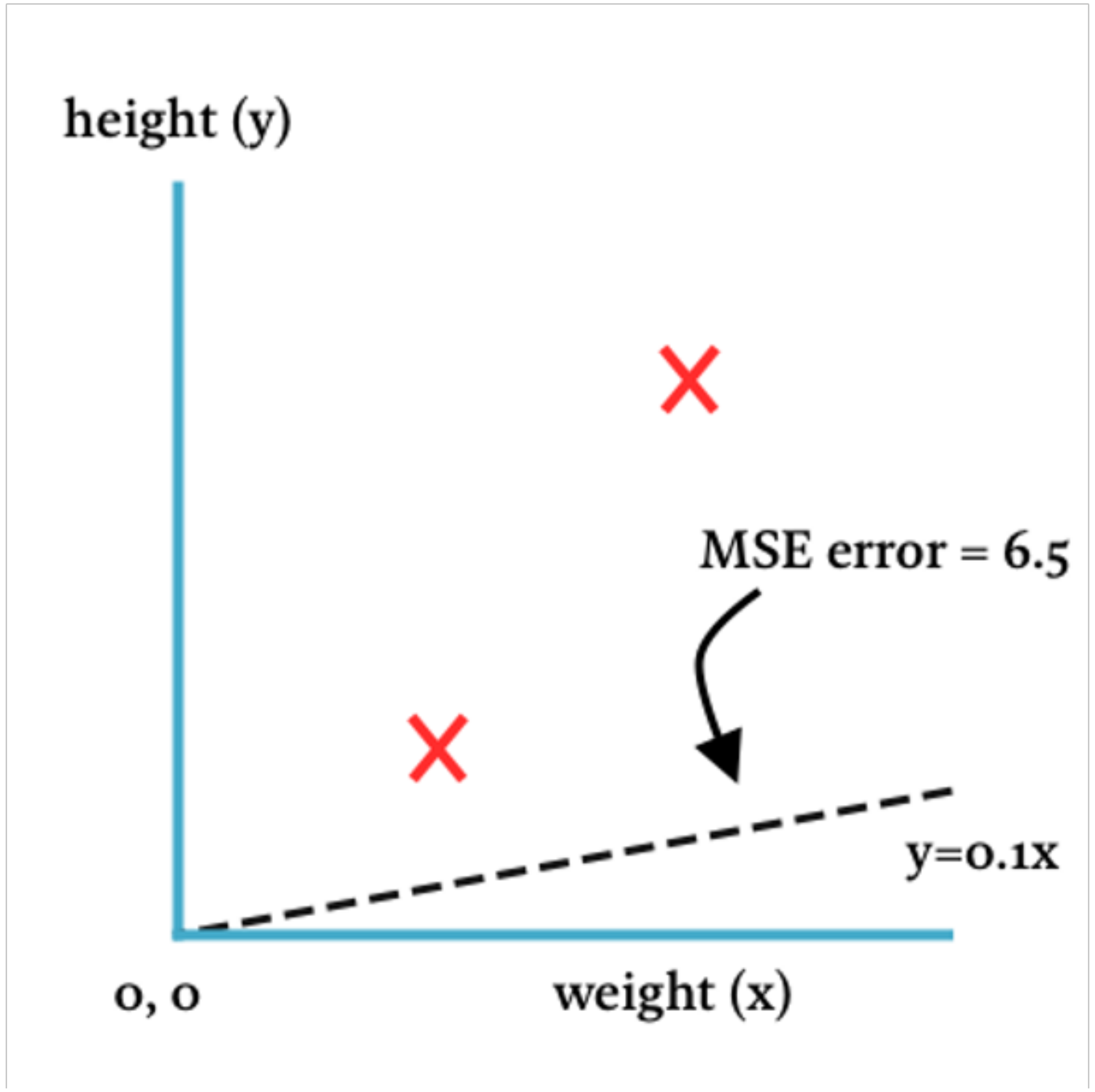

Gradient Descent (Worked out example)

- Now we improve
  - Gradient = First derivative
  - Descent = Move in decreasing direction

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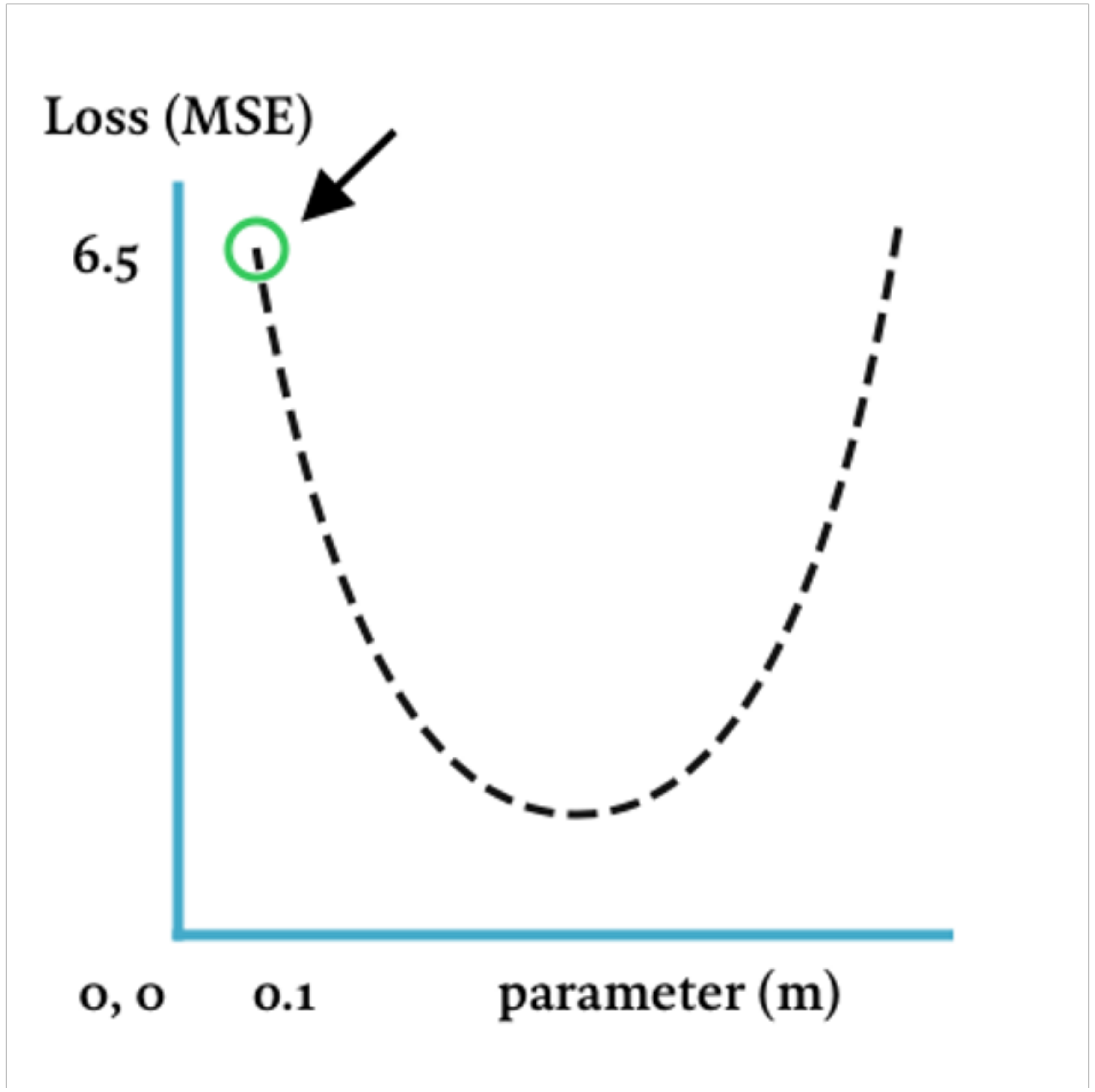

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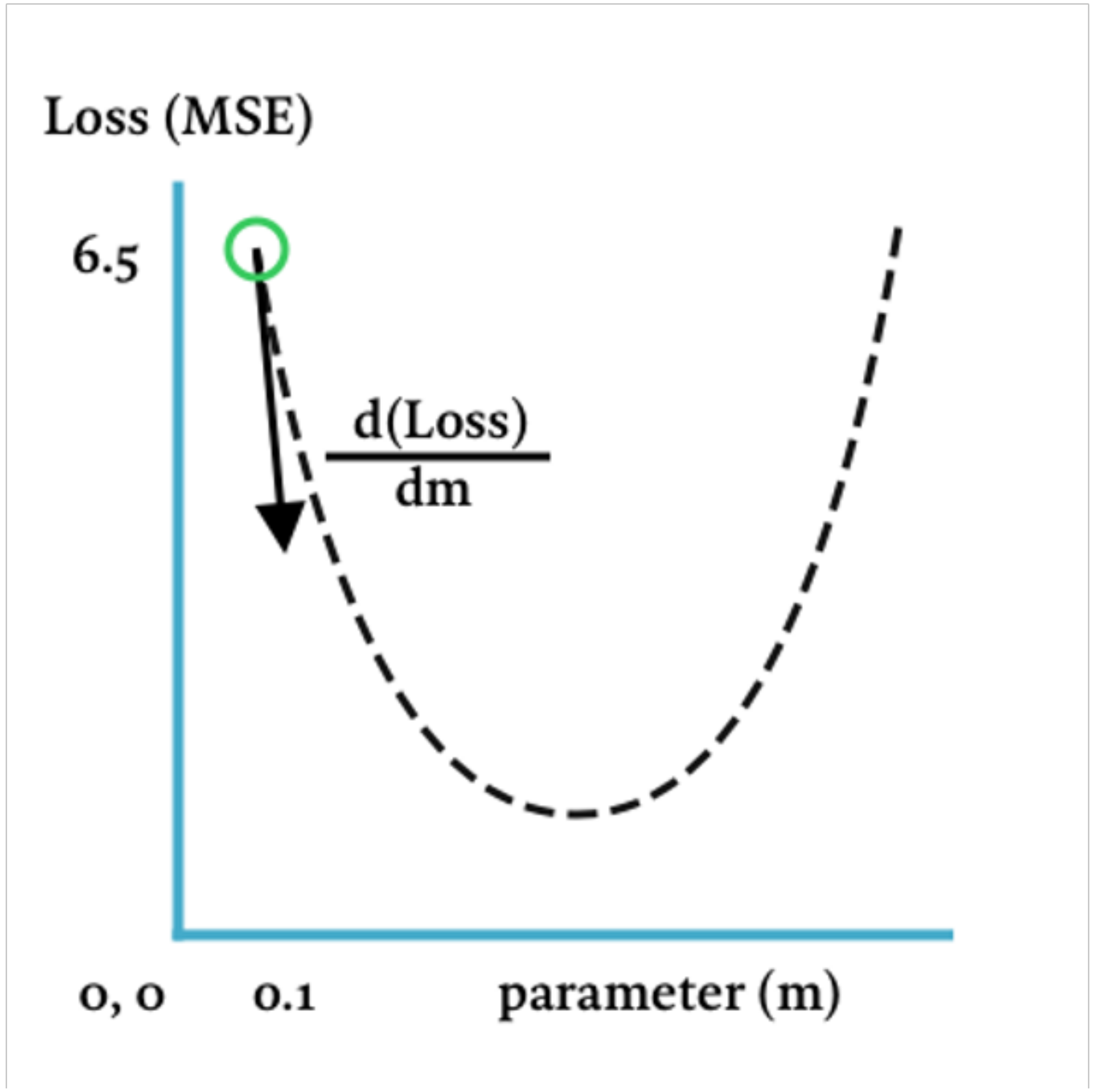
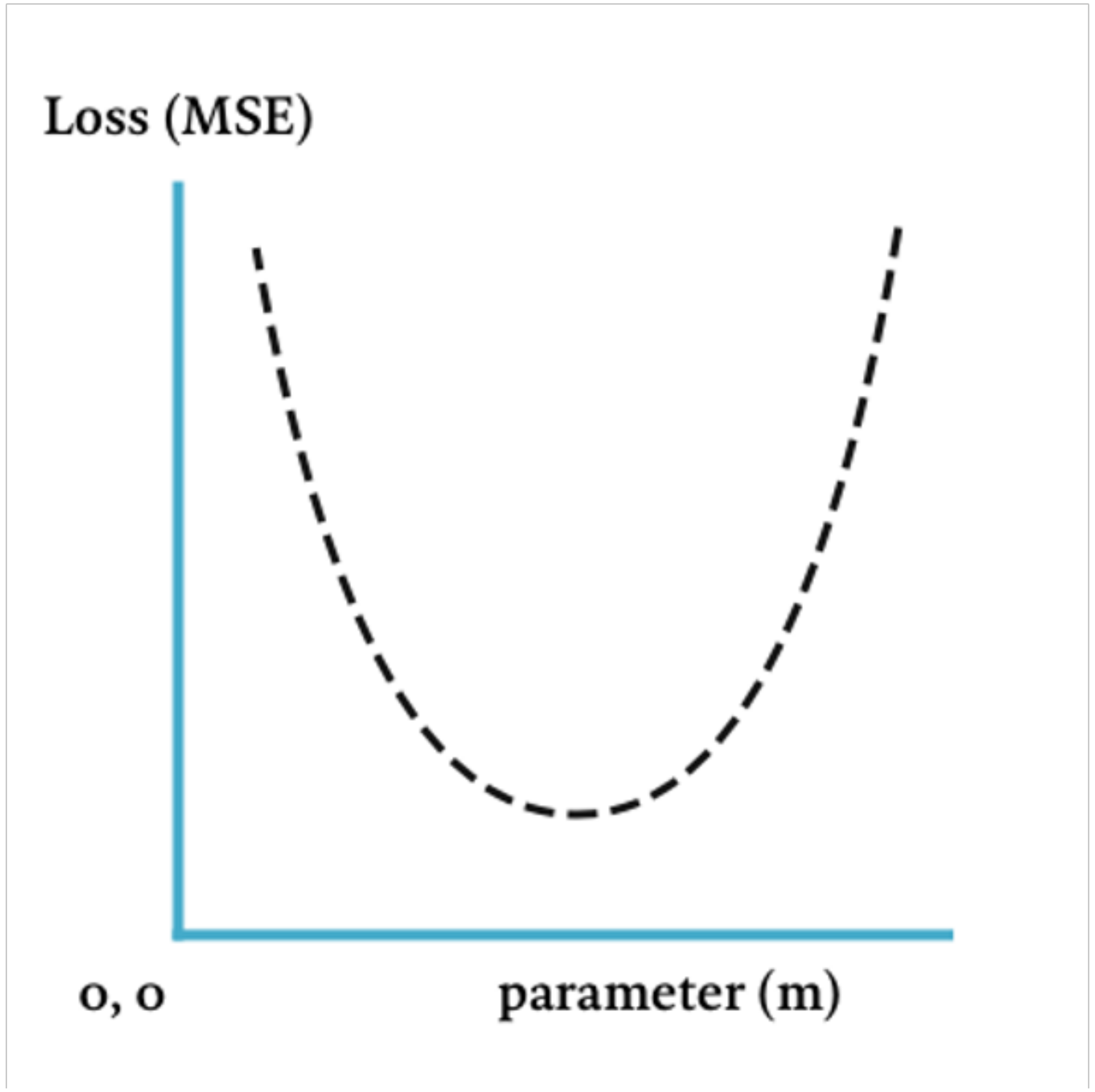


