HELMHOLTZ ZENTRUM
DRESDEN ROSSENDORF

Deep Learning Neural Network Block

HIDA_2025

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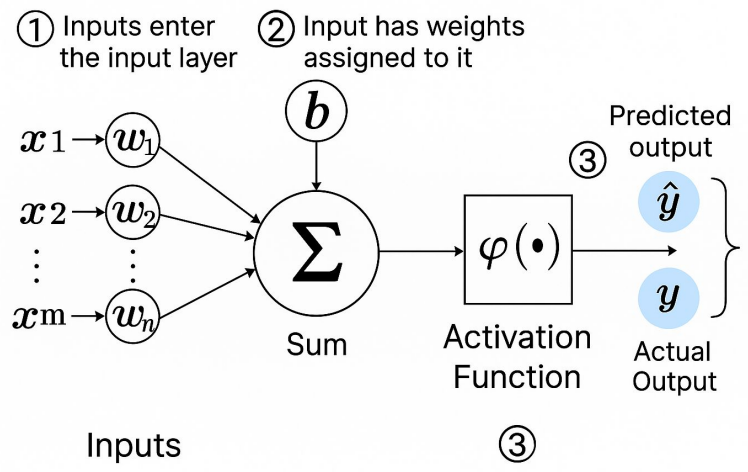
DRESDEN concept

Step 1: Forward Propagation

- **Inputs:** $x_1, x_2, x_3 \ldots\ldots x_m$
- Each input has an associated **weight:** w_1, w_2, w_3
- A single **neuron** in the hidden layer **computes**: $z = x_1w_1 + x_2w_2 + x_3w_3 + b$
- Output from the neuron after **activation** (e.g., sigmoid, ReLU): $\hat{y} = activation(z)$
- **Loss Function:** Measures the difference between prediction $\hat{y}$ and true label y.

  Example (MSE - Mean Squared Error): $Loss = \frac{1}{2}(y - \hat{y})^2$



Difference between predicted output and actual output

https://medium.com/@jainvidip/forward-and-backward-propagation-in-multilayered-neural-networks-a-deep-dive-d596e875dedf

Step 2: Backpropagation Concept

- **Goal:** Minimize the loss by adjusting weights.
- **Compute gradient:** Use calculus (chain rule) to compute the gradient of the loss w.r.t each weight.
- **Gradient Descent Rule:** Update weights in the opposite direction of the gradient:

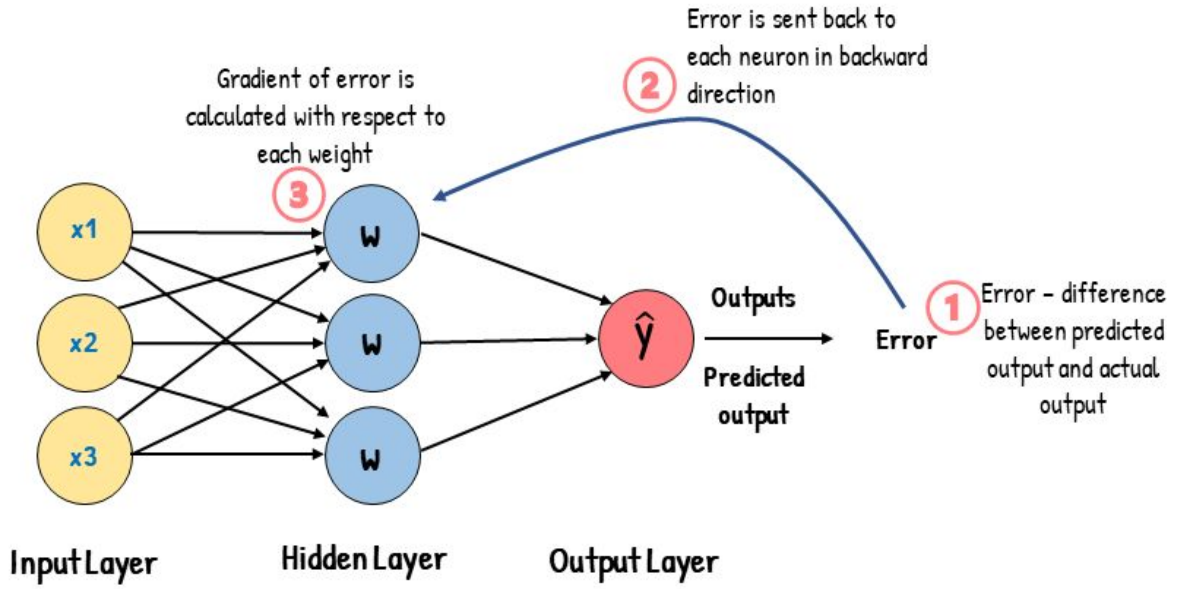
$$w_i^{new} = w_i^{old} - \eta \cdot \frac{\partial Loss}{\partial w_i}$$

where:

η = learning rate (controls how big each step is)

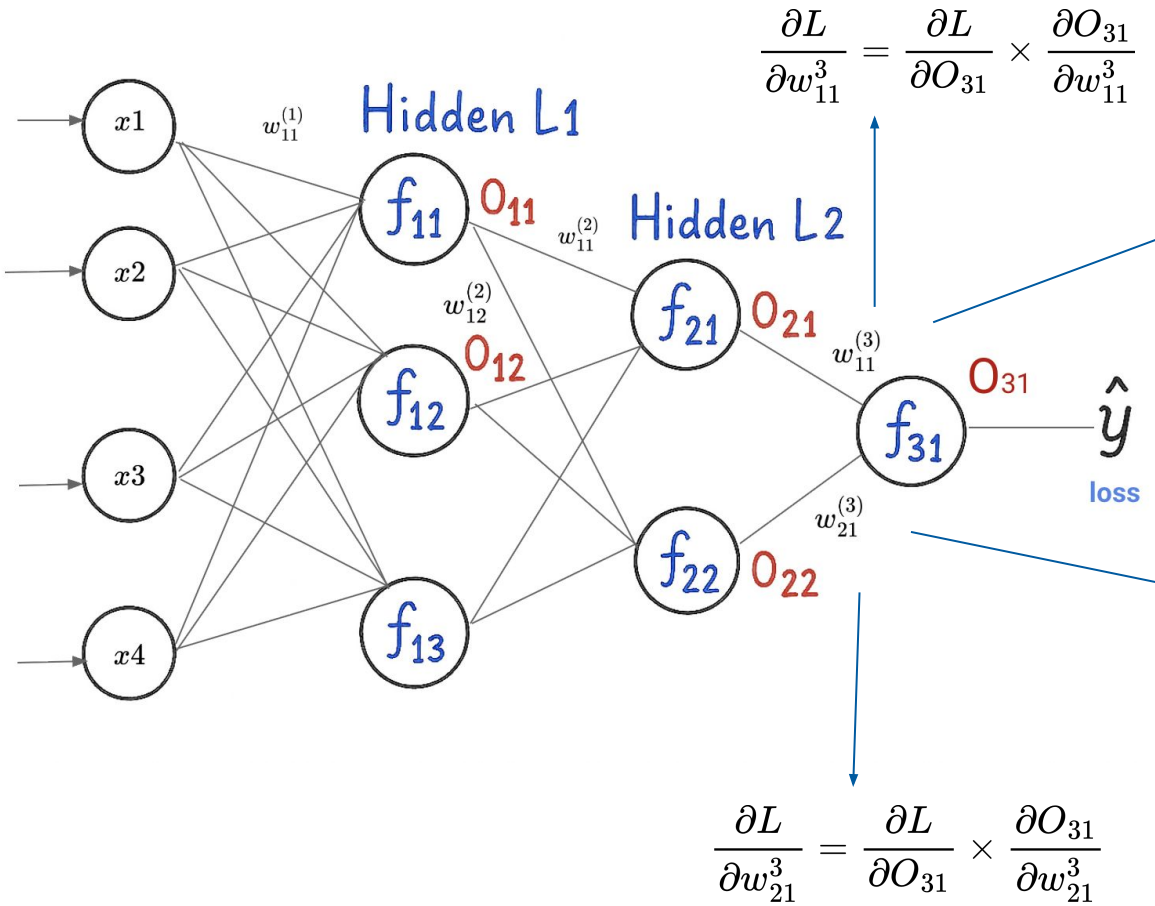
$\frac{\partial \text{Loss}}{\partial w_i}$ = how sensitive the loss is to weight w_i

- **Optimizer:** (Gradient Descent, Adam, RMSprop) do this updating process



https://vijaygadre.medium.com/deep-learning-explained-a-beginners-guide-42fd8e8a770b

CHAIN Rule in BACKPROPAGATION



$$w_{11,\ new}^{(3)} = w_{11,\ old}^{(3)} - \eta \cdot \frac{\partial L}{\partial w_{11,\ old}^{(3)}}$$

update weight | old weight | learning rate | gradient

$$w_{21,\ new}^{(3)} = w_{21,\ old}^{(3)} - \eta \cdot \frac{\partial L}{\partial w_{21,\ old}^{(3)}}$$

https://www.youtube.com/watch?v=cxPAvoIbsIk&list=PLZoTAELRMXVPGU70ZGsckrMdr0FteeRUi&index=8

CHAIN Rule in BACKPROPAGATION

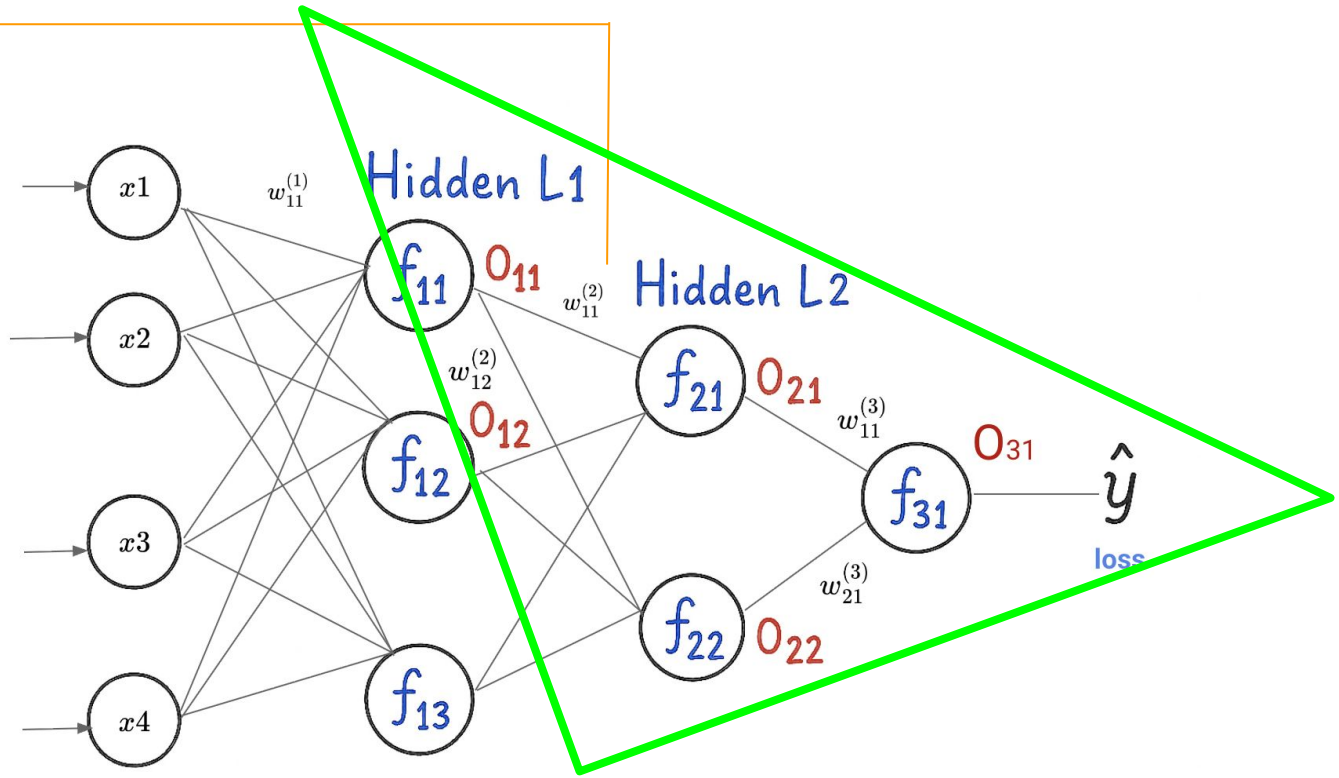
$$w^{(2)}_{11,\ new} = w^{(2)}_{11,\ old} - \eta \cdot \frac{\partial L}{\partial w^{(2)}_{11}}$$

