M-Lab CARTE AI Workshop 2025

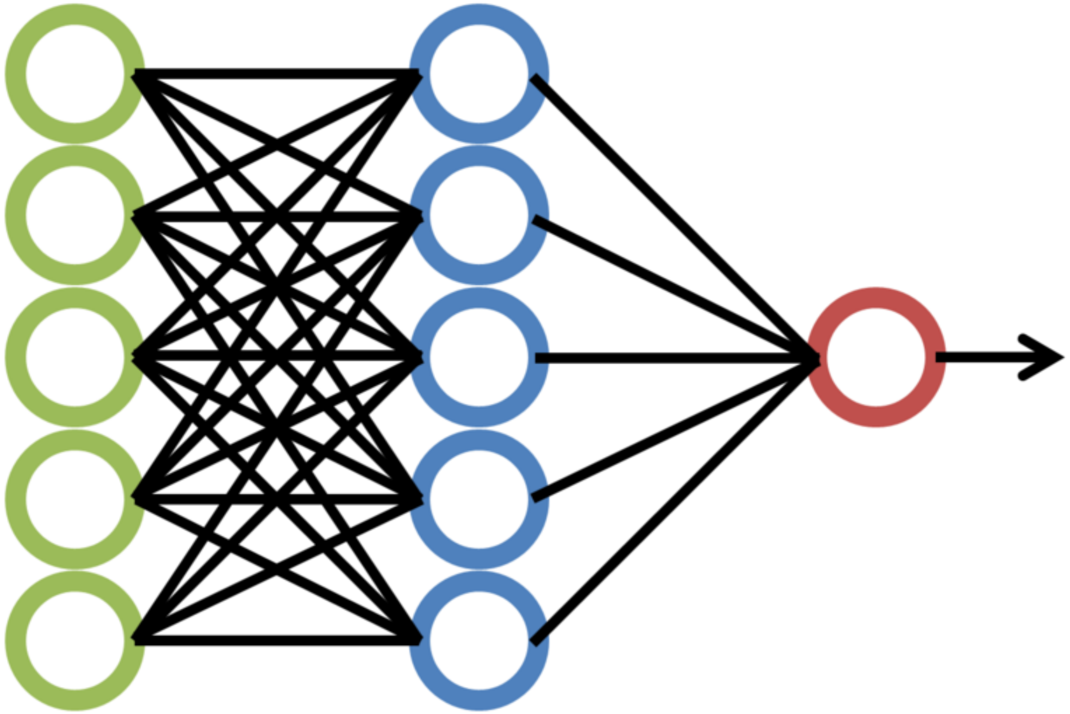
Neural Networks & Optimization

Overview

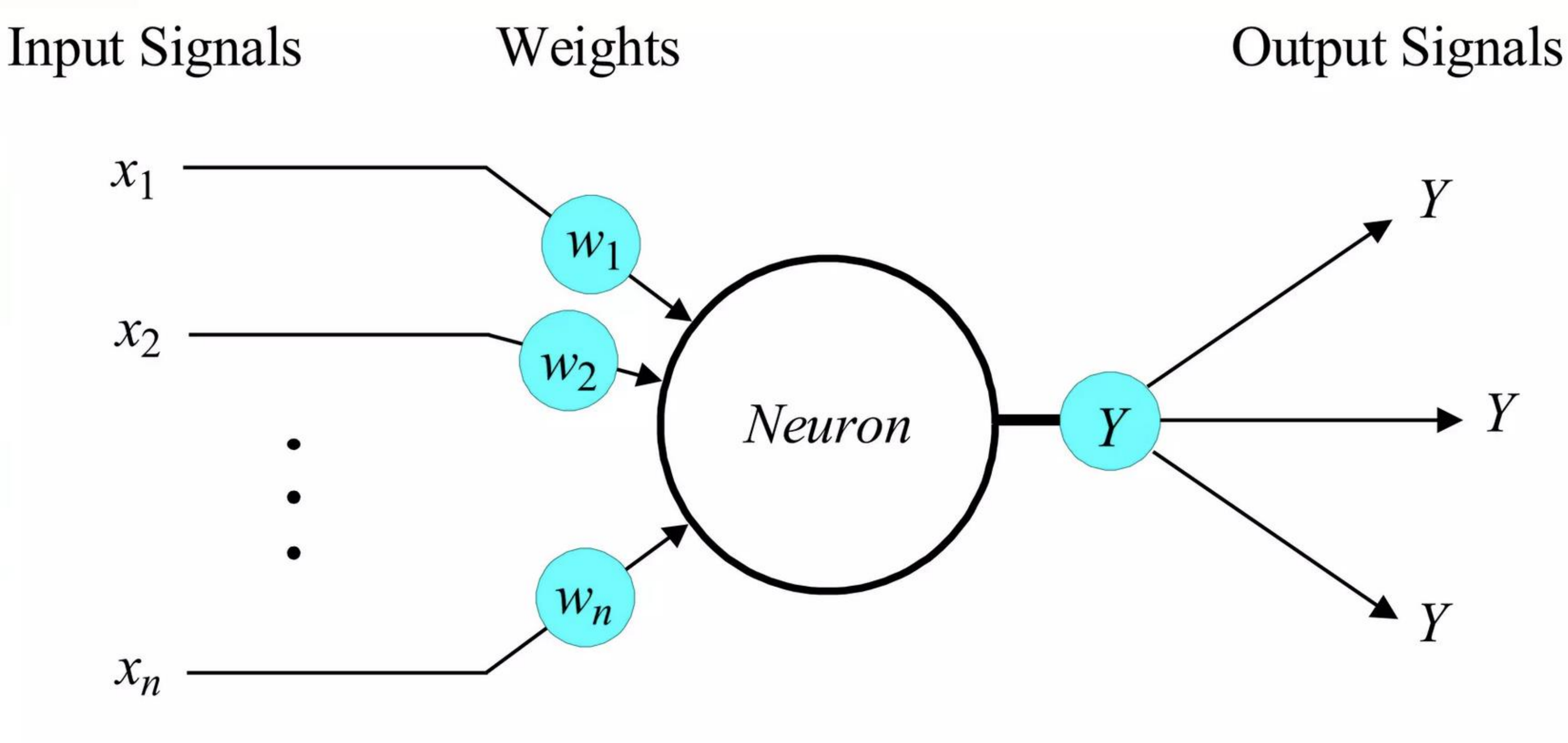
- This afternoon we will discuss the fundamentals of neural networks
- Neural networks drive nearly all modern AI tools
- We will also look at optimization
- Optimization is an example of a non-Machine Learning area of Artificial Intelligence

What is a neural network?

- Complex structure of interconnected computing nodes (neurons)