Gradient Descent (Worked out example)

- Why is the curve convex shaped?



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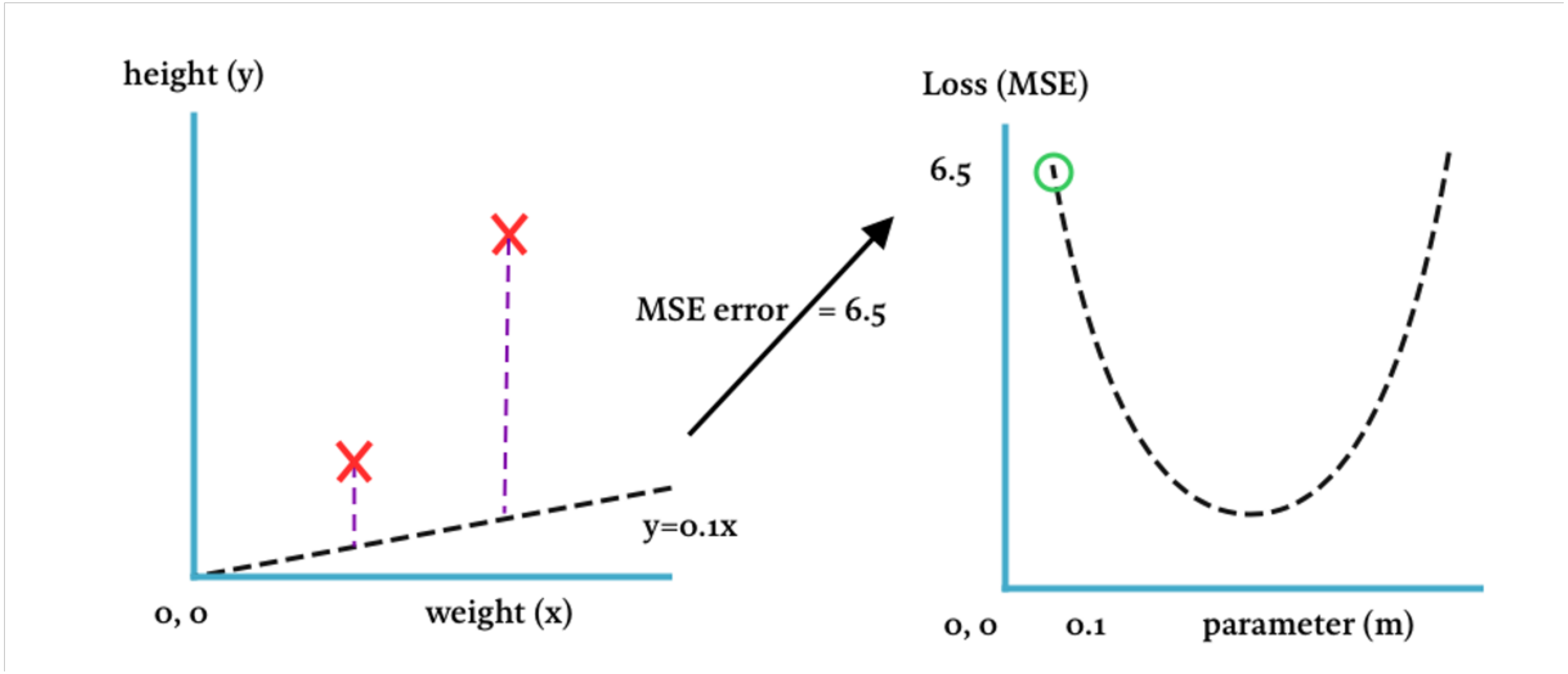

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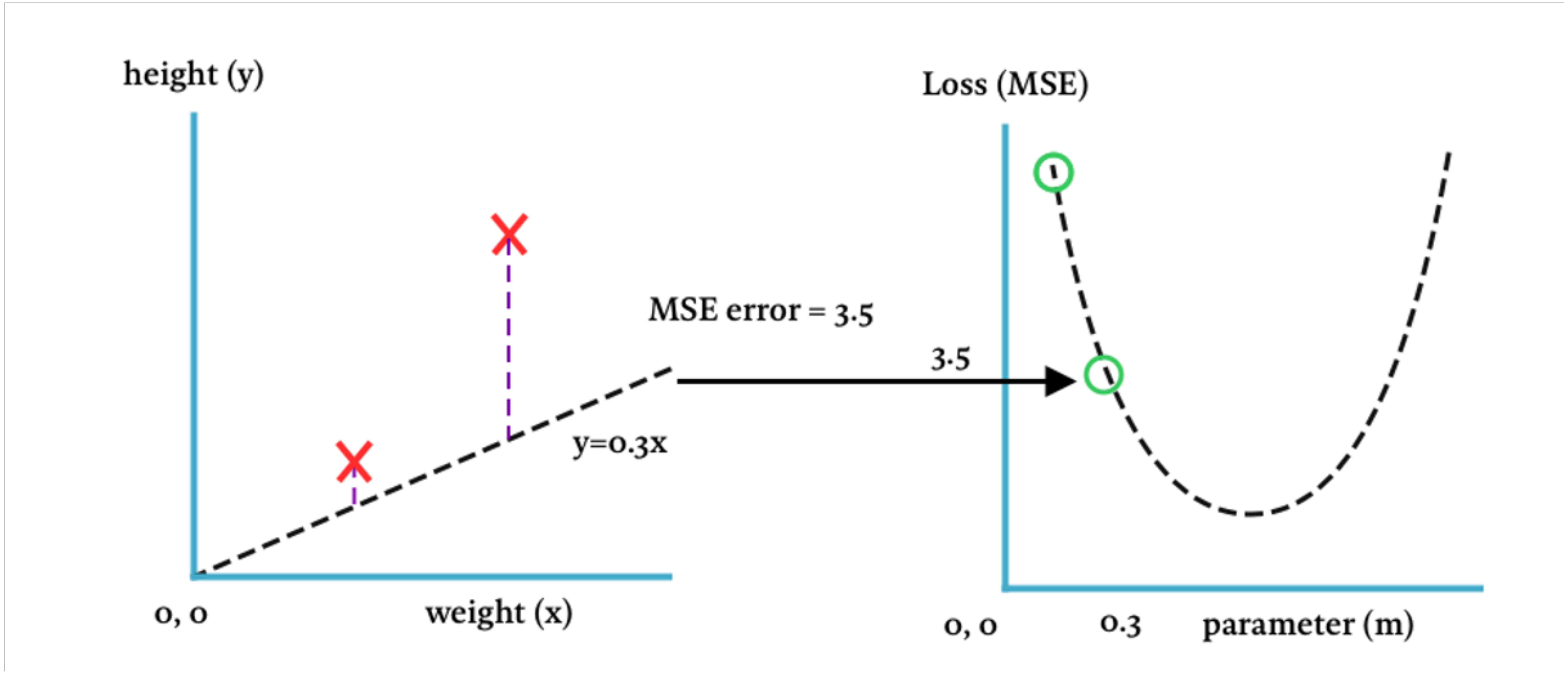

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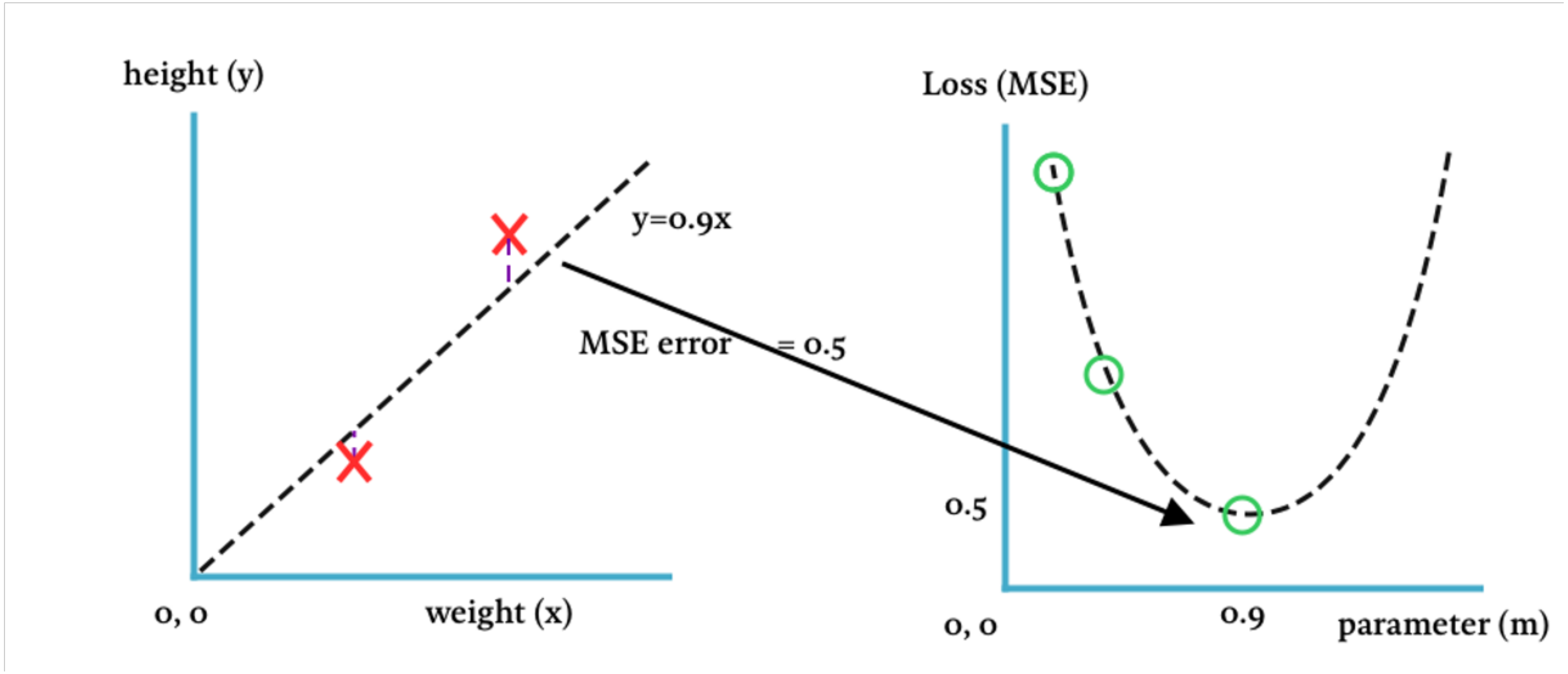