update weight

old weight

learning rate

gradient



$$\frac{\partial L}{\partial w^{(2)}_{11}} = \left(\frac{\partial L}{\partial O_{31}} \cdot \frac{\partial O_{31}}{\partial O_{21}} \cdot \frac{\partial O_{21}}{\partial w^{(2)}_{11}} \right) + \left(\frac{\partial L}{\partial O_{31}} \cdot \frac{\partial O_{31}}{\partial O_{22}} \cdot \frac{\partial O_{22}}{\partial w^{(2)}_{12}} \right)$$

https://www.youtube.com/watch?v=cxPAvoIbsIk&list=PLZoTAELRMXVPGU70ZGsckrMdr0FteeRUi&index=8

Exploding Gradients

$$\frac{\partial O_{31}}{\partial O_{21}} = \frac{\partial \left(w_{11}^{(3)} \cdot O_{21} \right)}{\partial O_{21}} = w_{11}^{(3)}$$

$$\frac{\partial L}{\partial w_{11}^{(2)}} = \left(\frac{\partial L}{\partial O_{31}} \cdot \frac{\partial O_{31}}{\partial O_{21}} \cdot \frac{\partial O_{21}}{\partial w_{11}^{(2)}} \right) + \left(\frac{\partial L}{\partial O_{31}} \cdot \frac{\partial O_{31}}{\partial O_{22}} \cdot \frac{\partial O_{22}}{\partial w_{12}^{(2)}} \right)$$

activation derivative

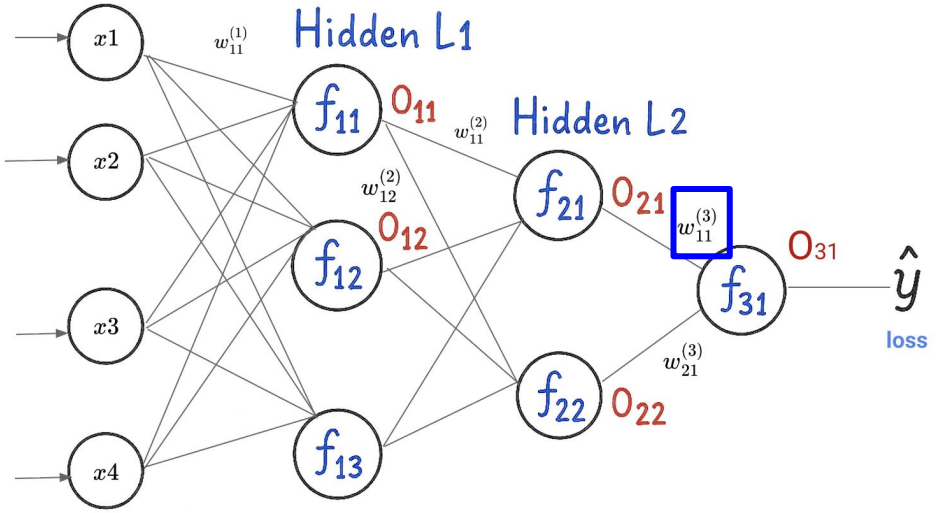
weights in layer 3

What Happens?

- If weights were very large, the outputs became very large
  - → **During backpropagation,** at each layer, they are multiplied by:
    - Weights of the layer
    - Activation derivatives
  - multiplying these large values made gradients very big → **exploding gradients**

Why Exploding Happens?

- If weights are **large (>1)**, every backward step **amplifies** the gradient.
- After many layers, the gradient becomes **huge** (exponential growth).



This made deep networks very hard to train.

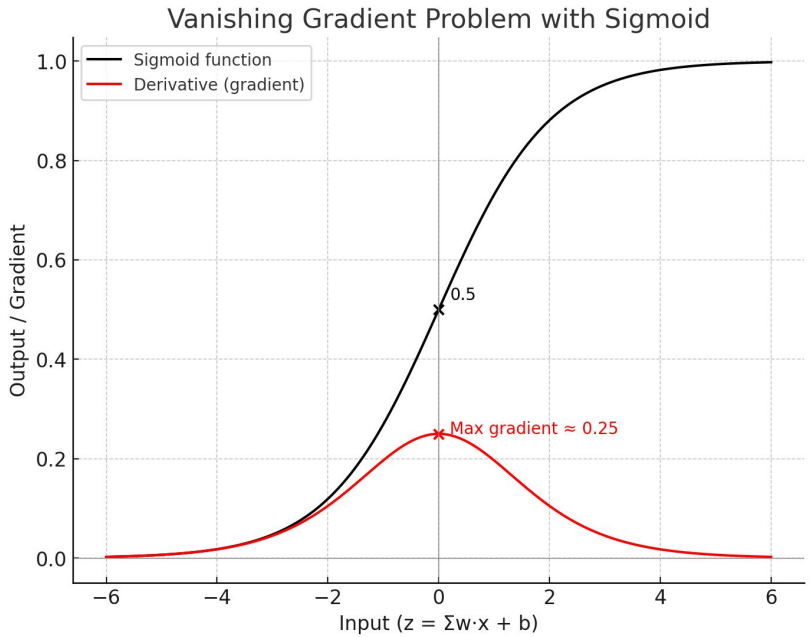
https://www.youtube.com/watch?v=cxPAvoIbsIk&list=PLZoTAELRMXVPGU70ZGsckrMdr0FteeRUi&index=8

Vanishing Gradients

What Happens?

- If weights were very small and we used sigmoid/tanh activations (which squash values close to 0)
  - → **During backpropagation,** multiplying these small values made gradients very tiny → **vanishing gradients**

$$w_{\text{new}} = w_{\text{old}} - \eta \cdot \text{gradient}$$



Why Vanishing Happens?

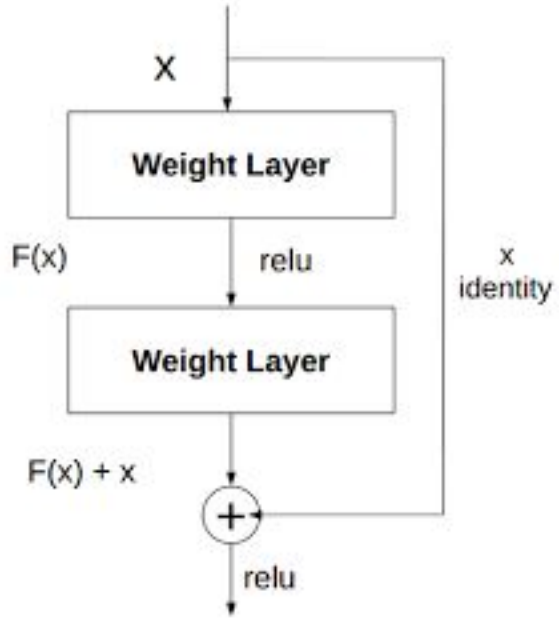
- If each gradient is small (< 1), the product shrinks toward 0.
- When the gradient becomes almost zero:
  - The update step is extremely tiny: $w_{\text{new}} \approx w_{\text{old}}$
  - Early layers receive almost no update

This makes training slows down or even stops

https://www.youtube.com/watch?v=JIWXbzRXk1I&list=PLZoTAELRMXVPGU70ZGsckrMdr0FteeRUi&index=10

What is the solution now?

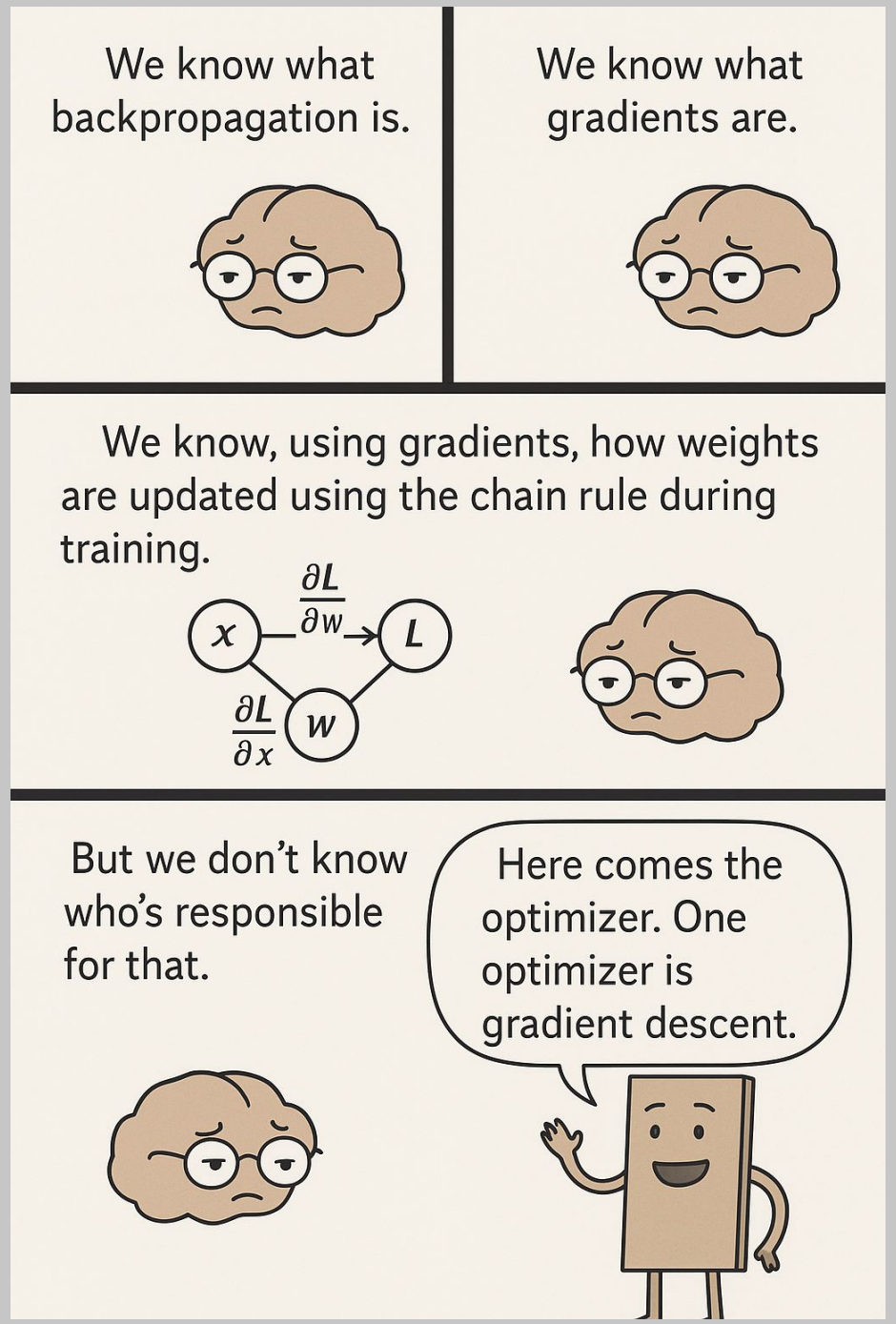
- **ReLU activations** → prevent values from shrinking too much.
- **Batch Normalization** → keeps activations well-scaled, not too large or too small, making training more stable.
    - output → BatchNorm (normalize) → Activation function (like ReLU or tanh)
- **Skip Connections** → Creates a shortcut that jumps over some layers. So, during propagation, gradient does not get multiplied repeatedly by small numbers through many layers and hence, gradient doesn't vanish. For example **ResNets**.
- **Normalize input data (standard scaler/MinMax scaler form sklearn):** Scale training data to a small range (like 0–1) → This prevents very large or very small numbers that could shrink gradients during backpropagation.
- **Proper Weight Initialization** → Xavier, He initialization



https://www.researchgate.net/publication/354907417_Scalable_deeper_graph_neural_networks_for_high-performance_materials_property_prediction