- Can identify patterns and trends in complex data
- NNs operate on the principle of “learning” from data, using a process that mimics how biological brains learn

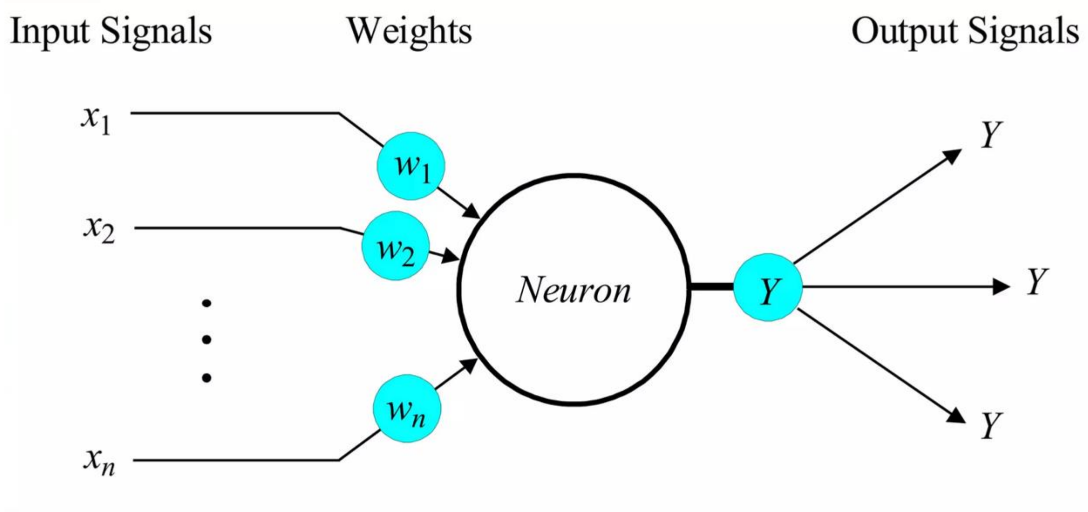


View inside an artificial neuron



View inside an artificial neuron

- Behaves like a linear regression model:
- $w_1 x_1 + w_2 x_2 + \ldots + w_n x_n$
- Weights correspond to how much the neuron “cares” about each input