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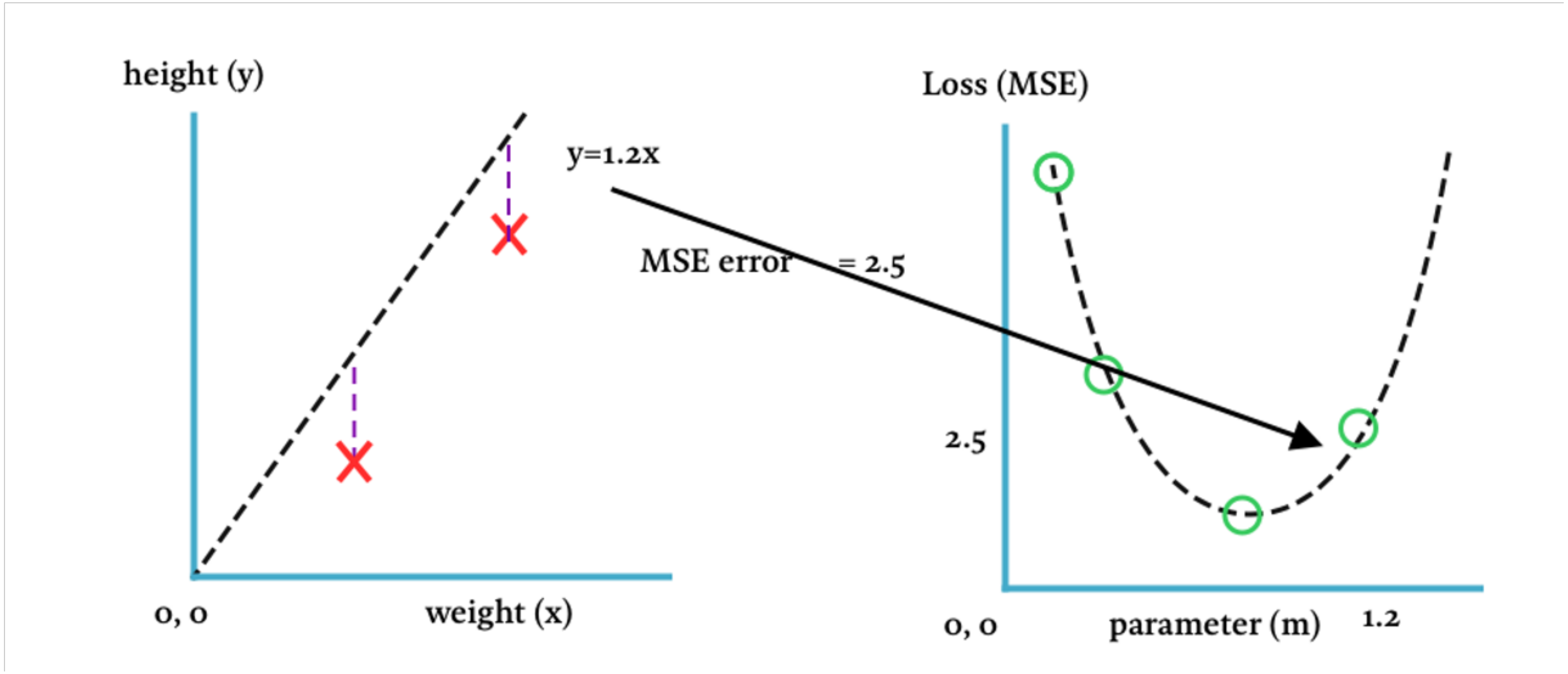
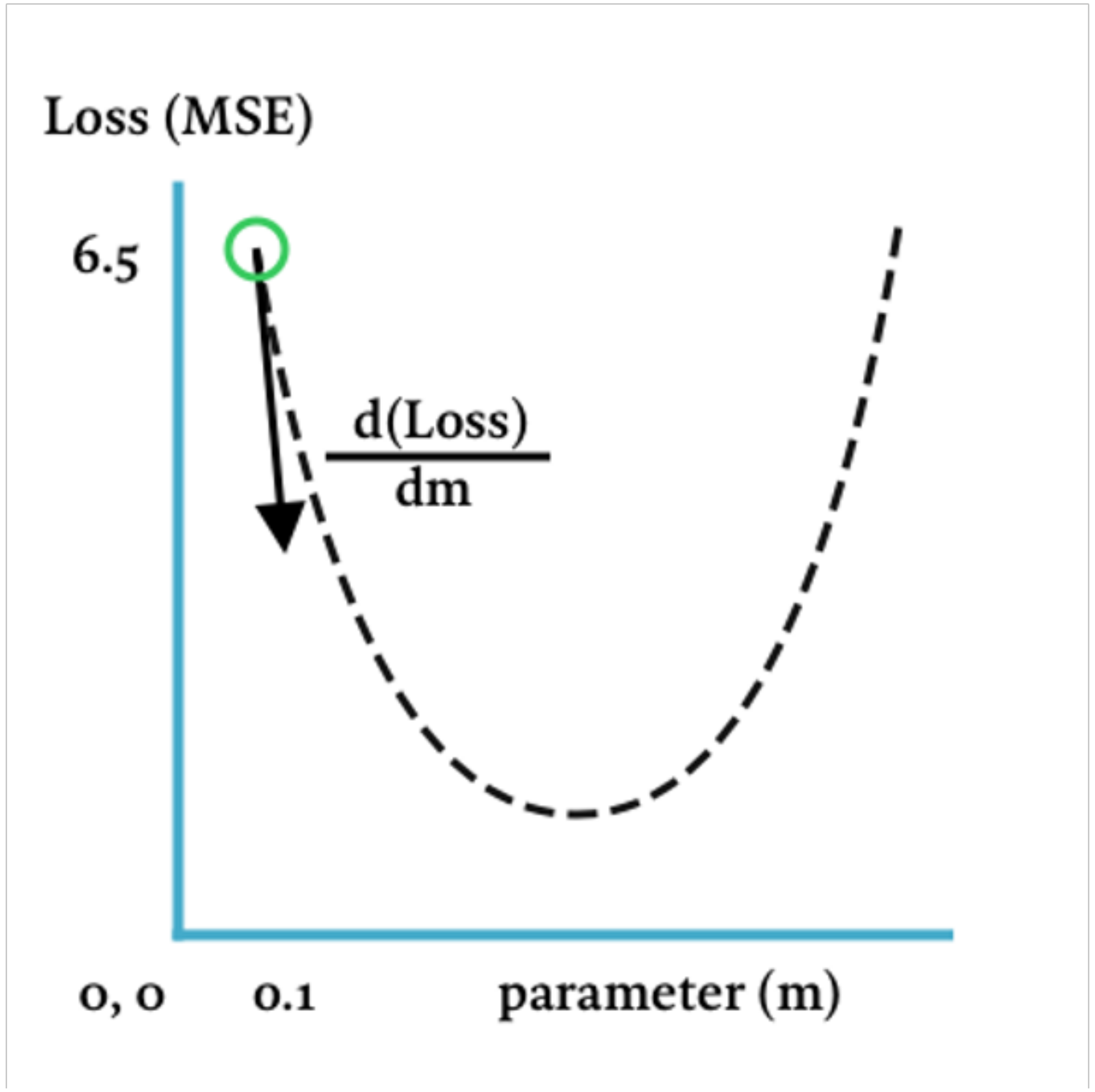


Gradient Descent (Worked out example)

- Step 3: Perform a gradient descent step
  - Calculate gradient



Gradient Descent (Worked out example)

- Step 3: Perform a gradient descent step
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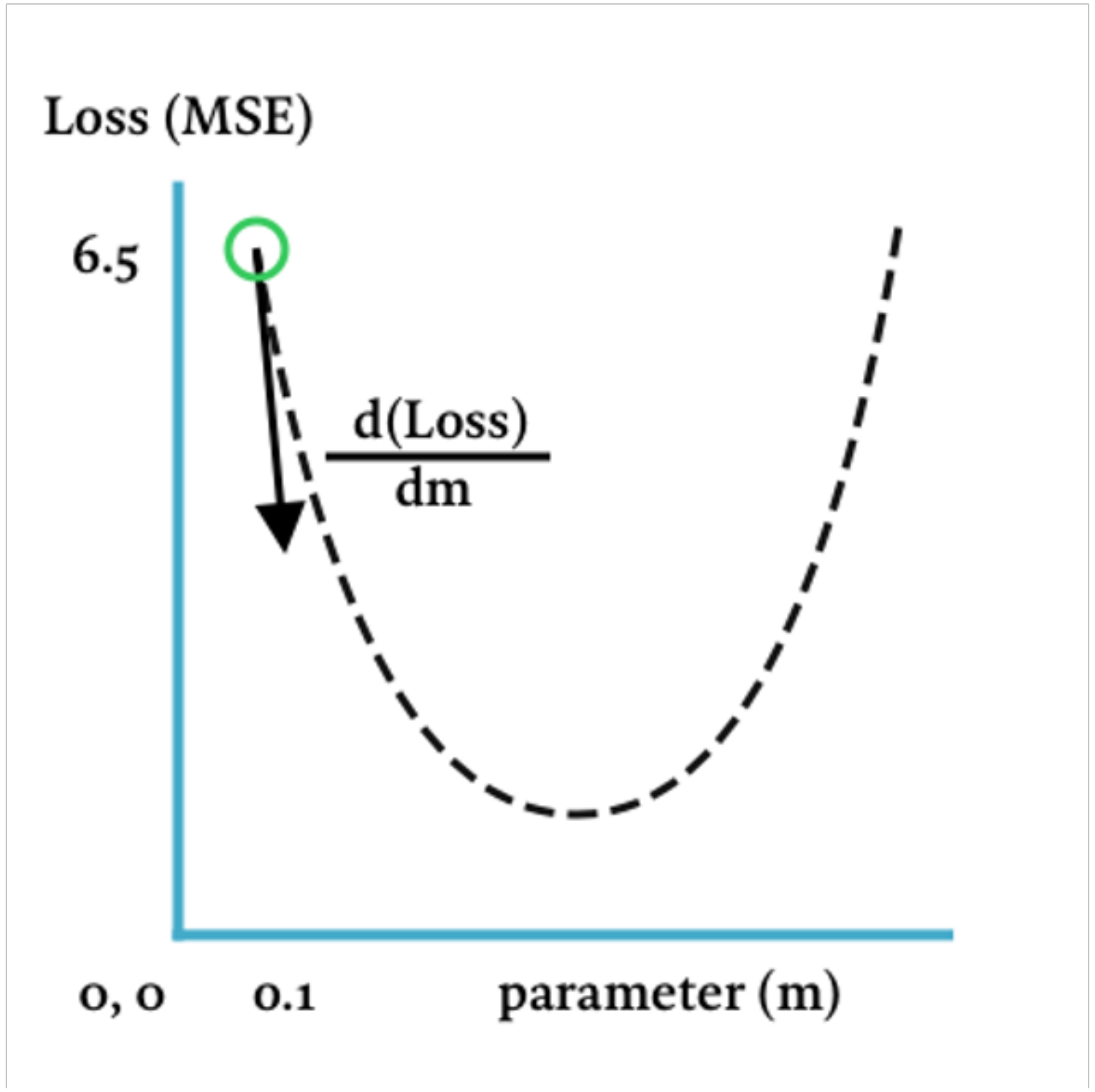
$$\mathbf{m}_{\text{new}} = \mathbf{m}_{\text{old}} - \left[-\frac{d(\text{Loss})}{dm} \right] \times \text{step\_size}$$