What is Optimizer

Adjusts a model’s weights to reduce the loss



Gradient Descent

Idea:

Gradient Descent is a method used to find the lowest point (minimum) of a curve or surface. Think of it like trying to find the bottom of a valley when you're walking downhill.

- Imagine you are **standing on top of a hill**
- You want to **reach the lowest point**
- You **can't see the whole hill**, but you **can feel the slope** under your feet
- So you take **small steps downhill each time**

generated by chatgpt

This method is called Gradient Descent.

Direction of Gradients vs Our Step

Gradient = points uphill

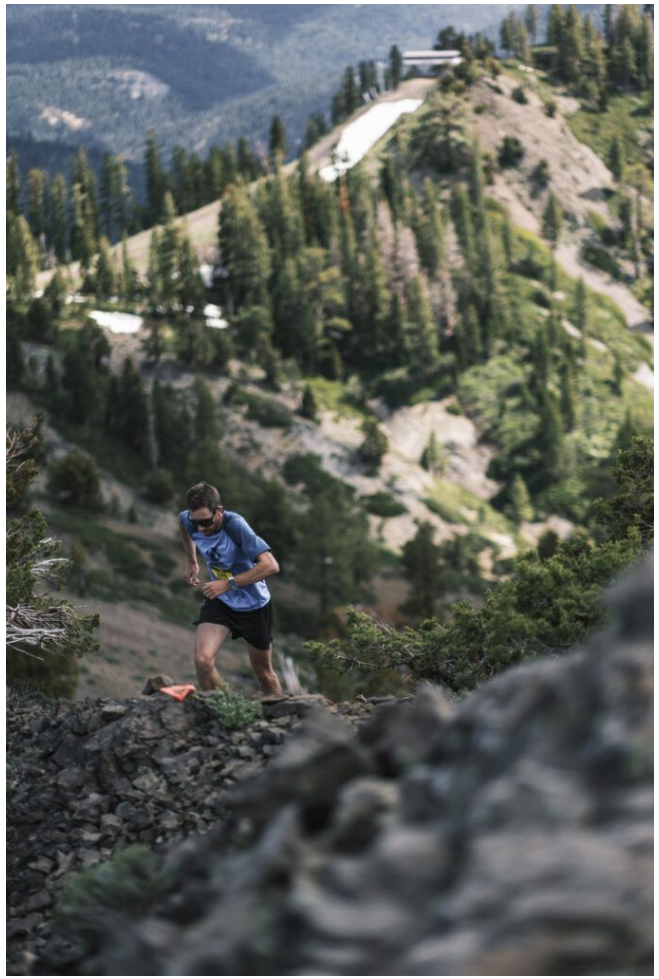
We want to go downhill → **go opposite the gradient**

The **gradient is like an arrow** showing where the ground goes **up the fastest**

If you walk **with the arrow** → **you go up the hill** (loss increases)

Our goal is to **reach the bottom** (make loss small)

So we **move opposite the arrow (gradient)** → this takes us **downhill**

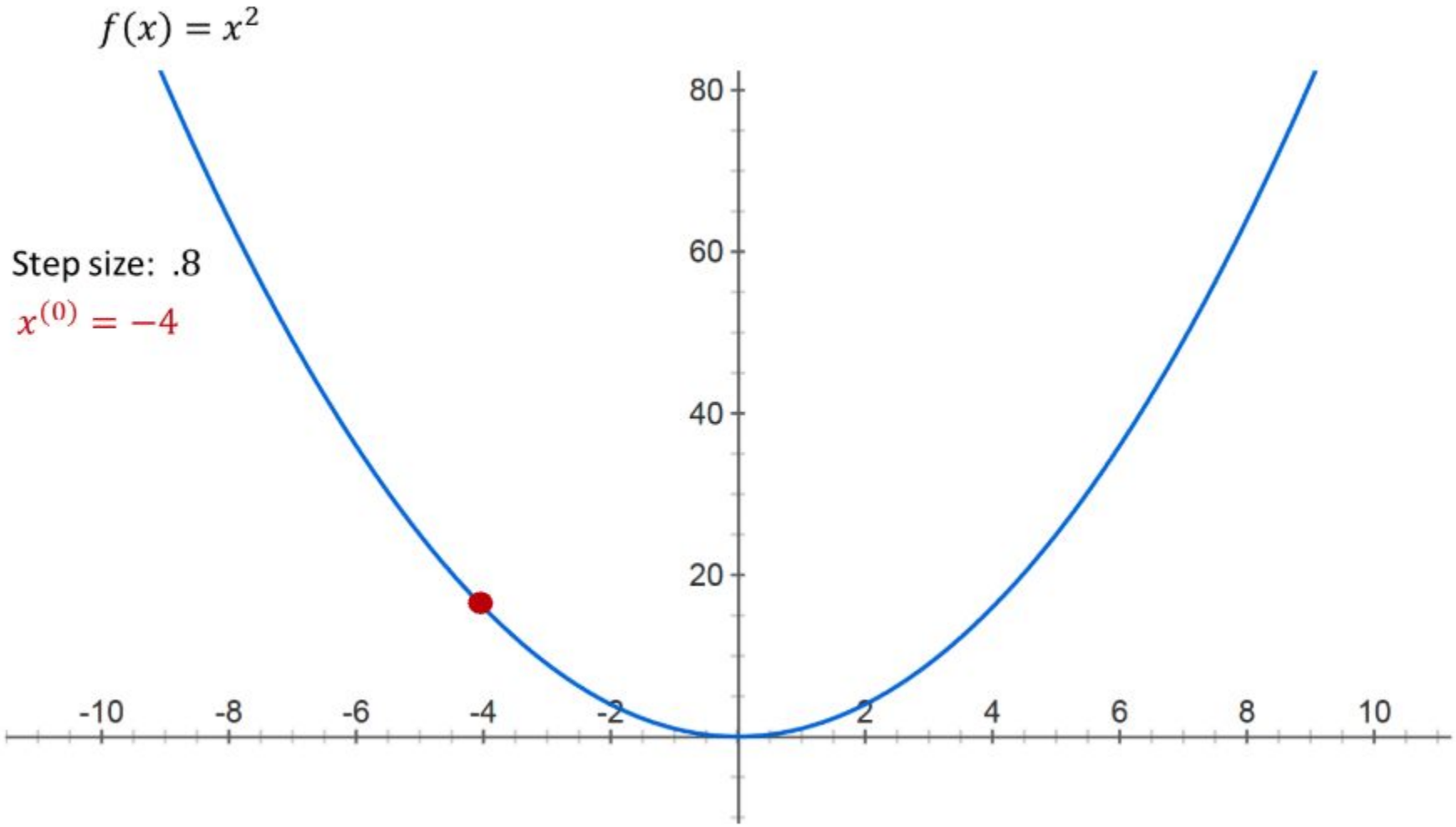


generated by chatgpt

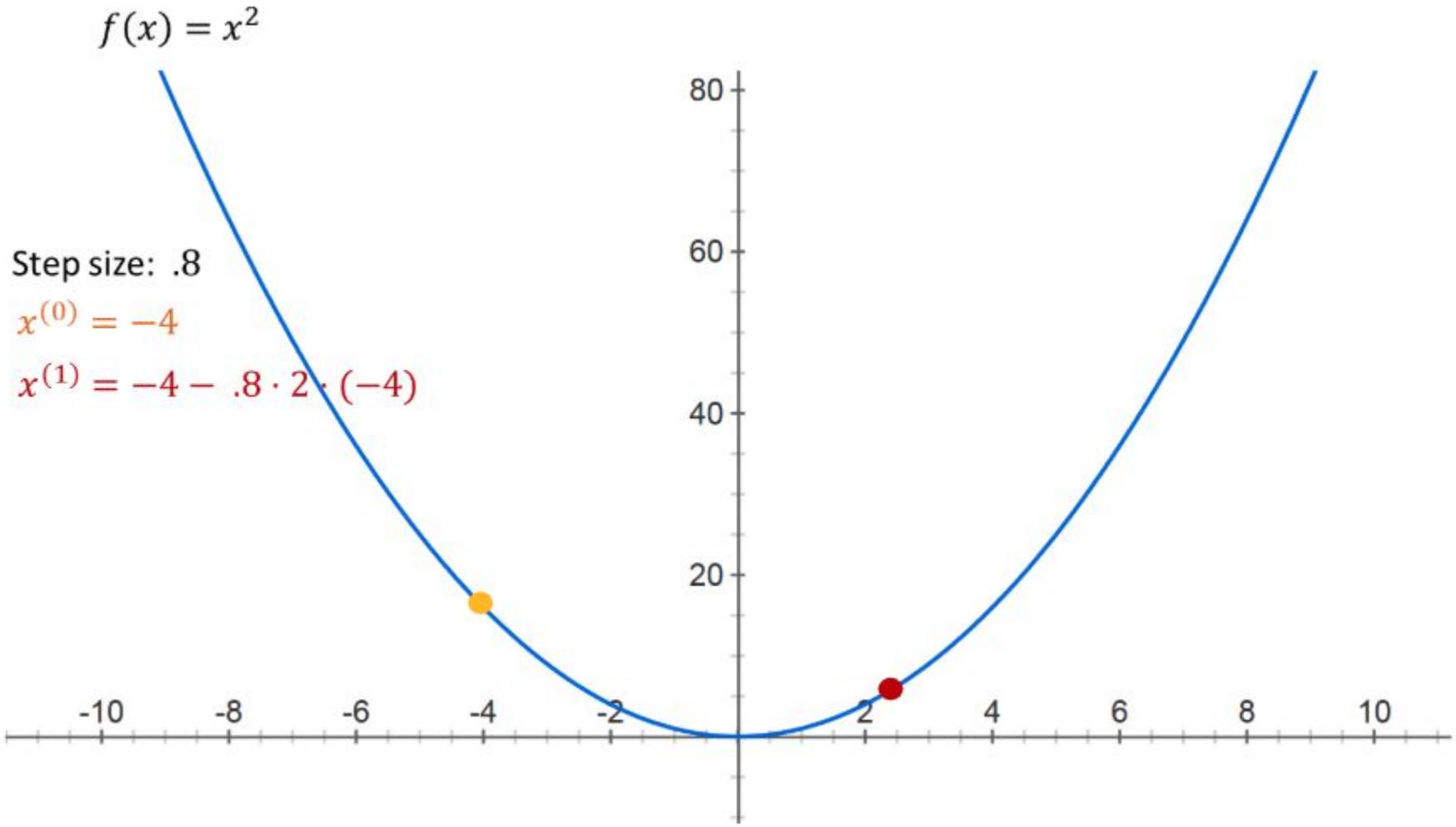
This is the **main reason** why we **subtract** the derivative (gradient) from the old weight in gradient descent.