Visualization

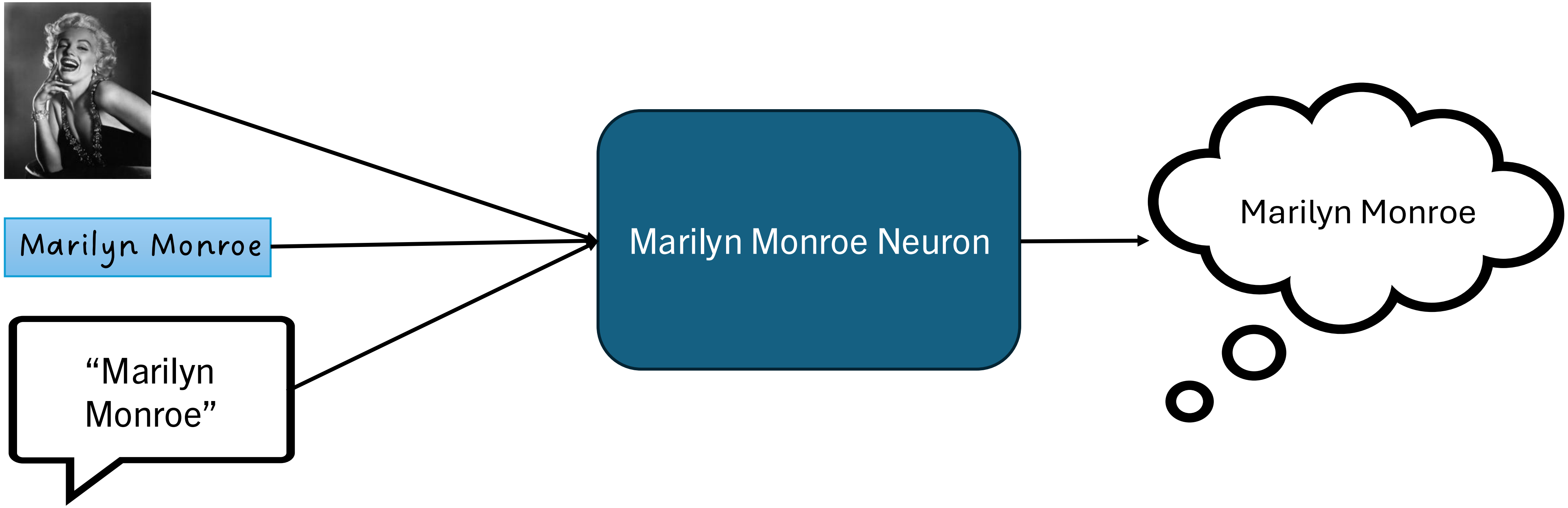
https://neuron.carte.training/

The Marilyn Monroe neuron

- Study conducted on patients with epilepsy
- Researchers use specialized equipment to measure the “excitement” of individual neurons in a patient’s brain
- Measuring a neuron, the researchers showed patients a series of images
- In each patient, they found around five neurons that fired when the patient looked at a specific person

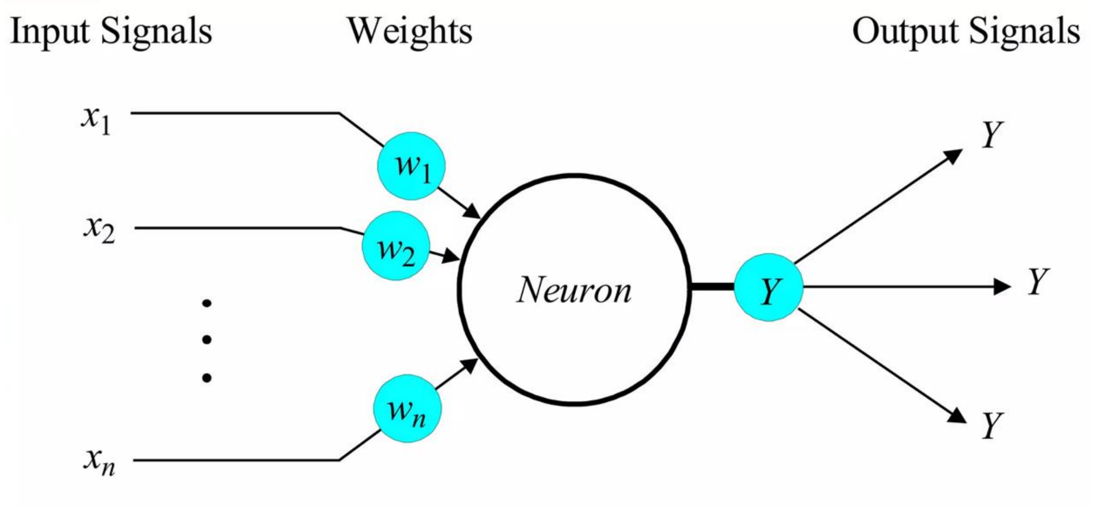
Back to the brain: the Marilyn Monroe Neuron