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- Step 3: Perform a gradient descent step
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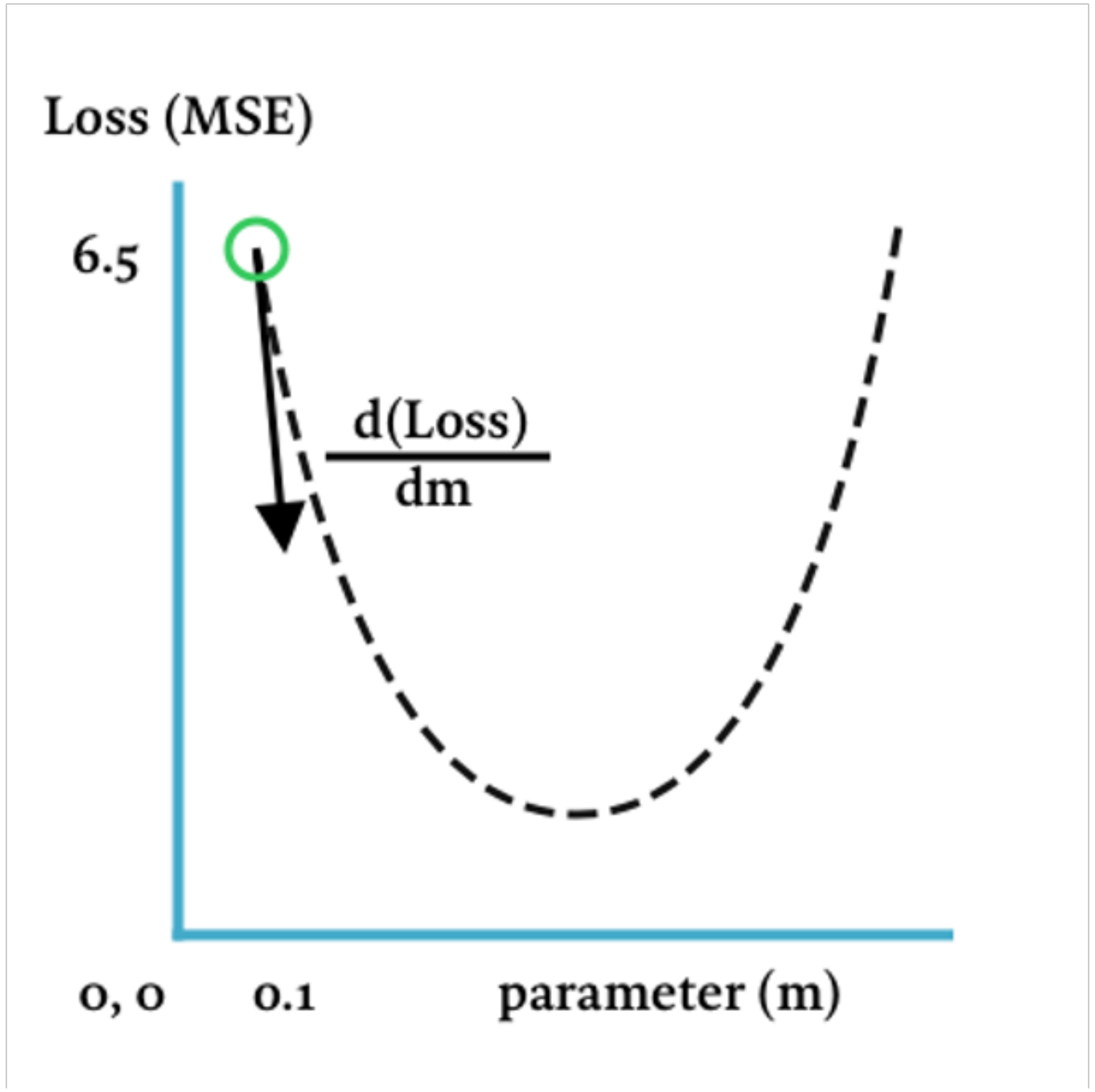
  - Update parameters

$$\mathbf{m}_{new} = \mathbf{m}_{old} - \left[- \frac{d(Loss)}{dm}\right] \times \text{step\_size}$$

$$\mathbf{m}_{new} = 0.1 - \left[- 2\right] \times 0.1$$

$$\mathbf{m}_{new} = 0.3$$



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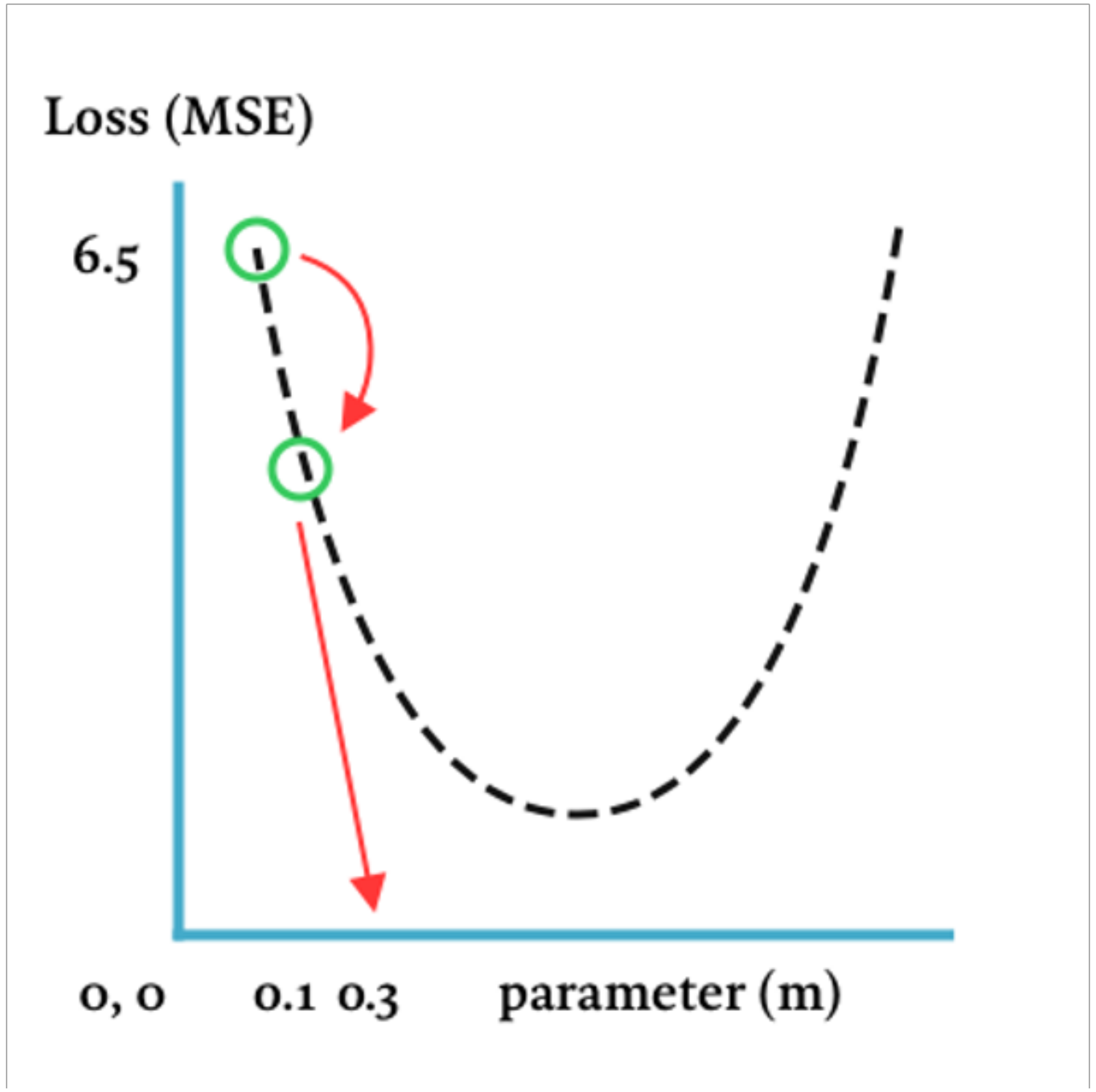
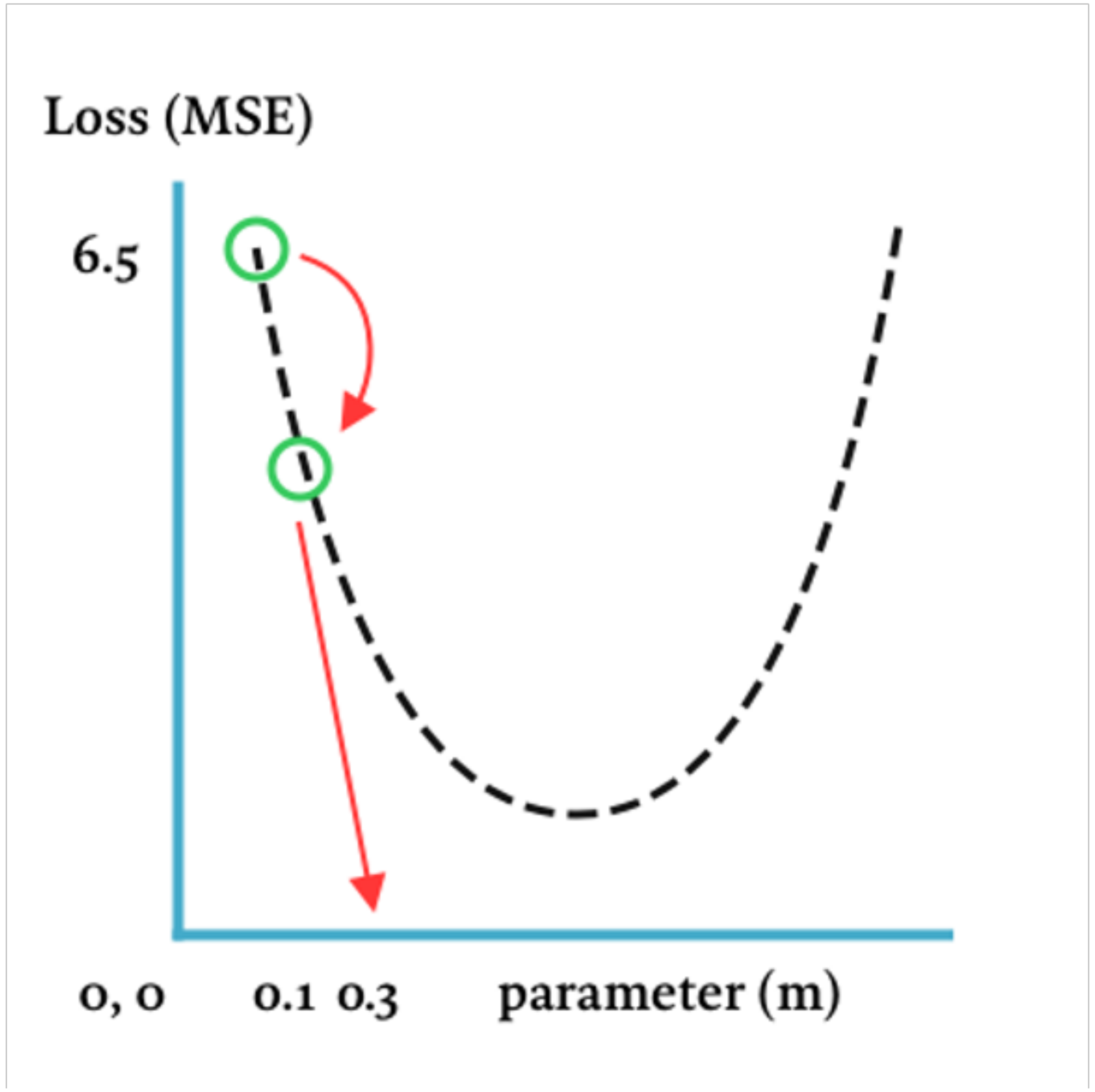


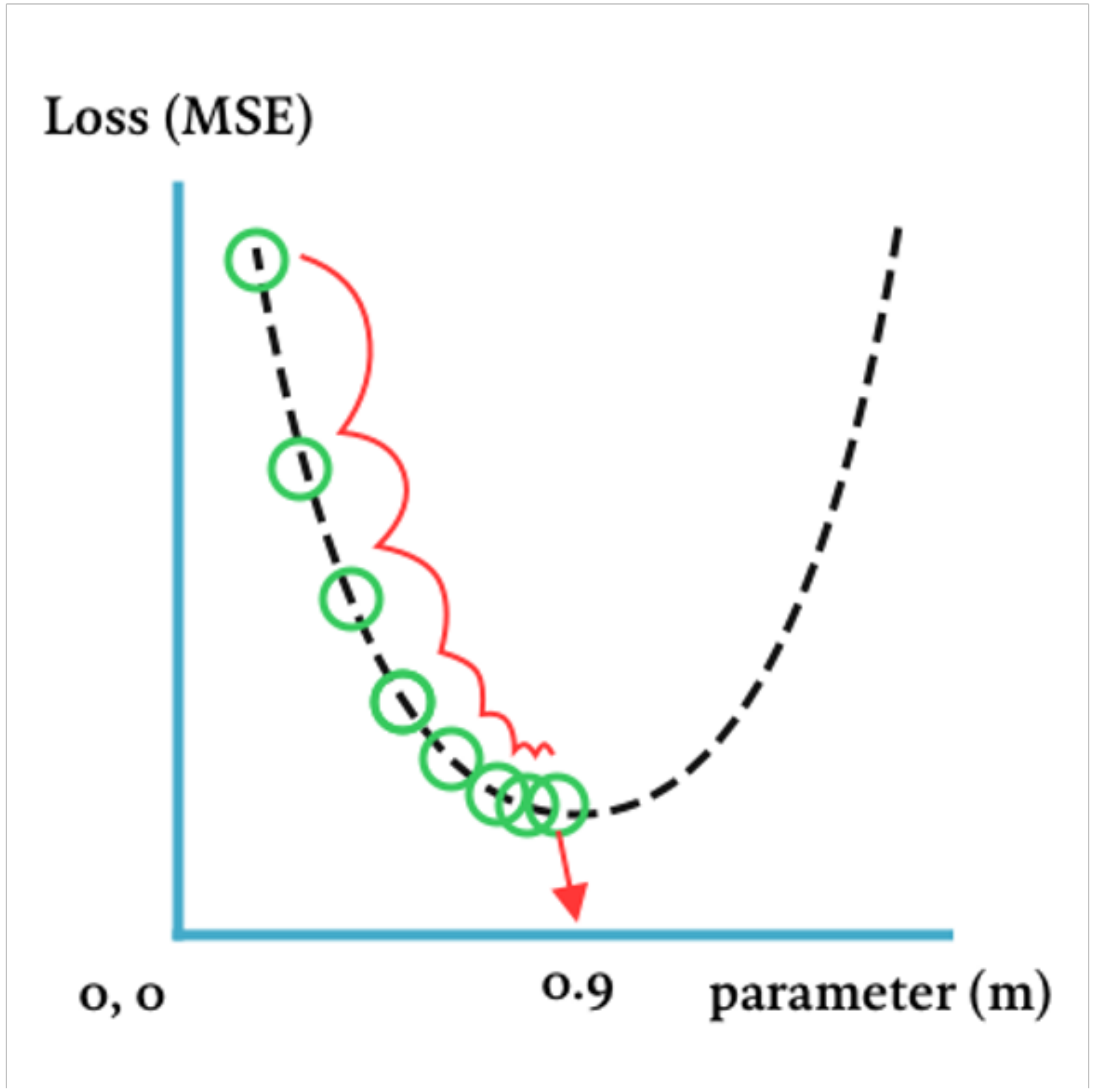
Gradient Descent (Worked out example)