$$w_i^{new} = w_i^{old} - \eta \cdot \frac{\partial Loss}{\partial w_i}$$

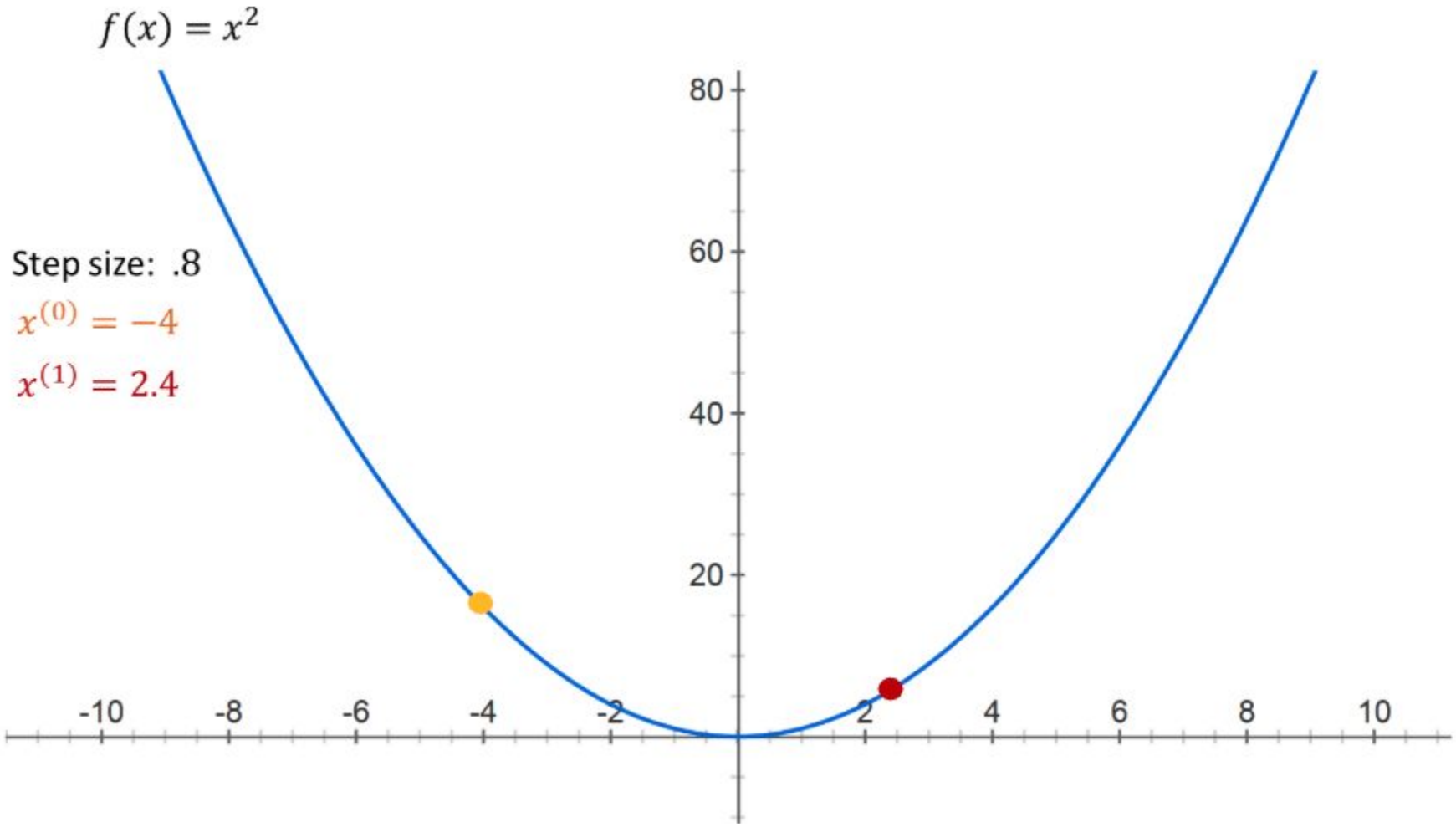
How Weights Change in Gradient Descent



How Weights Change in Gradient Descent



How Weights Change in Gradient Descent



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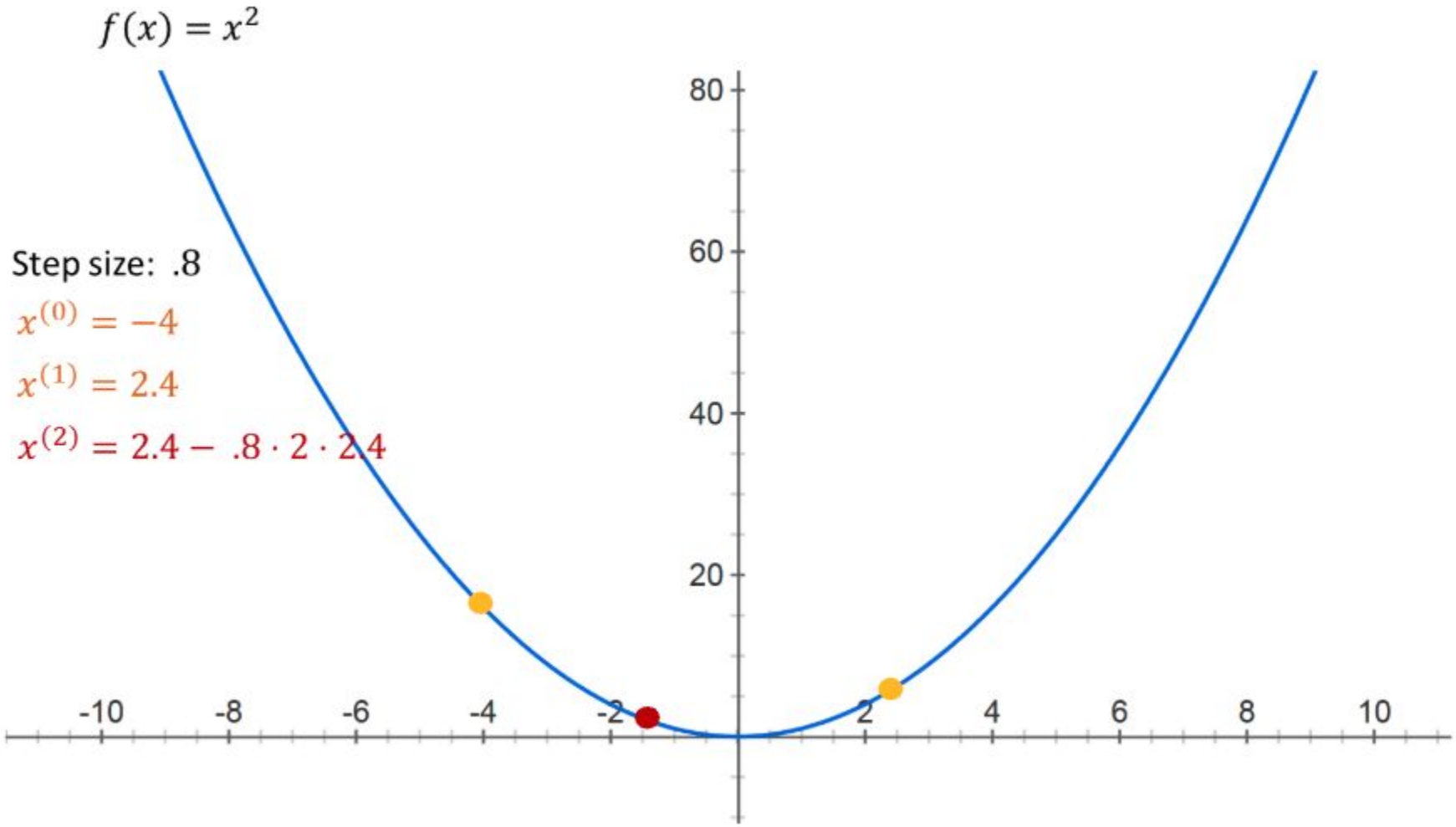
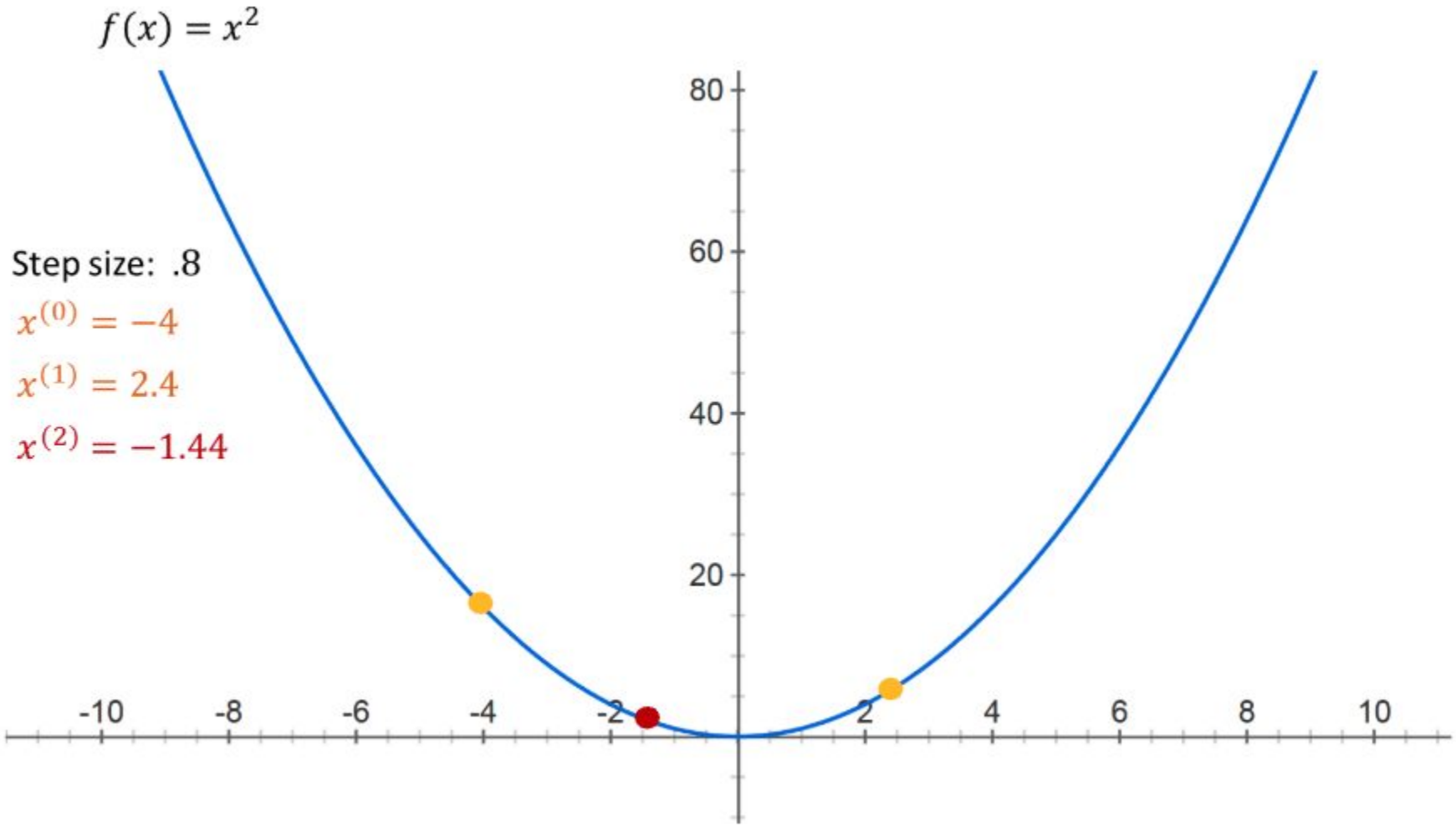
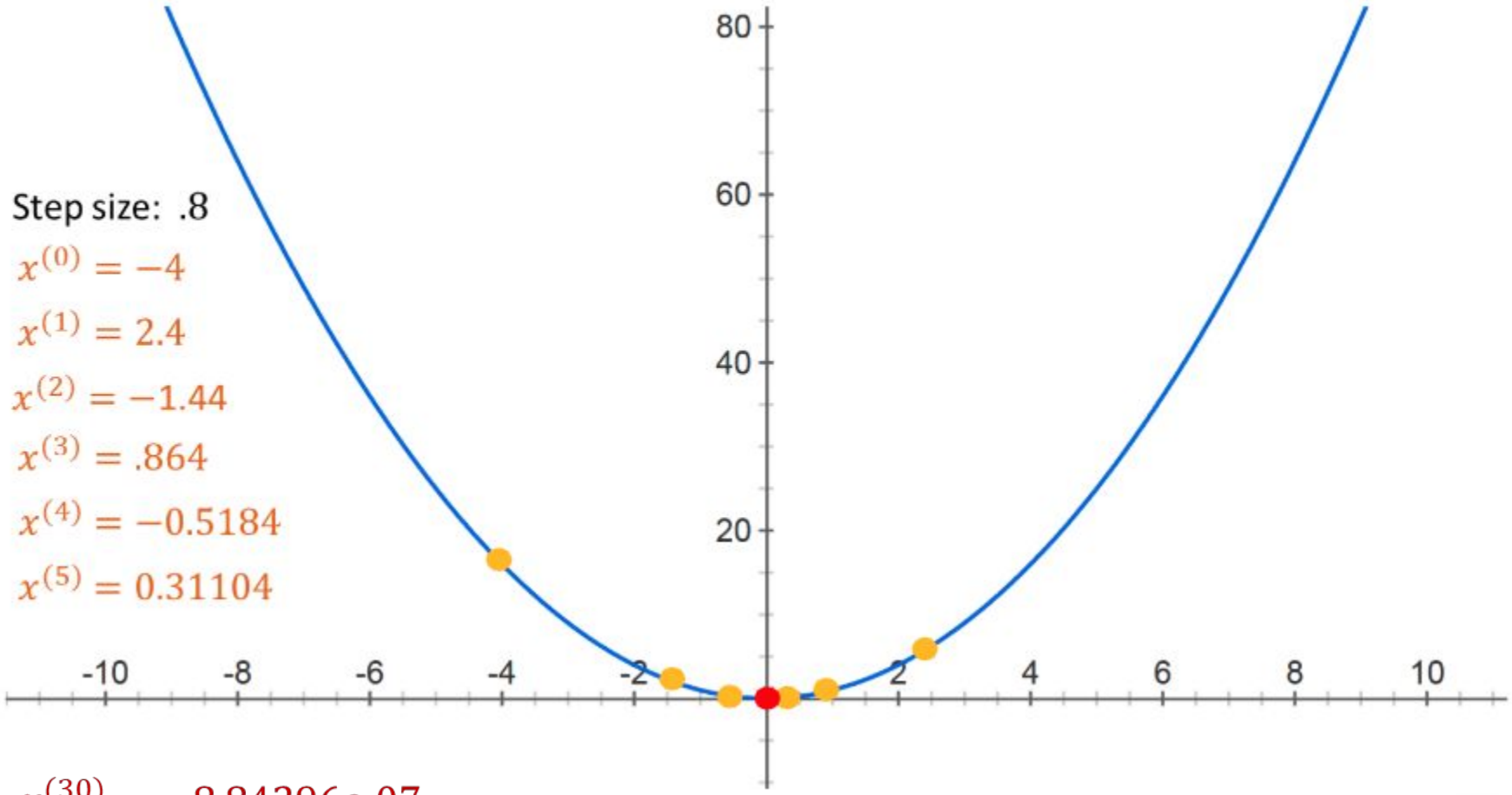