- Once a “celebrity” neuron was identified, the researchers wanted to know if it would still fire for representations other than images



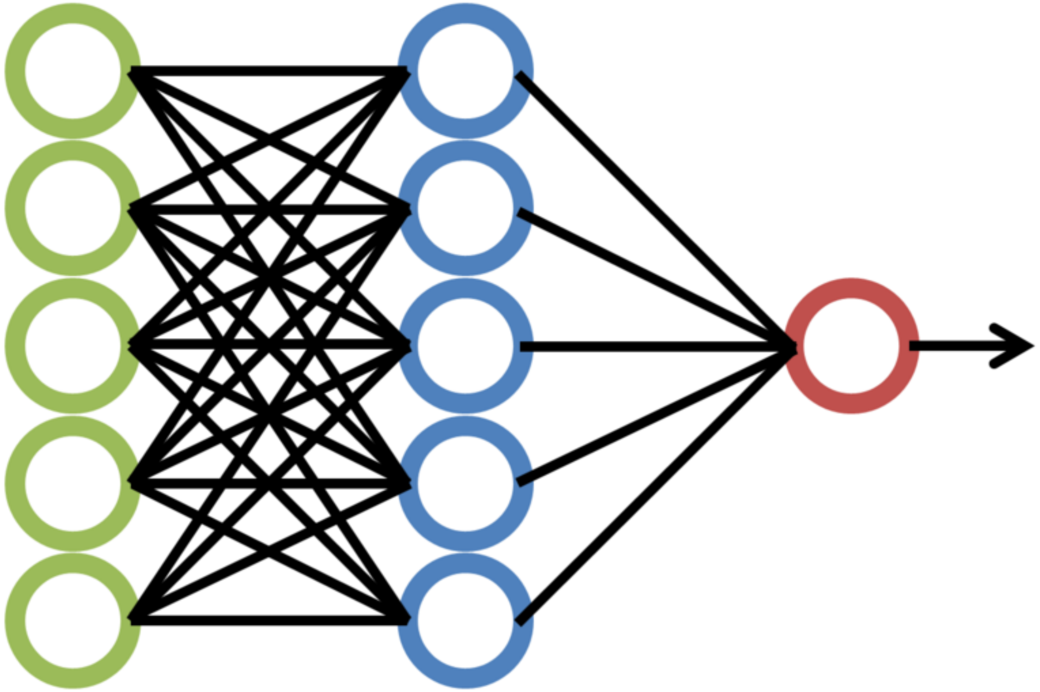
Marilyn Monroe ANN

- Weights would be high from neurons that react to different representations of Marilyn Monroe
- Weights would be low for neurons that react to other people, or concepts



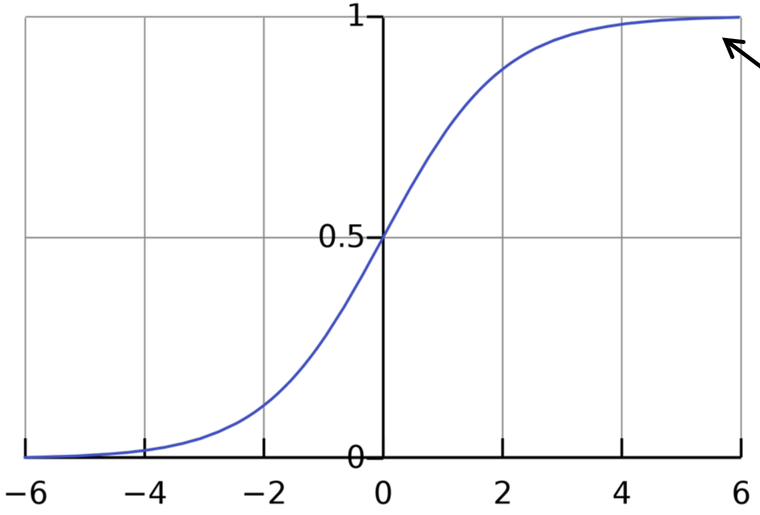
ANNs

- Each neuron considers the responses of the neurons in the previous layer
- It learns to pay attention to the neurons that are excited about what it's excited about
- Ignores the neurons that are excited about other things



Activation Functions

- Basic approach: when I see enough activity, I get excited
- Below threshold: 0
- Above threshold: 1
- More useful: gradually increase excitement as we see more activity
- In practice: many different activation functions!