- Step size/ Learning rate
  - Hyper-parameter
  - Cant be too large or too small



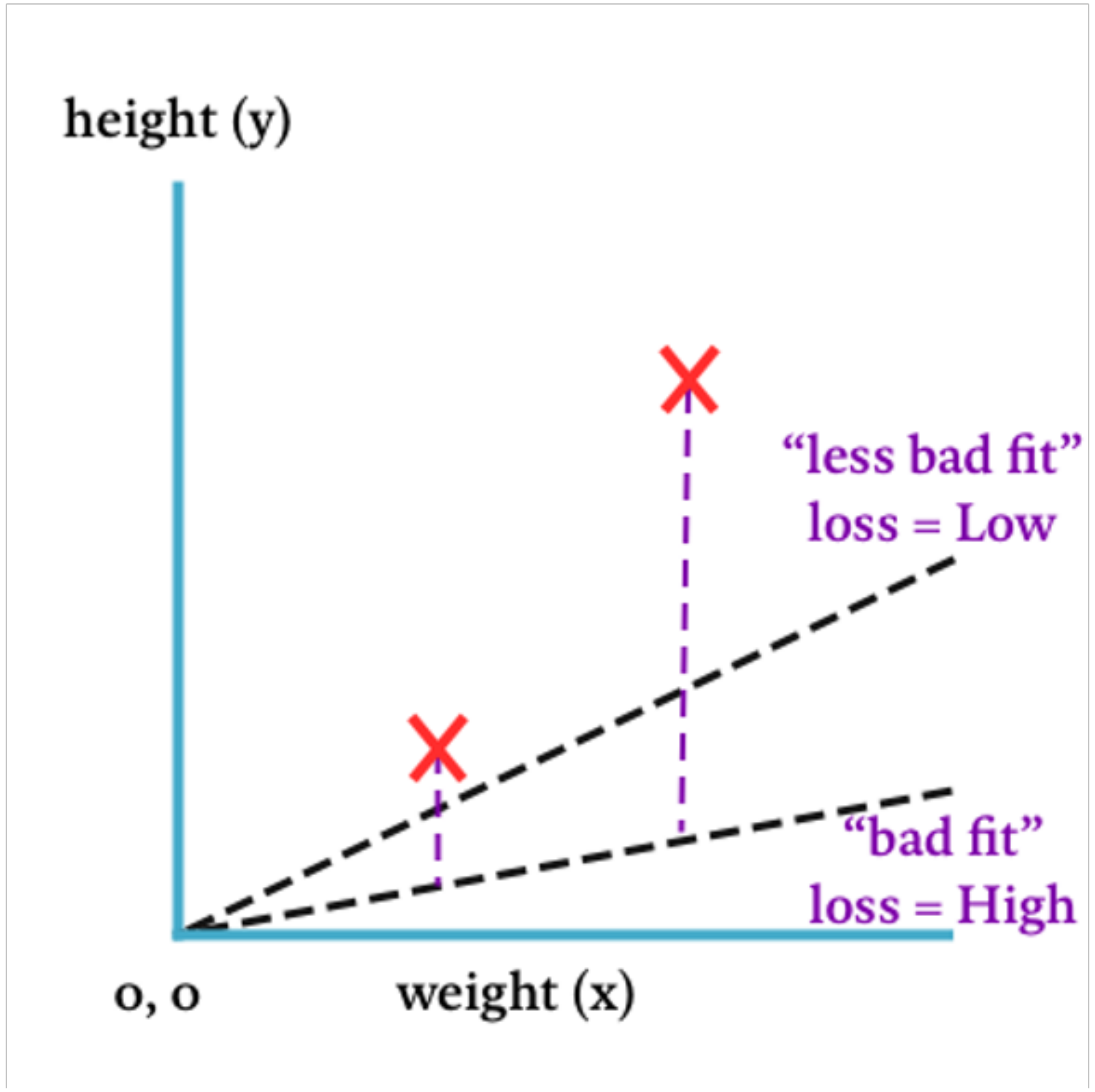
Gradient Descent (Worked out example)

- Step size/ Learning rate trick
  - Momentum
  - Faster convergence



Gradient Descent (Worked out example)

- Step 3: Perform a gradient descent step
  - One step complete

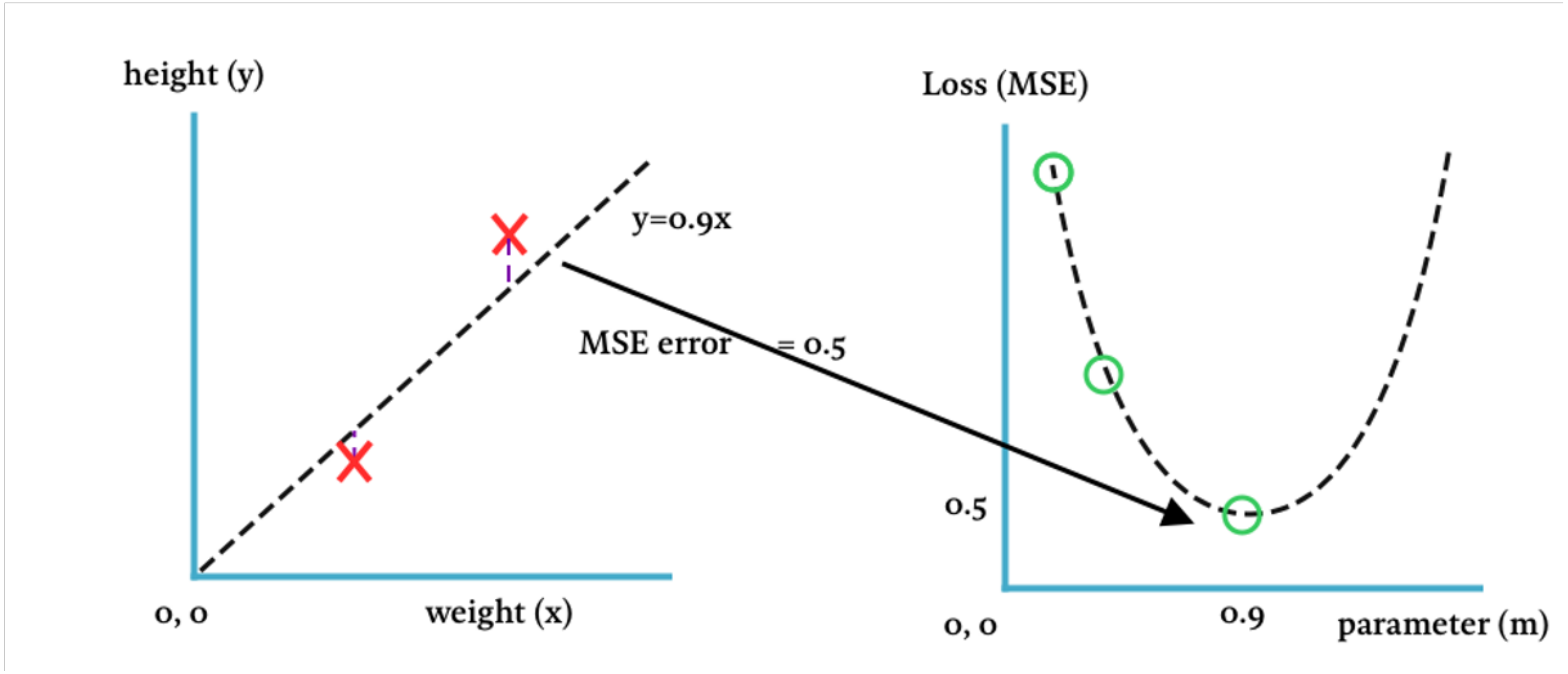


Gradient Descent (Worked out example)

- Step 4: Repeat Step 3 until stopping criteria is met

Gradient Descent (Worked out example)

- Step 4: Repeat Step 3 until stopping criteria is met
  - Solution found at m = 0.9



Gradient Descent (Worked out example)

- Step 4: Repeat Step 3 until stopping criteria is met
  - Gradient = 0
  - Update < Threshold
  - Max iterations

Revisit

- Key words
  - First order
  - Iterative
  - Local minimum
  - Differentiable

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  - First order: Differentiate loss once
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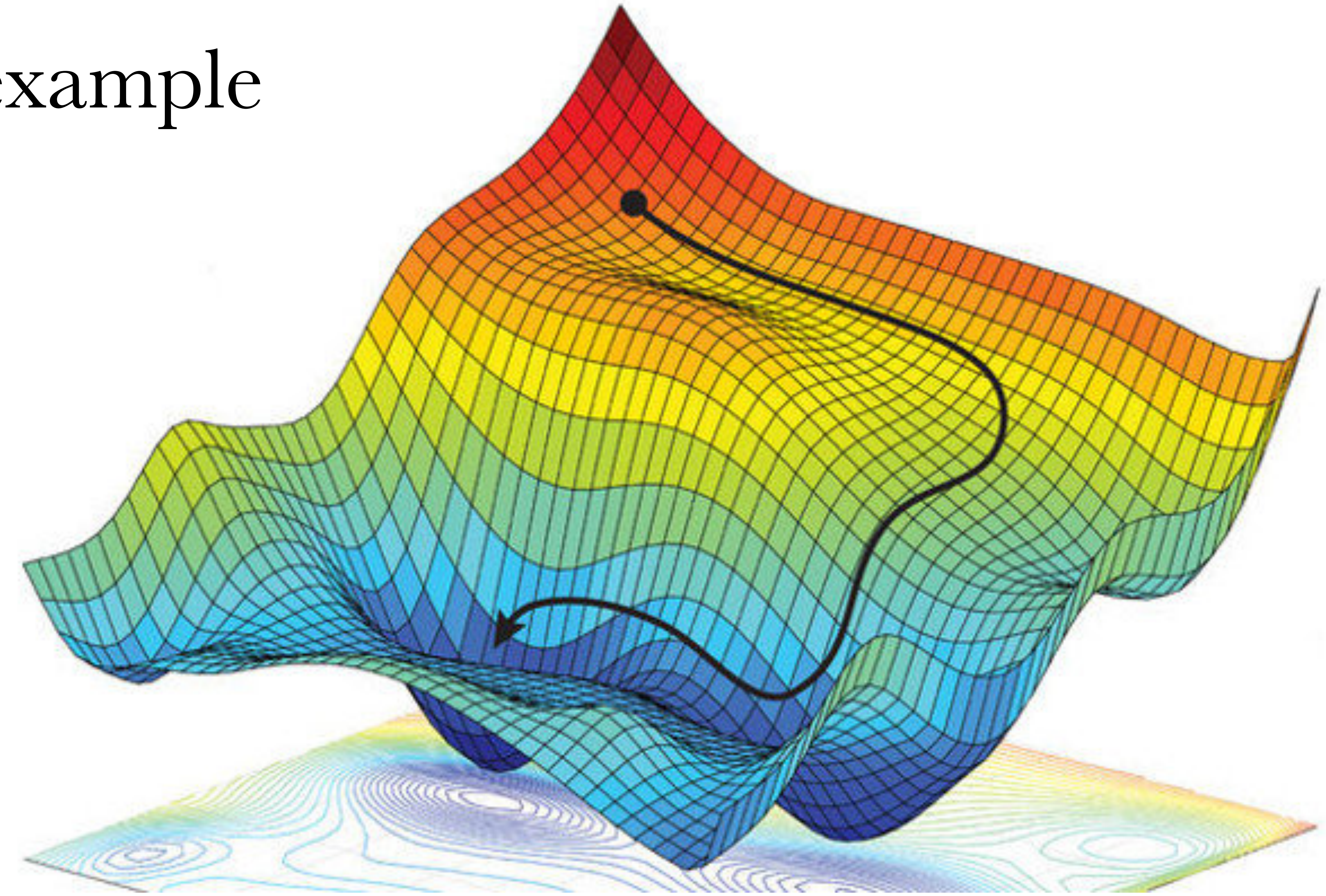
Revisit