How Weights Change in Gradient Descent



How Weights Change in Gradient Descent

$f(x) = x^2$



Step size: .8

$x^{(0)} = -4$

$x^{(1)} = 2.4$

$x^{(2)} = -1.44$

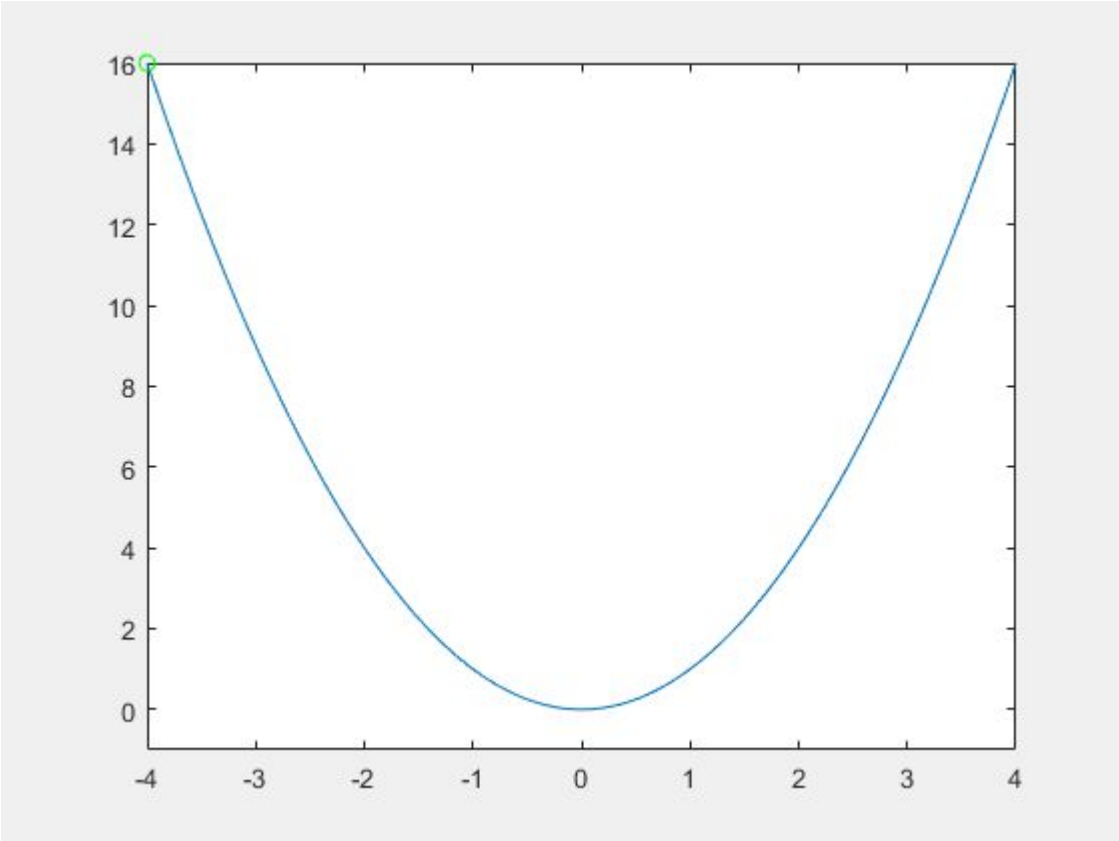
$x^{(3)} = .864$

$x^{(4)} = -0.5184$

$x^{(5)} = 0.31104$

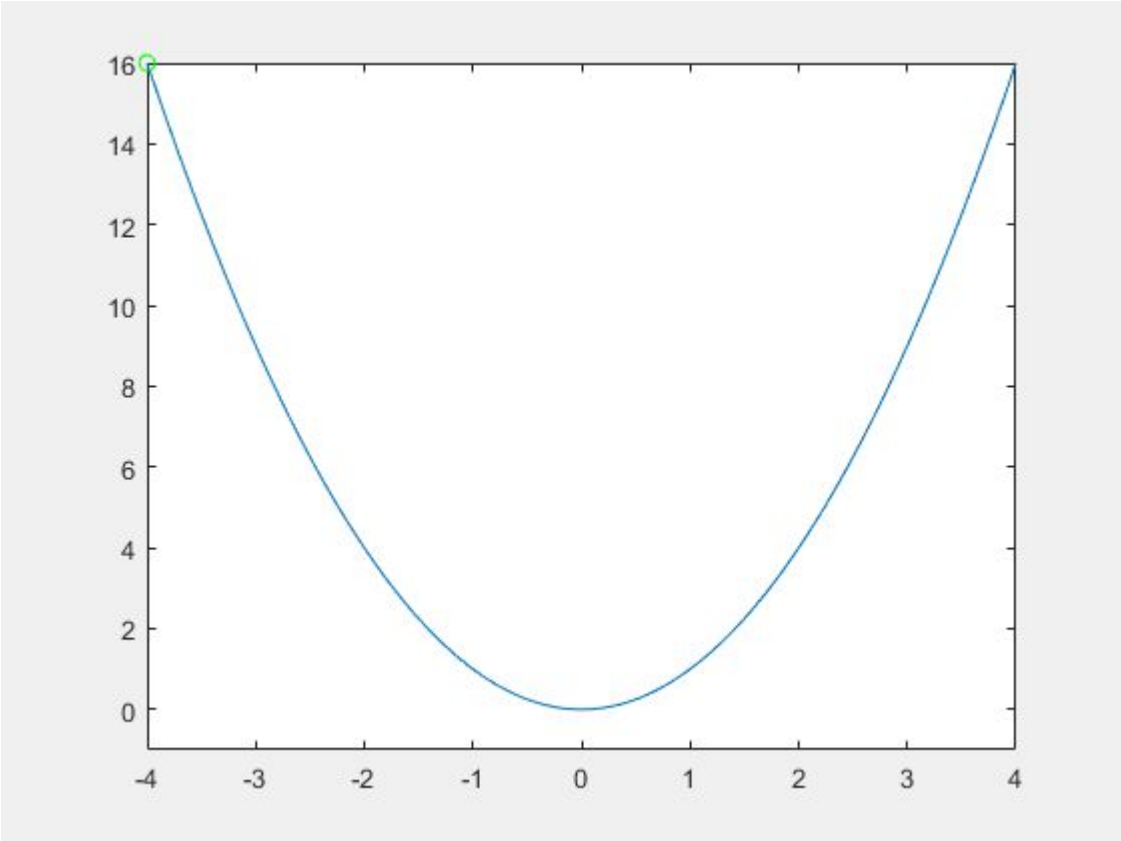
$x^{(30)} = -8.84296e\text{-}07$

Gradient Descent



Step size: .9

Gradient Descent



Step size: .2

Gradient Descent Summary

- The network has one single set of weights (shared by all samples → input data)
- At the start → weights are randomly initialized once
- One training round (called an epoch):
  - Send all samples through the network → **forward propagation**
  - Calculate loss for all samples
  - Compute gradients for all samples→ **backpropagation**
  - Calculate gradients with respect to loss for all samples and then **average** all gradients
  - Update the weights once using this average gradient