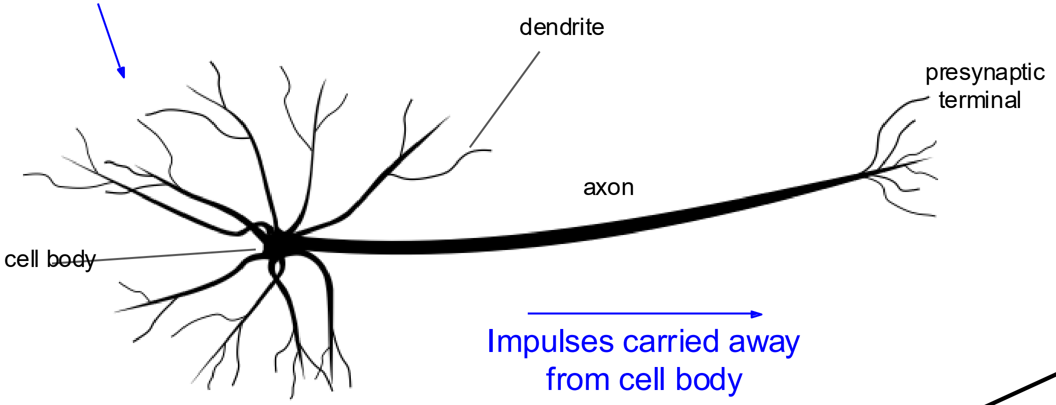
Desired value gets max output

The Neuron Metaphor

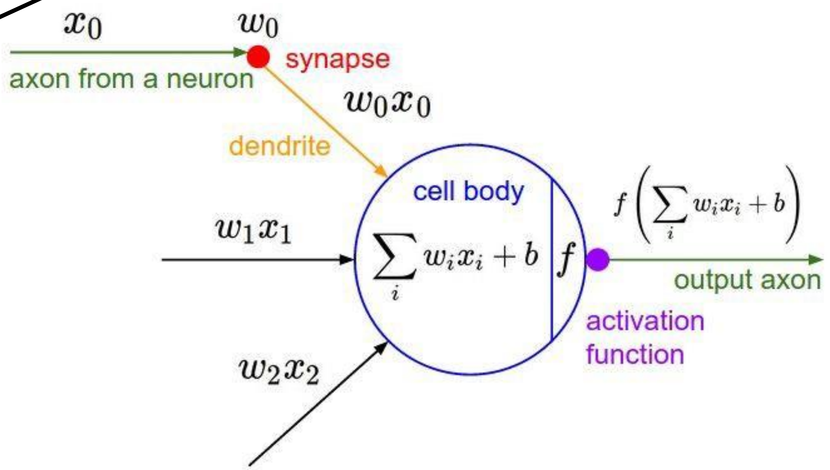
- Neural networks were inspired by our understanding of the brain and how neurons interact.
- An artificial neuron in a neural network takes in multiple inputs, applies a function to them, and generates an output – mirroring the basic functionality of a biological neuron.
- This analogy has been extremely useful for explaining and visualizing how these artificial structures work.