- Key words
  - First order: Differentiate loss once
  - Iterative: Optimal value by repeated updates
  - Local minimum: Each iteration, lowest point in neighborhood
  - Differentiable: Loss function allowed for differentiation

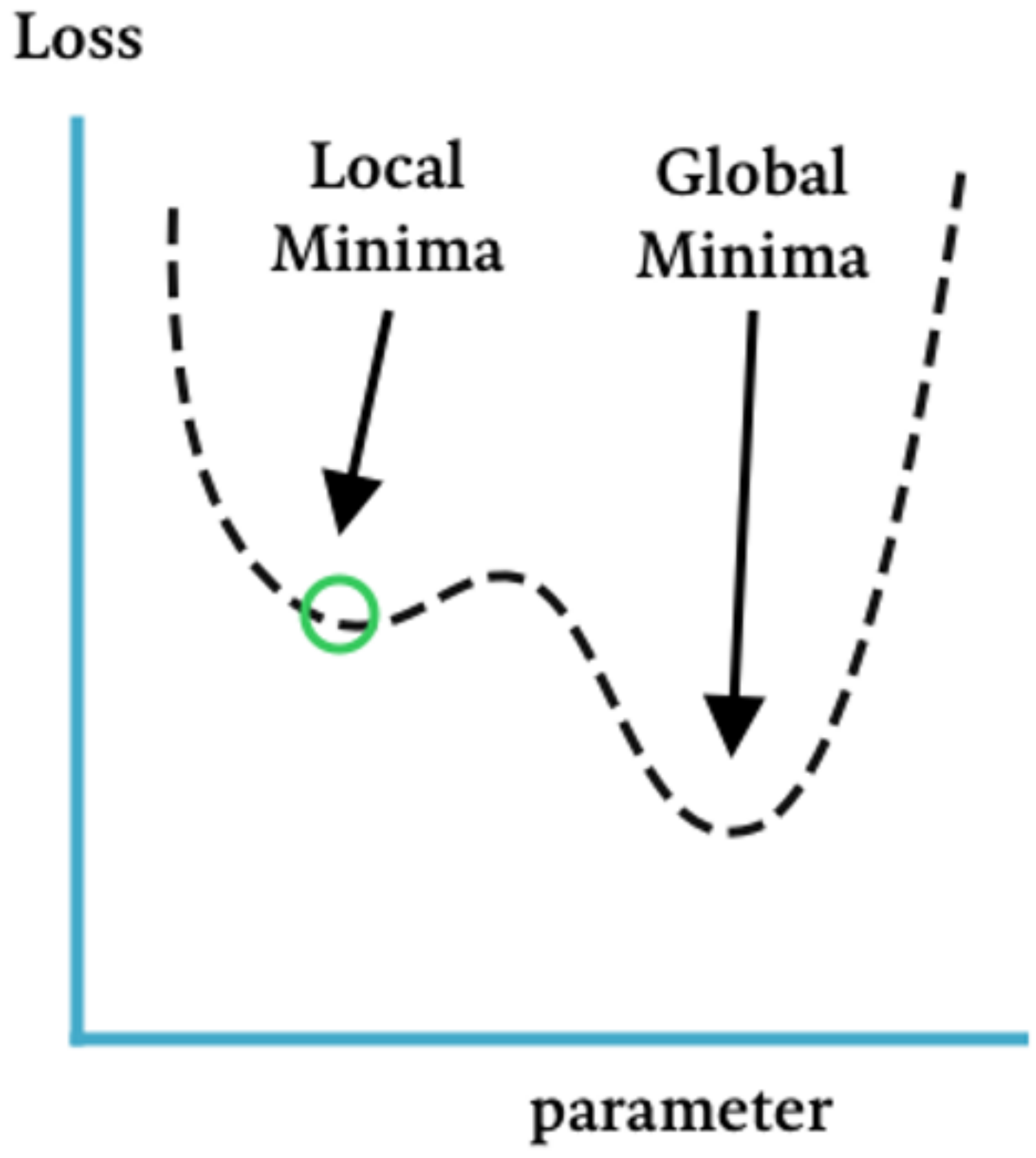
Gradient Descent Analogy

- Think of a multi-dimensional example



Problems with Gradient Descent

Problems with gradient descent

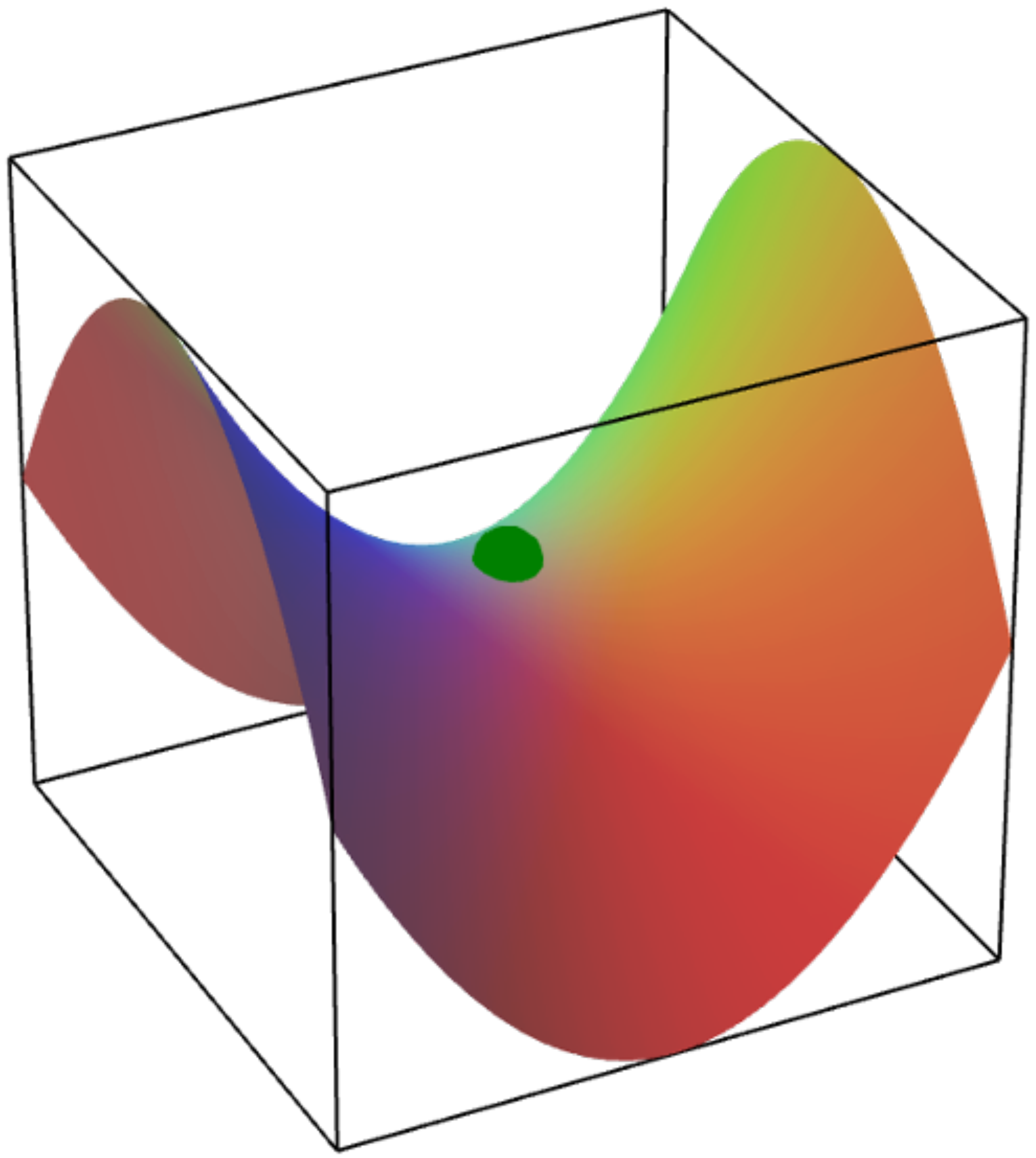


- Non-convex loss landscape

Problems with gradient descent

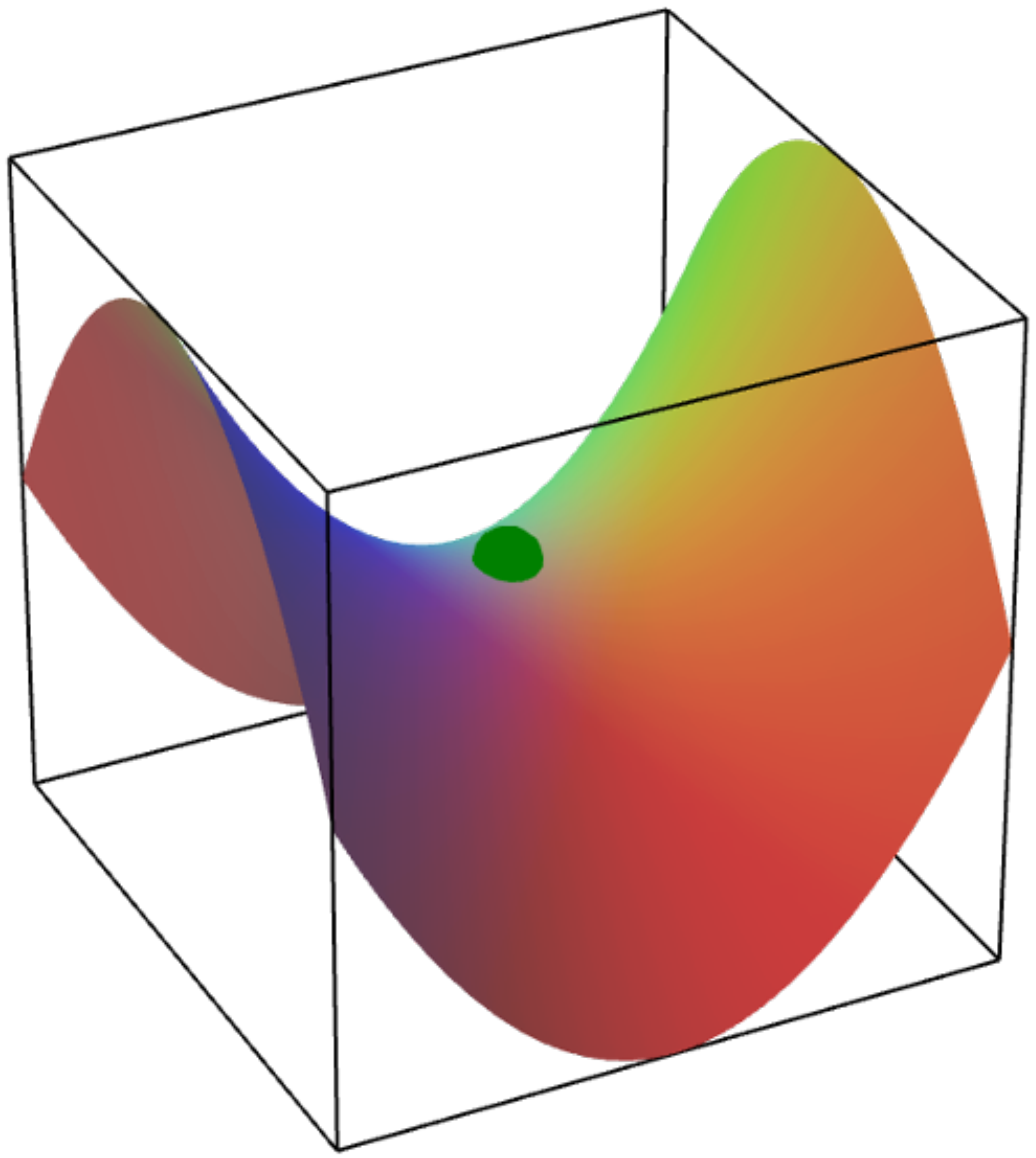
- Non-convex loss landscape
  → Stuck in local minima