❗ **Problem: Using all samples each time makes training very slow on large datasets.**

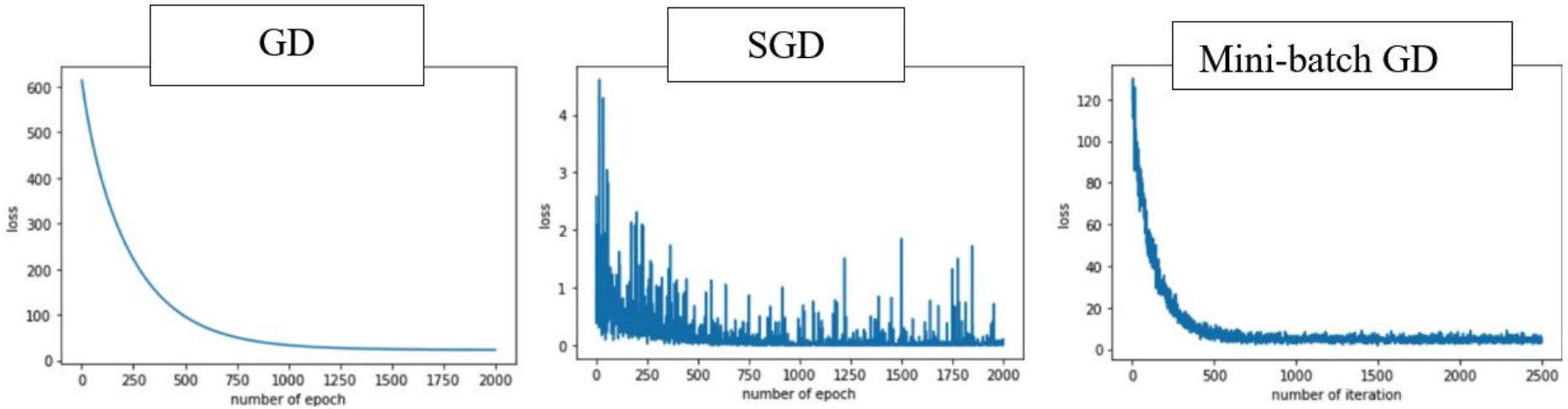
Solution

Stochastic Gradient Descent (SGD)

- A faster version of Gradient Descent
- Uses one sample at a time instead of all samples together
  - Pick one sample
  - Do forward & backward → compute error (gradient)
  - Update weights immediately
  - Repeat for all samples → this completes **1 epoch**

Mini-batch SGD

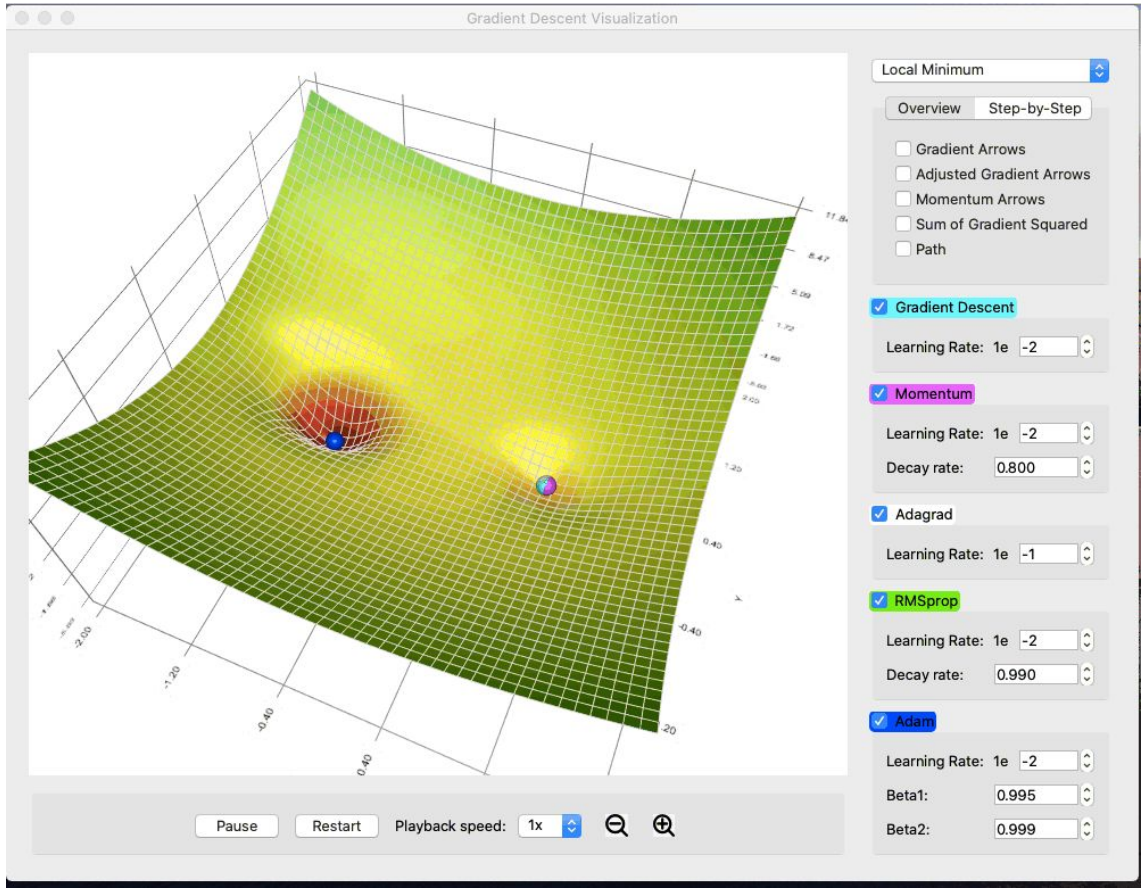
- Instead of 1 sample or all samples, take a **small group** (like 32 or 64).
- Compute average error for that group.
- Update weights.
- Repeat with the next mini-batch until the whole dataset is used → **1 epoch.**



https://medium.com/data-science/deep-learning-optimizers-436171c9e23f

Variants of Stochastic Gradient Descent (SGD)

- SGD with Momentum
  - remembers past direction → makes learning smoother
- Adagrad
  - Instead of one learning rate for everything, it gives each weight its own learning rate.
  - Weights that need bigger updates get them, while stable ones move less.
- RMSprop
  - Adagrad slows down too much over time.
  - RMSprop fixes this by keeping learning rates from becoming too small.
- Adam
  - Combines the ideas of Momentum and RMSprop.
  - Learns fast, adapts well, and works great for deep learning.



ADAM is the most popular choice this days.

https://github.com/lilipads/gradient_descent_viz

Training

After choosing how the model learns using optimizers,

- ❏ we must decide **what data to learn from**
- ❏ **and how to check its learning**.

Training: Dataset Splitting & Evaluation

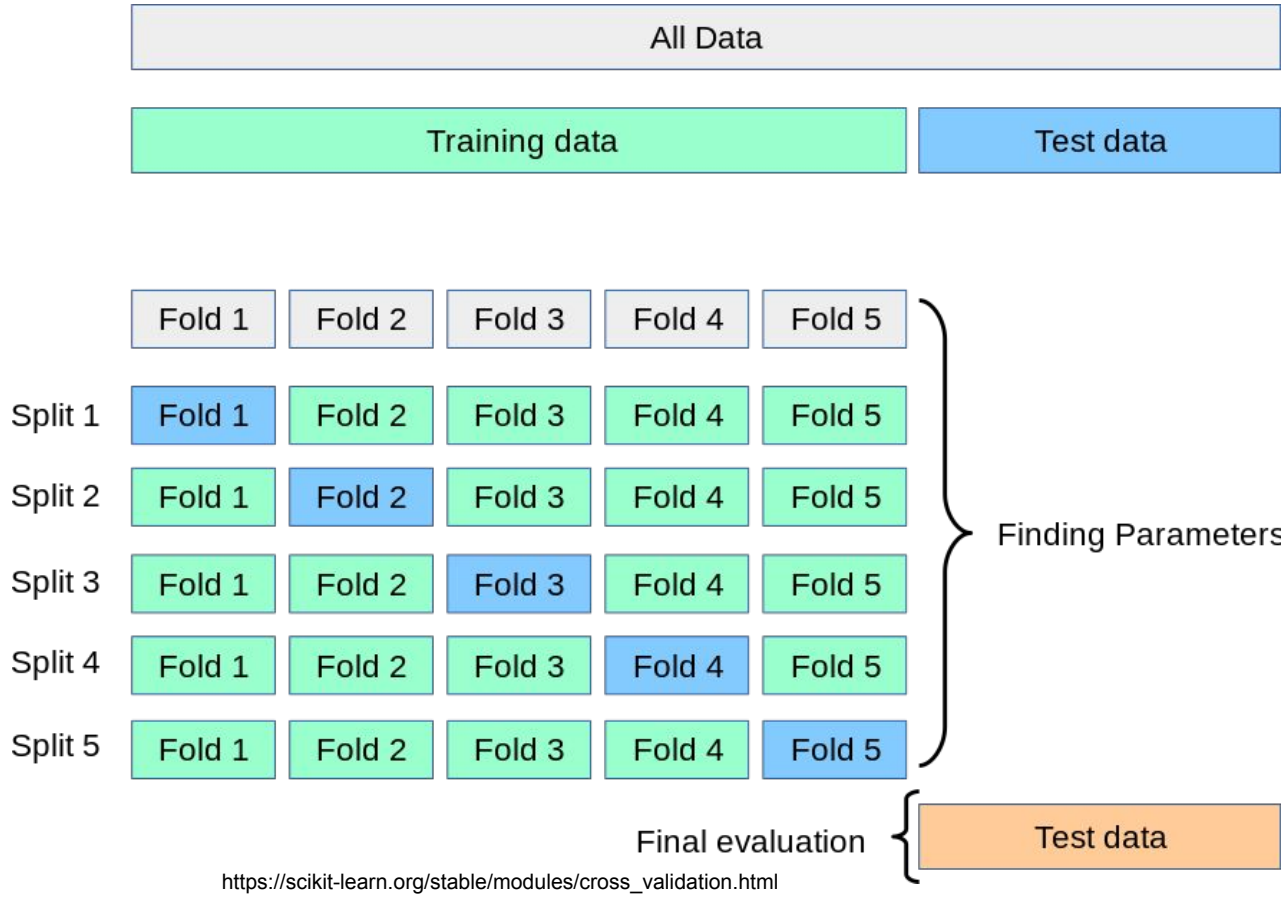
Dataset Splitting

- **Library**: `scikit-learn` (`train_test_split, KFold`)

- **Why**:
  - **Train set → model learns**
  - **Validation set → tune hyperparameters**
  - **Test set → unbiased evaluation**

Cross Validation

- Split data into k folds.
- Train on k-1 folds, validate on remaining fold. Repeat for all folds.



https://scikit-learn.org/stable/modules/cross_validation.html

Why: more reliable performance estimate, reduces overfitting risk.