Problems with gradient descent



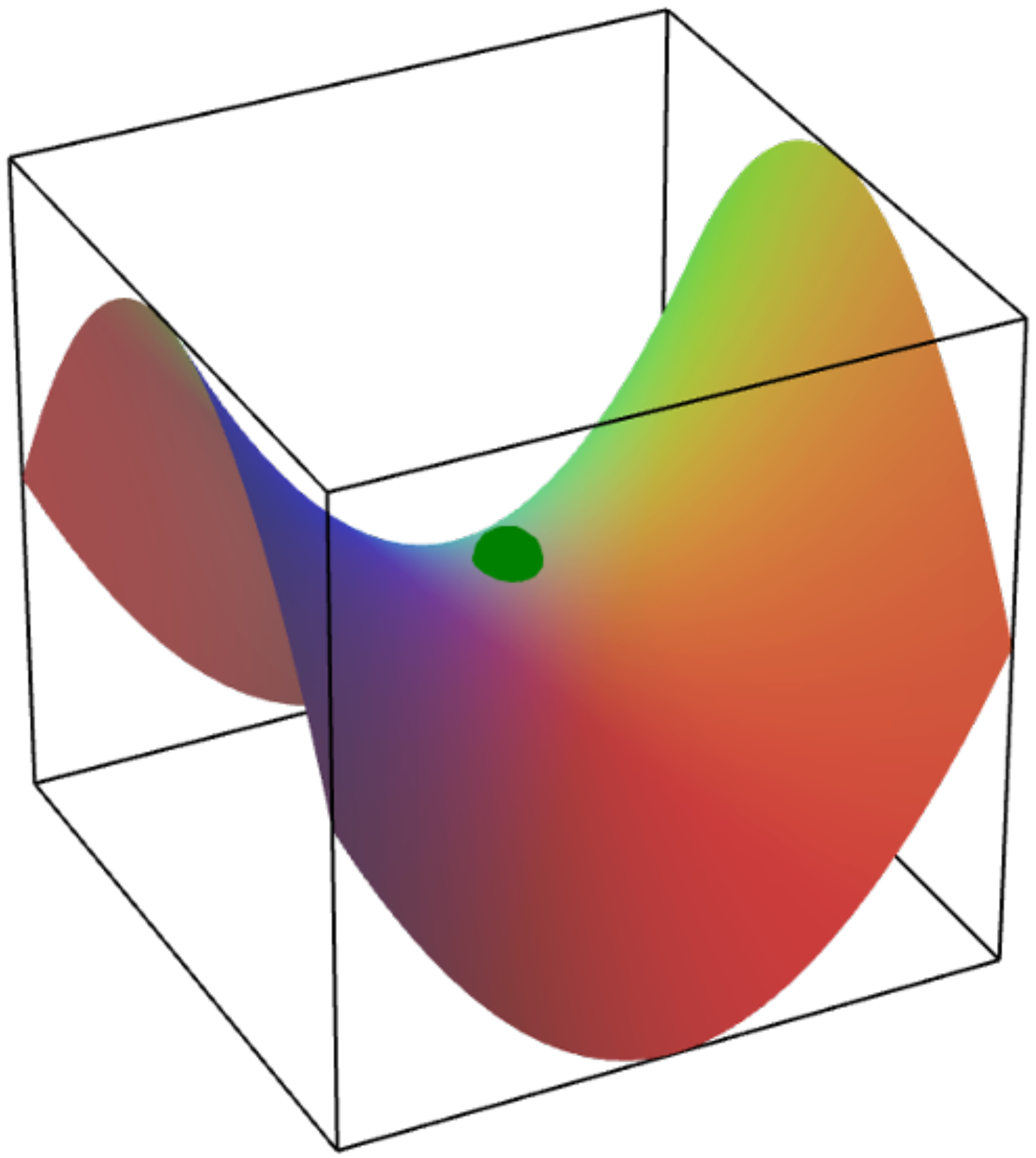
- Non-convex loss landscape
  - → Stuck in local minima
  - → Stuck in a saddle point

Problems with gradient descent



- Non-convex loss landscape
  → Stuck in local minima
  → Stuck in a saddle point
- No convergence guarantees

Problems with gradient descent



- Non-convex loss landscape
  - → Stuck in local minima
  - → Stuck in a saddle point
- No convergence guarantees
  - → Sub optimal solutions
  - → No incentive to update parameters

More Problems with gradient descent

- When scale and dimensionality of data is high

More Problems with gradient descent

- When scale and dimensionality of data is high
  - Model (10,000 params) to classify images
  - 100,000 images
  - Each image 1 Megapixel= 1,000,000 features

More Problems with gradient descent

- When scale and dimensionality of data is high
  - Model (10,000 params) to classify images
  - 100,000 images
  - Each image 1 Megapixel= 1,000,000 features
  - At each step, ~(1,000,000,000,000,000 + 10,000) computations to obtain gradients?

More Problems with gradient descent

- When scale and dimensionality of data is high
- How to perform gradient descent here?

Stochastic Gradient Descent

Stochastic Gradient Descent

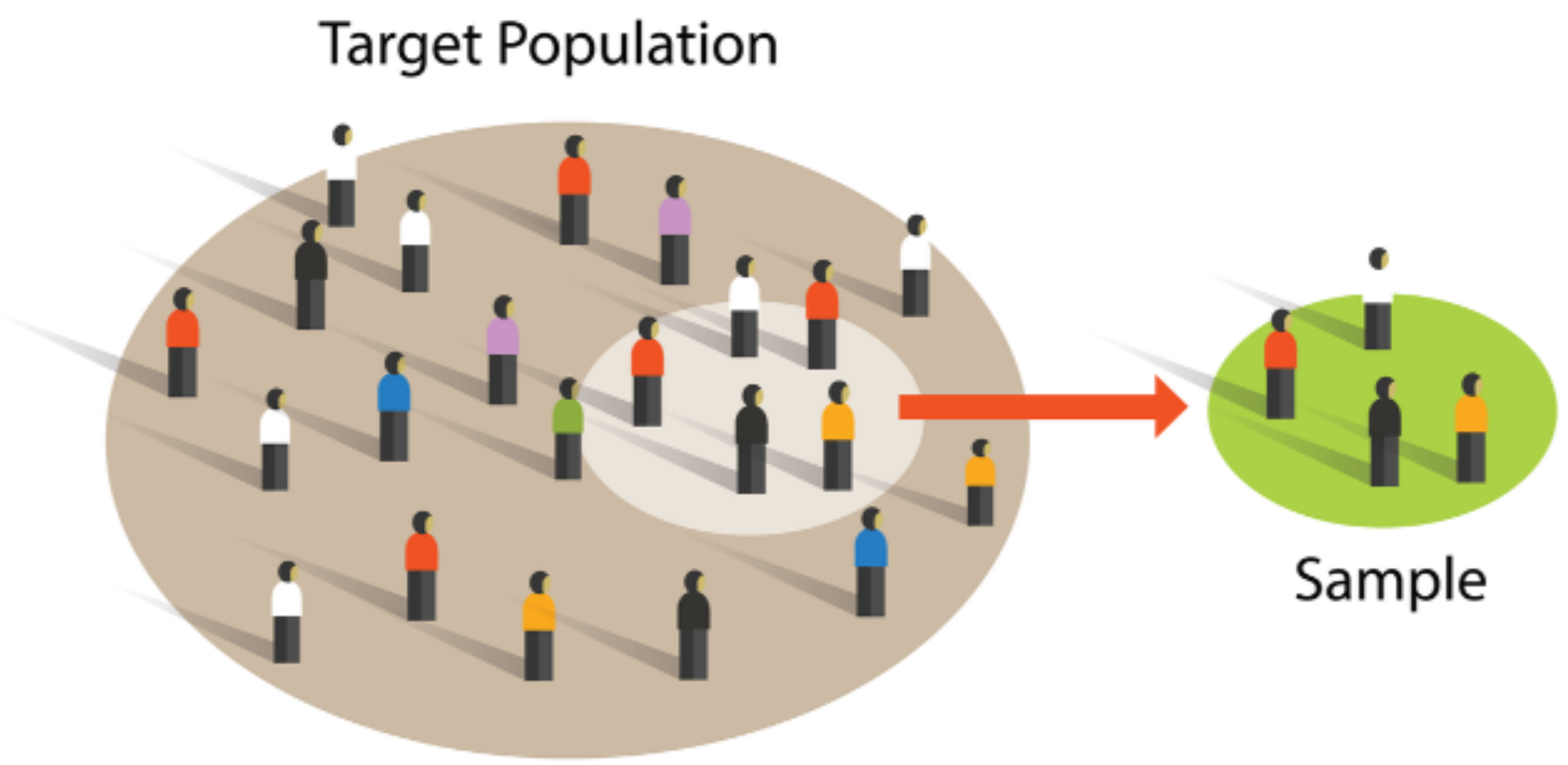
- Stochastic approximation of the true gradient

Stochastic Gradient Descent

- Stochastic approximation of the true gradient
  - Use less data
  - Take approximate steps
  - Take them faster!!

Stochastic Gradient Descent

- Use less data
  - Randomly sample a batch

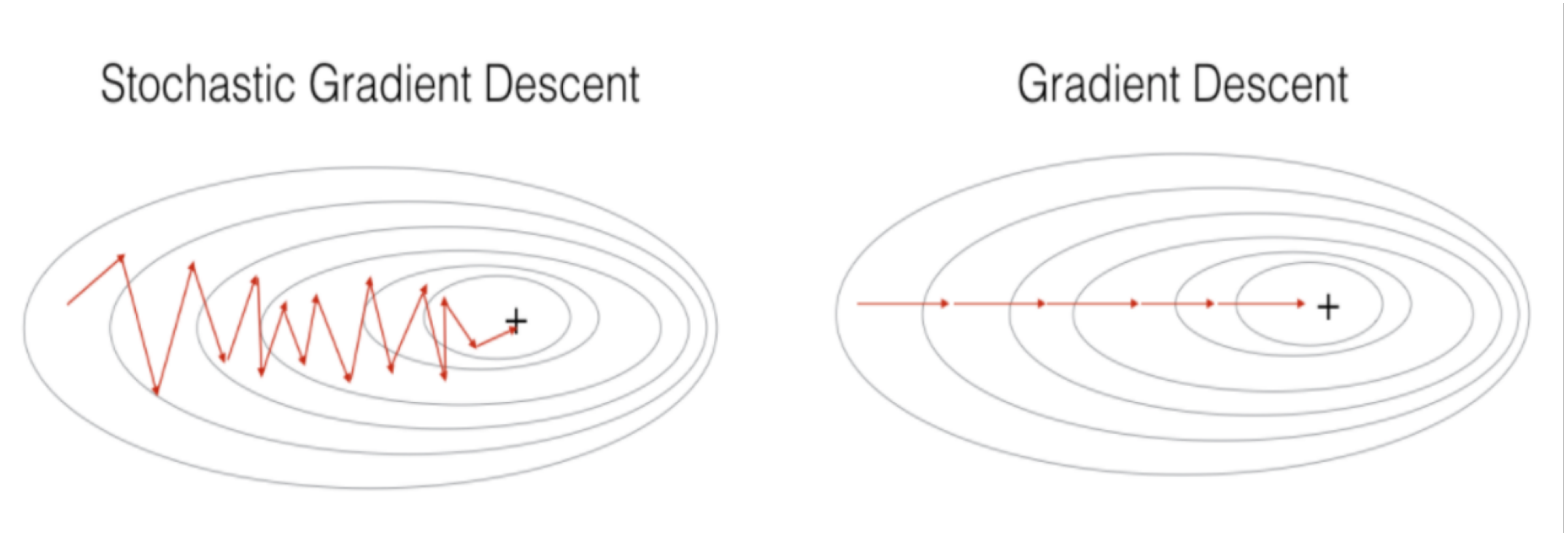


Stochastic Gradient Descent

- Use less data
  - Randomly sample a batch
  - Batch Gradient Descent (true gradient)
  - SGD/ Mini-Batch Gradient Descent (sample size >= 1)

Stochastic Gradient Descent

- Take approximate steps
  - 2D view of going down the valley



Stochastic Gradient Descent

- Take approximate steps
  - 2D view of going down the valley
  - Smaller variance = better estimate

Stochastic Gradient Descent

- Take steps faster
  - Mini-batch enables parallelism
  - Enables use of a GPU

Stochastic Gradient Descent

- SGD and variance
  - High variance near optimal solution (example)
  - Early stopping

Stochastic Gradient Descent

- SGD in Neural Networks
  - Backpropagation = calculate a single stochastic gradient

Stochastic Gradient Descent

- SGD in Neural Networks
  - Backpropagation = calculate a single stochastic gradient
  - Implementation challenges:

    → Step-size?

    → Mini-batch size?

More Optimizers

- Adaptive moment estimation (Adam)

More Optimizers

- Adaptive moment estimation (Adam)
  - **Separate learning rate** (based on moments)
  - Includes momentum
  - Recommended as default*

More Optimizers

- Adaptive Gradient (AdaGrad)

More Optimizers

- Adaptive Gradient (AdaGrad)
  - Learning rate based on frequency of features
  - Suitable for sparse data (e.g., language)
  - Accumulates gradients and scales each weight
  - Disadvantage: infinitesimally small learning rates

More Optimizers

- Adaptive Gradient (AdaDelta)

More Optimizers

- Adaptive Gradient (AdaDelta)
  - **Solves the problems with AdaGrad**
  - Smaller updates

More Optimizers

- Resilient Back-propagation (Rprop)

More Optimizers

- Resilient Back-propagation (Rprop)
  - **Only takes sign of gradients for update**
  - Invariant to initialization of hyper-parameters
  - Reinforcement Learning?