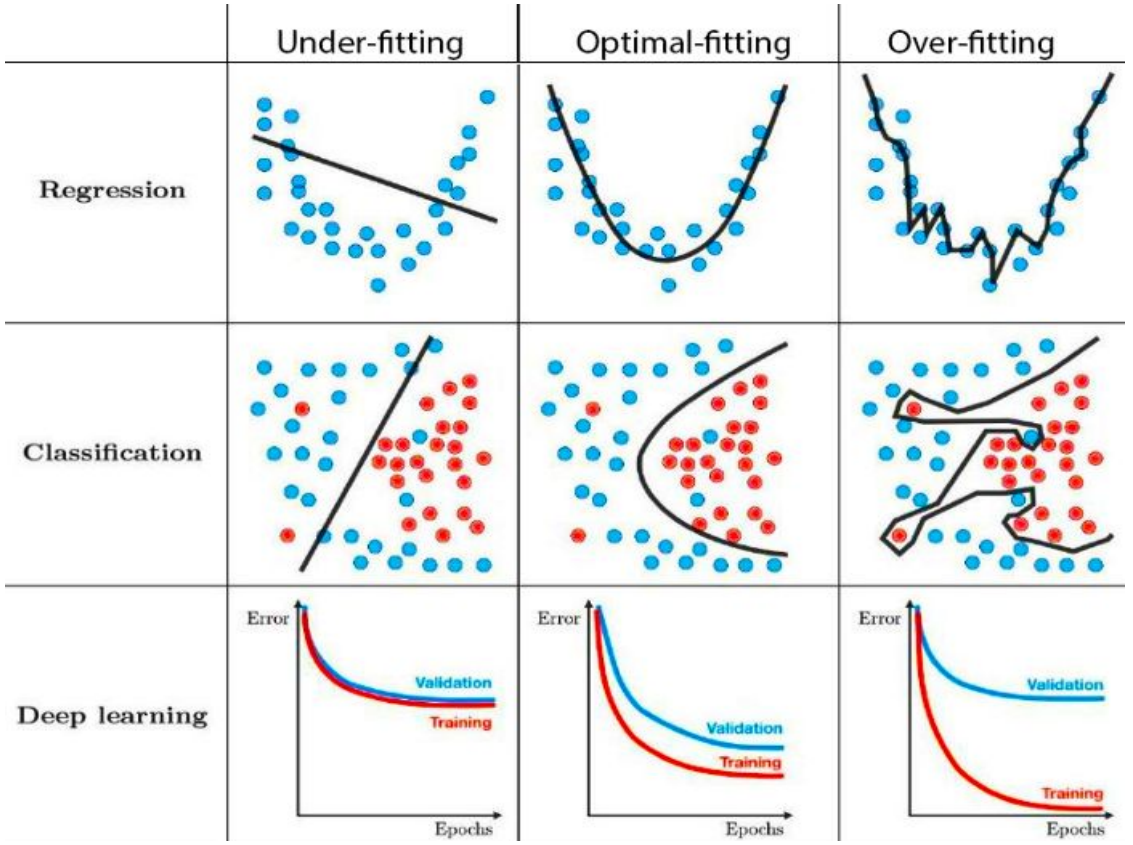
Training Challenges: Overfitting/Underfitting

What is Overfitting?

- Model learns the training data *too well*, including noise and random details.
- Performs well on training data but poorly on new, unseen data.

What is Underfitting?

- Model is **too simple** to learn the patterns in the data.
- Performs poorly on both training and new data → hasn't learned enough.



https://towardsdatascience.com/techniques-for-handling-underfitting-and-overfitting-in-machine-learning-348daa2380b9/

Why Overfitting/Underfitting happen?

Overfitting — model memorizes training data

- Model too complex (many parameters, layers, neurons)
- Small dataset (not enough examples)
- Trains too long without stopping

Underfitting — model fails to learn

- Model too simple (few parameters, shallow)
- Trains too little (stopped early)
- Features not informative

Solution

- Dropout
- L1/L2 regularization
- Early Stopping
- Data Augmentation
- Weight Initialization

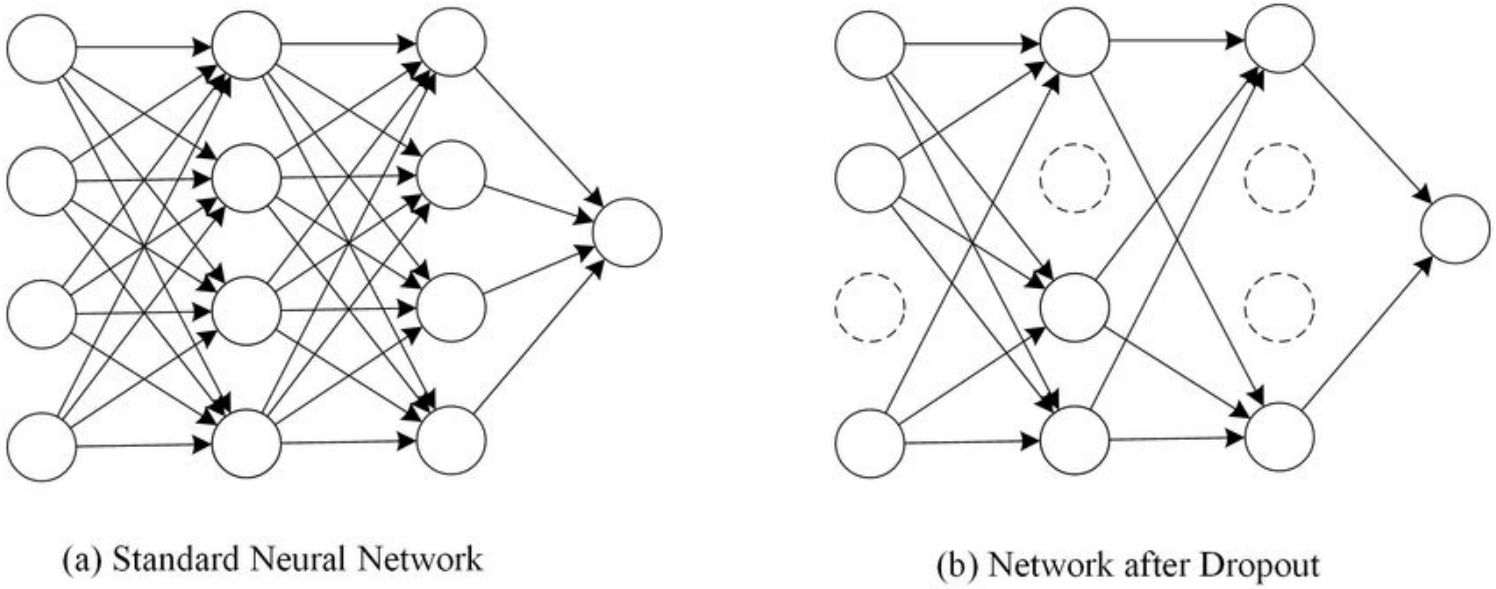
Solution: Dropout

What is Dropout?

- Regularization technique to reduce overfitting.
- Randomly **turns off** some neurons during training

Why Dropout helps?

- Forces the network to learn more robust patterns instead of memorizing.
- Makes models less overfitted and more generalizable



(a) Standard Neural Network

(b) Network after Dropout

https://www.researchgate.net/figure/Dropout-neural-network-model-a-is-a-standard-neural-network-b-is-the-same-network_fig3_309206911

Solution: Regularization

Regularization = Adding a penalty to the loss function to reduce overfitting

- Stops the model from depending too much on any one weight.
- Makes the model simpler (with smaller or fewer weights).

L1 Regularization (Lasso)

$$\text{Loss} = \text{Prediction Error} + \lambda \sum |w|$$

- Adds **absolute value** of weights to loss
- Pushes many weights to zero → removes unimportant features

L2 Regularization (Ridge)

$$\text{Loss} = \text{Prediction Error} + \lambda \sum w^2$$

- Adds **squared values of weights** to the loss
- Makes all weights smaller and smoother → none becomes too large

Solution: Early Stopping

What it is?

- Stop training when validation performance starts to drop

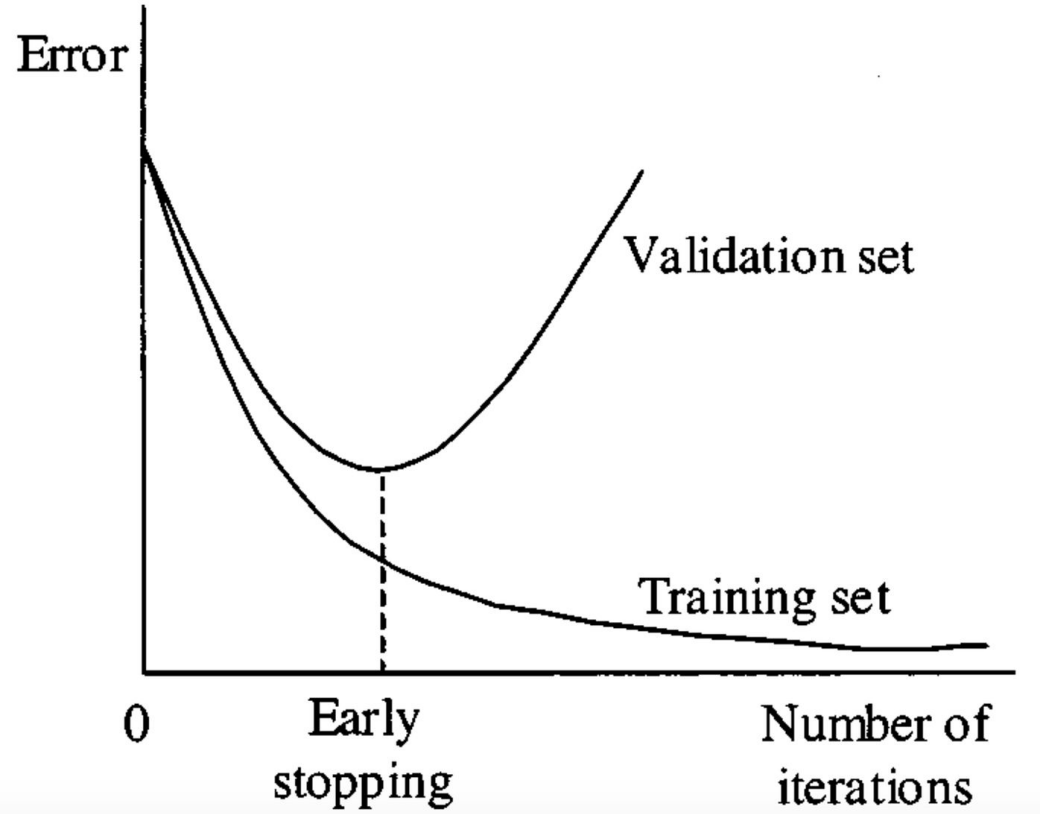
Why it helps:

- Prevents overfitting on training data
- Helps model generalize better to new data

Note: Requires **splitting** data into three sets:

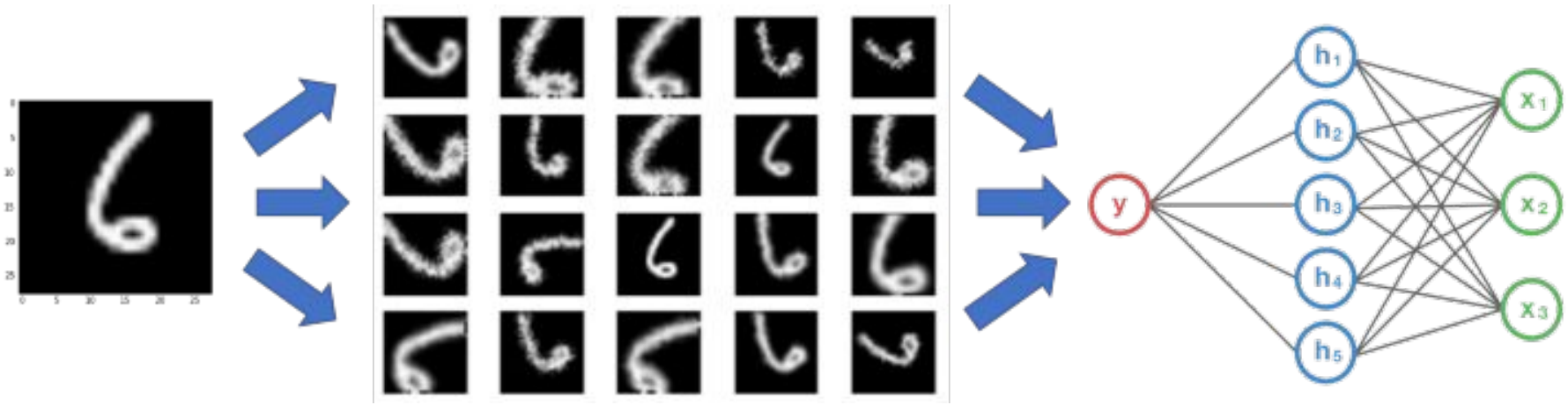
- **Train, Validation, and Test**.

Takeaway: Stop at the right time → less overfitting



https://www.researchgate.net/figure/Early-stopping-based-on-cross-validation_fig1_3302948

Solution: Data Augmentation



https://medium.com/data-science/rethinking-data-augmentations-a-causal-perspective-e0b7810579a7

What is Data Augmentation?

- Artificially increase the size of a training dataset.
- Creates new training examples by making small changes to existing data (like flipping, rotating, or cropping images).

Why it helps?

- Gives the model more varied data to learn from.
- Prevents the model from memorizing training data.
- Improves generalization to unseen data.

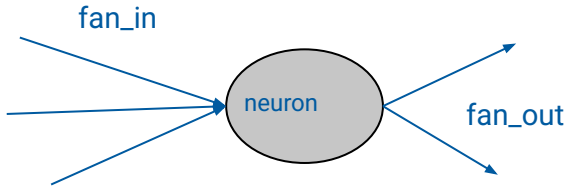
Takeaway: Makes training data richer → avoid overfitting.

Weight Initialization

- Weight should be small but should not be very small
- Weight should not be same, rather should have good variance.

Technique:

1. Uniform Distribution $W_{ij} \sim U\left(-\frac{1}{\sqrt{\text{fan\_in}}}, \frac{1}{\sqrt{\text{fan\_out}}}\right)$



2. Xavier/Gorat Distribution

   a. **Xavier Normal** $W_{ij} \sim \mathcal{N}\left(0, \frac{2}{\text{fan\_in} + \text{fan\_out}}\right)$

   b. **Xavier Uniform** $W_{ij} \sim U\left(-\frac{\sqrt{6}}{\sqrt{\text{fan\_in} + \text{fan\_out}}}, \frac{\sqrt{6}}{\sqrt{\text{fan\_in} + \text{fan\_out}}}\right)$

   } good with sigmoid activation function

3. He init

   a. **He uniform** $W_{ij} \sim U\left(-\frac{\sqrt{6}}{\sqrt{\text{fan\_in}}}, \frac{\sqrt{6}}{\sqrt{\text{fan\_in}}}\right)$

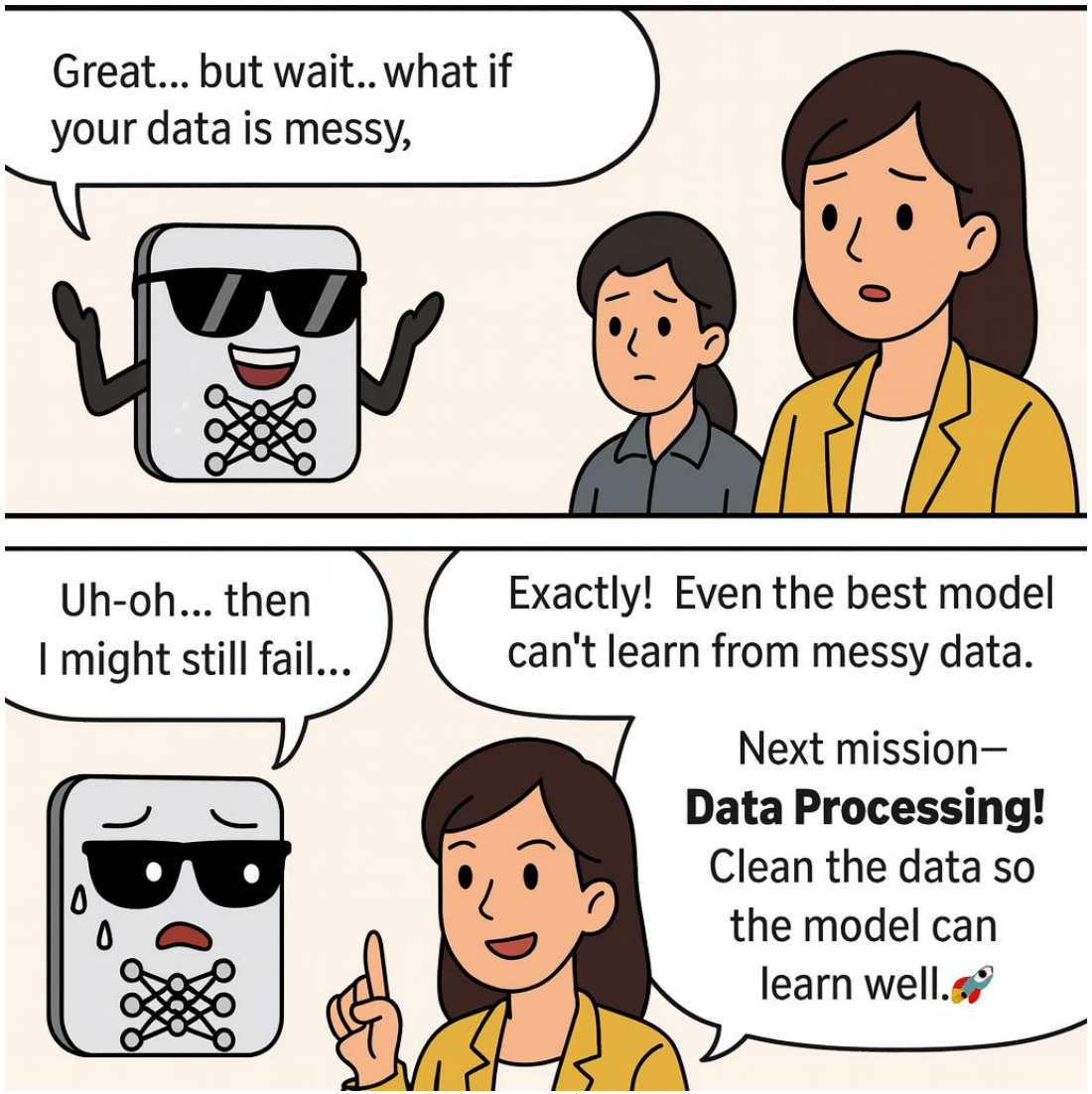
   b. **He Normal** $W_{ij} \sim \mathcal{N}\left(0, \frac{2}{\text{fan\_in}}\right)$

   } good with RELU activation function

https://www.youtube.com/watch?v=tMjdQLylyGI&list=PLZoTAELRMXVPGU70ZGsckrMdr0FteeRUi&index=15

Regularized… but Still Failing?

Next Mission: Data Processing!



generated by chatgpt

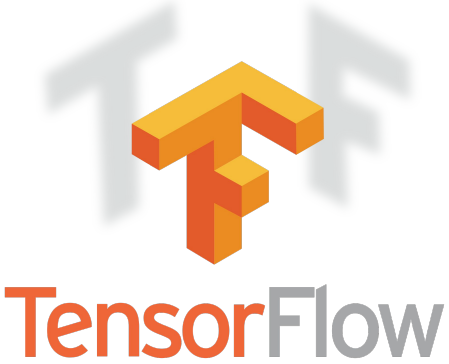
Data Preprocessing

- **Libraries**:
  - **pandas → data cleaning, handling missing values (fillna, dropna)**
  - **scikit-learn → normalization (MinMaxScaler)** →scales values to range [0,1].
    → **standardization** (**StandardScaler**)→rescales data to mean=0, std=1.

- **Why**: Models converge faster & avoid bias from different scales.

Hyperparameter Tuning Tools

- **Goal:** Find best values for learning rate, batch size, dropout, layers, etc.
- **Grid Search:** Tries all combinations (slow but thorough)
- **Random Search:** Tries random combinations (faster, often good enough)
- **Optuna:** Smart search — automates tuning, works with **PyTorch**, **TensorFlow**, etc.



Deep Learning Models & Transfer Learning

Types of Models

- **Fully Connected (Dense)** → each neuron connects to all in next layer; general tasks.
- **CNN (Convolutional Neural Networks)** → captures spatial patterns; best for images.
- **RNN (Recurrent Neural Networks)** → sequence learning; used for text, time series.
- **Transformers** → parallel processing, attention mechanism; state-of-the-art in NLP & vision.

Frameworks

- **TensorFlow** (Google) → scalable, production-ready.
- **PyTorch** (Meta) → flexible, research-friendly.
- **Keras** → high-level API, fast prototyping (runs on TensorFlow).

Transfer Learning

- Start with a **pretrained model** (e.g., ResNet, BERT).
- Fine-tune on your dataset.
- **Why it helps**:
  - Much **faster training** (because most features are already learned)
  - Works well even with **less data**
  - Often gives **better performance** than training from scratch

TensorFlow / PyTorch

TensorFlow:
Built by Google for large-scale deployment

Strong tools:

- **TensorFlow Serving** → tool to send trained models to servers.
- **TensorFlow Lite** → tool to shrink models to run on **phones, IoT devices**.
- **TensorFlow.js** → run in the **browser**.
- **Direct TPU support** → runs very well on Google's special AI hardware.

Great for mobile, web, production pipelines

PyTorch:

- PyTorch started as a **research-first framework** (built by Facebook AI).
- Focus: easy debugging, Pythonic, simple, flexible experiments → researchers loved it.
- But it didn't originally have strong deployment tools.
- TensorFlow was earlier for **production pipelines**, so companies adopted it.

Today: This is changing! PyTorch has **TorchServe, TorchScript, ONNX** for deployment. It's catching up fast. But TensorFlow still has more tools integrated for production at giant scale.

Thank You Any Questions?

Time for exercise

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HZDR