More Optimizers

- Choice of optimizer matters
  - Convergence time
  - Type of problem/ data

Recap

Recap

- Optimization
  - Maximize or minimize an objective function to find best fit parameters

Recap

- Gradient Descent
    - Iterative algorithm that uses gradients to solve optimization

Recap

- Stochastic Gradient Descent
  - Uses random sampling to apply gradient descent on data with high scale and dimensionality

Thank You!

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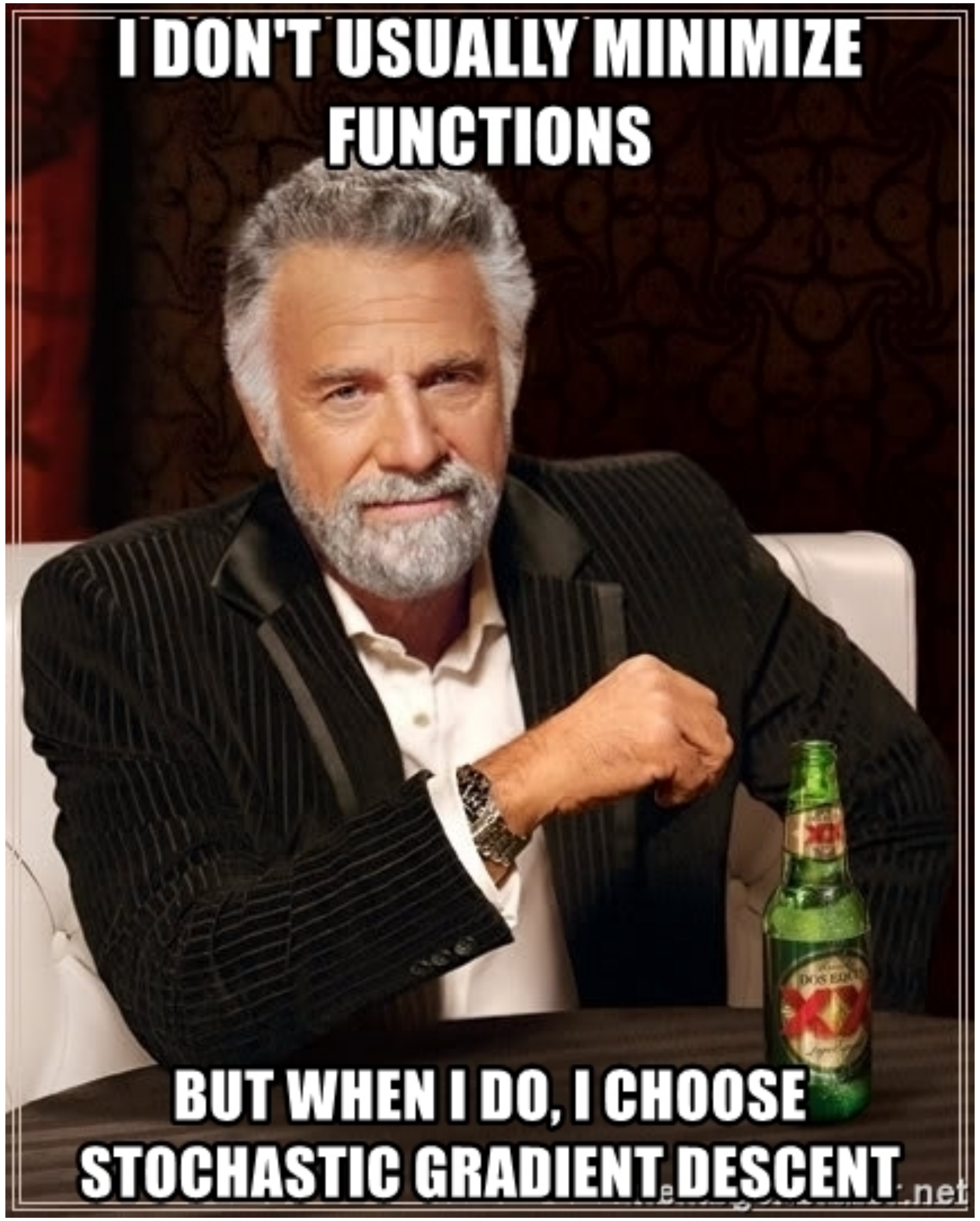
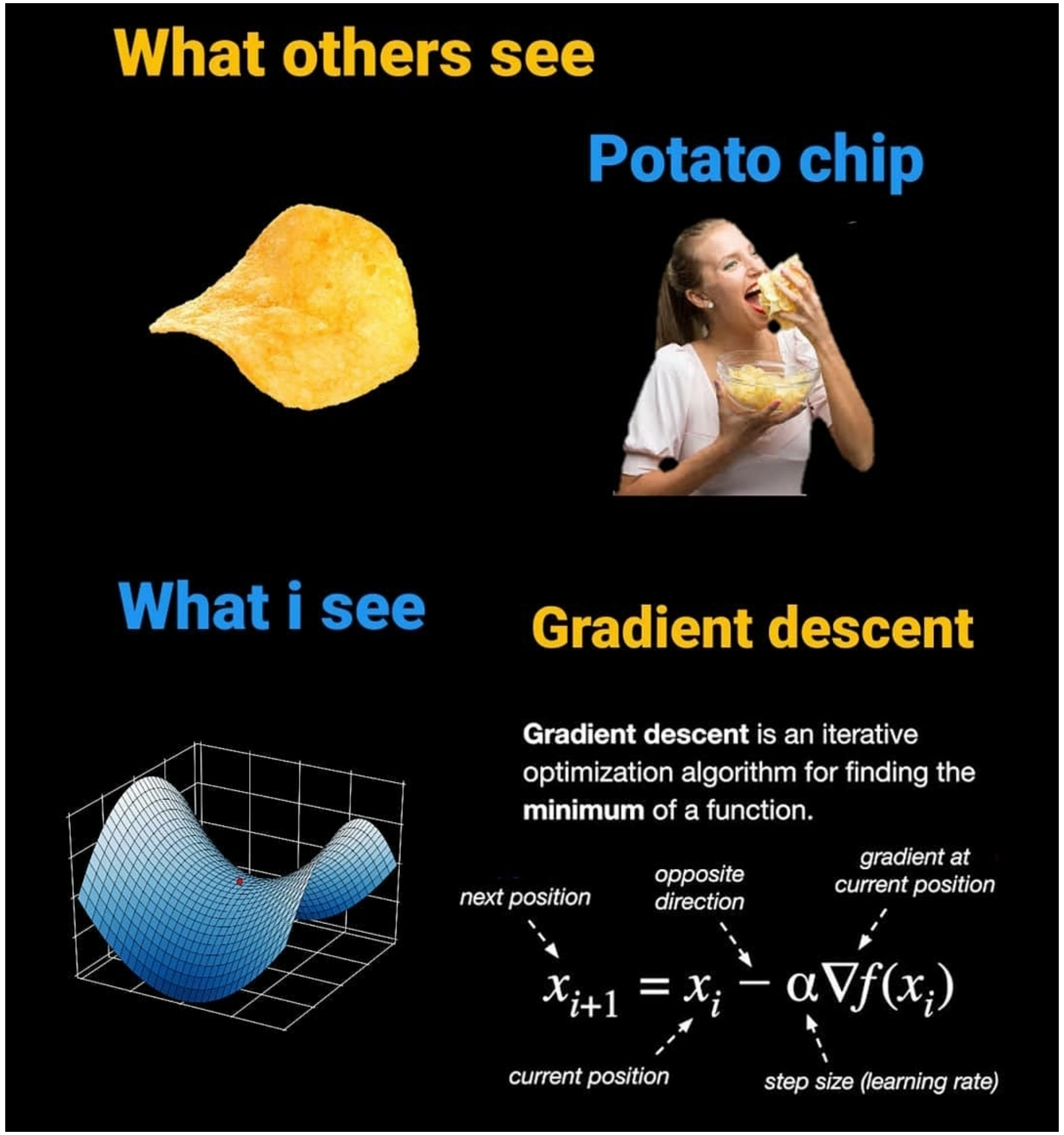
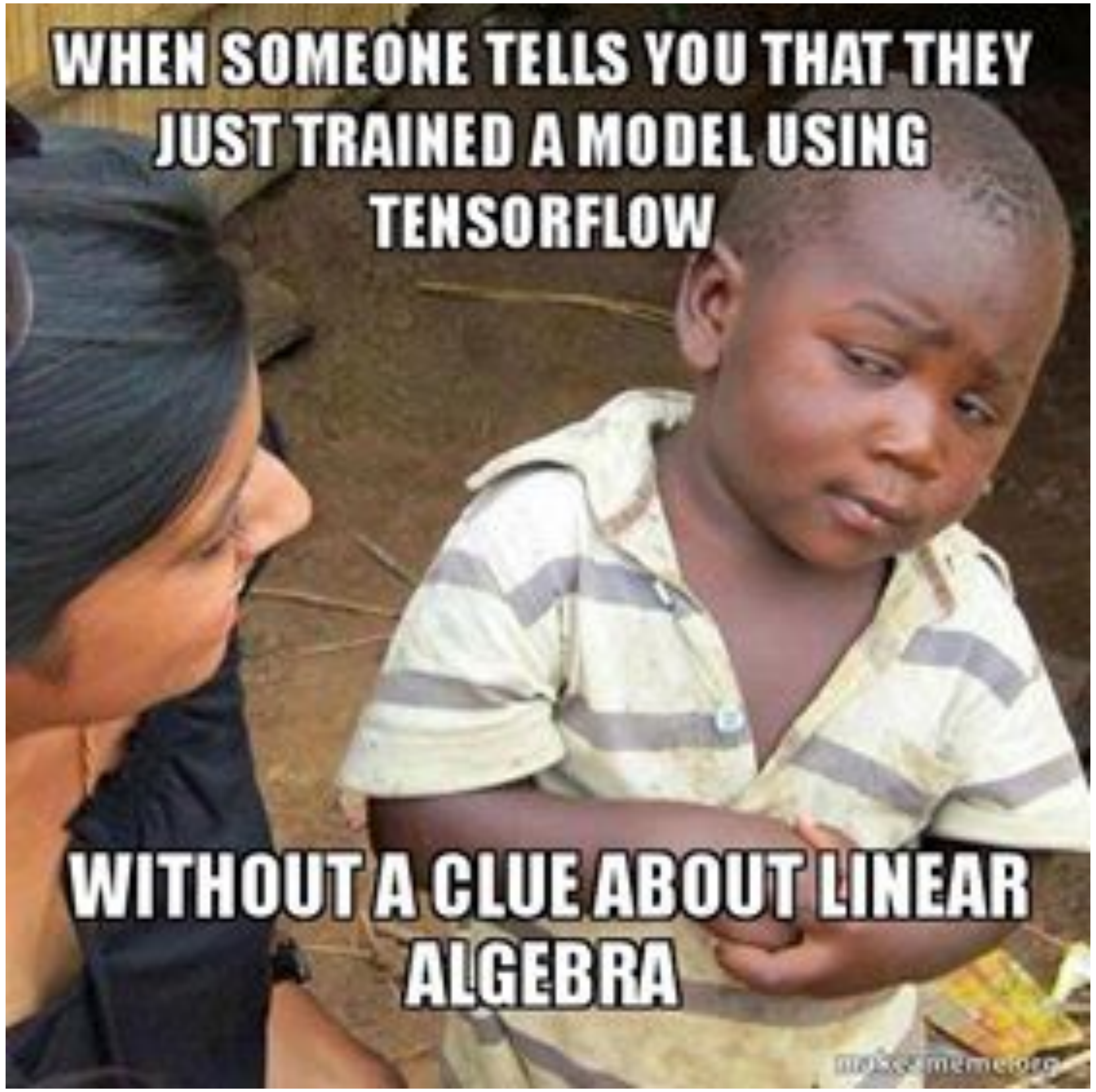
But wait… there's more…


I DON'T USUALLY MINIMIZE FUNCTIONS
BUT WHEN I DO, I CHOOSE STOCHASTIC GRADIENT DESCENT


What others see
Potato chip
What i see
Gradient descent
Gradient descent is an iterative optimization algorithm for finding the **minimum** of a function.
next position
opposite direction
gradient at current position
$x_{i+1} = x_i - \alpha \nabla f(x_i)$
current position
step size (learning rate)


WHEN SOMEONE TELLS YOU THAT THEY JUST TRAINED A MODEL USING TENSORFLOW
WITHOUT A CLUE ABOUT LINEAR ALGEBRA


Global
minimum
Stochastic
gradient
descent