The Neuron Metaphor

Impulses carried toward cell body



Impulses carried away from cell body



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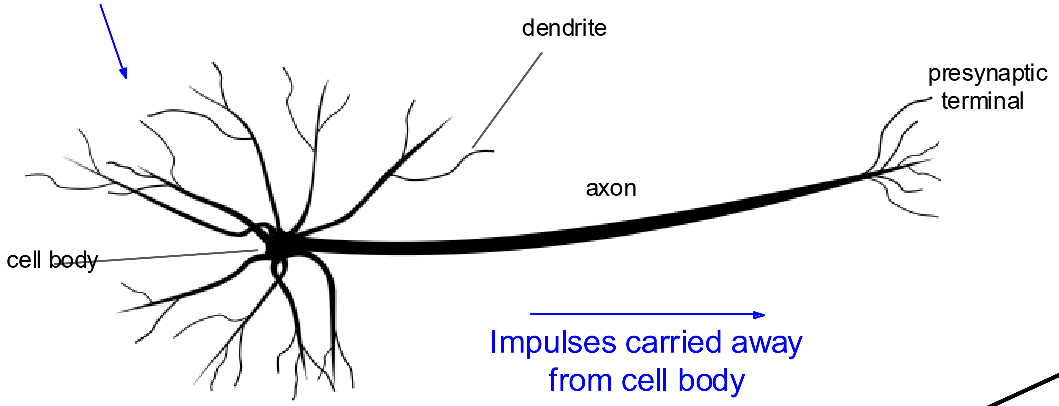

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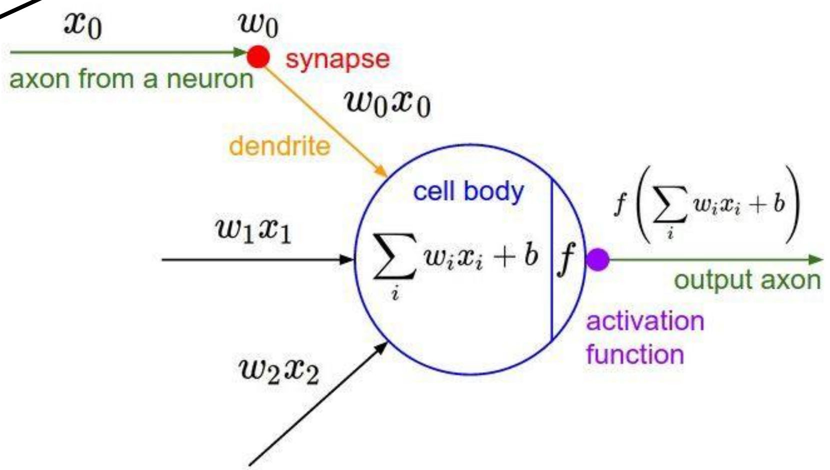
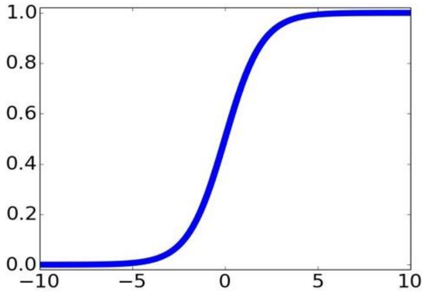




sigmoid activation function

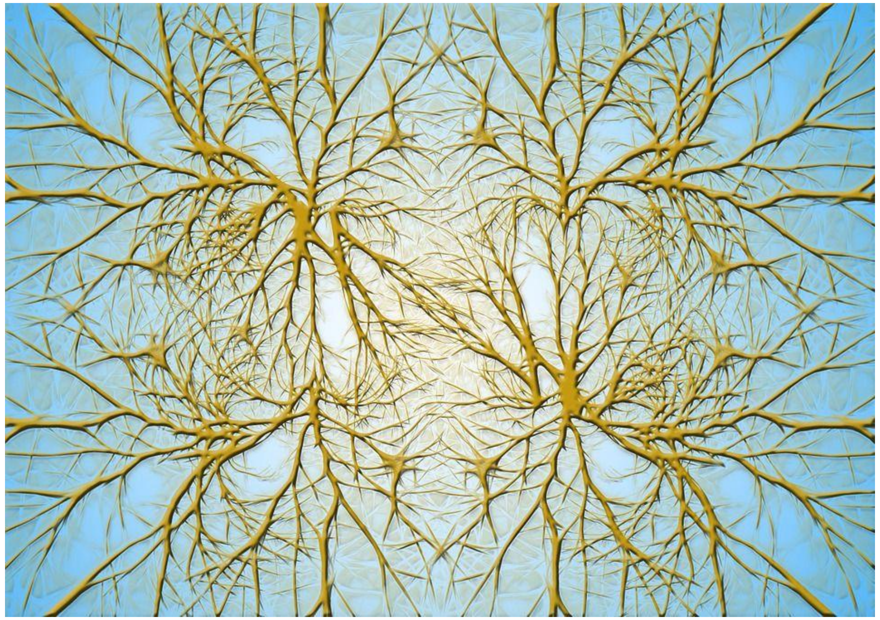
$$\frac{1}{1+e^{-x}}$$

Training the Network

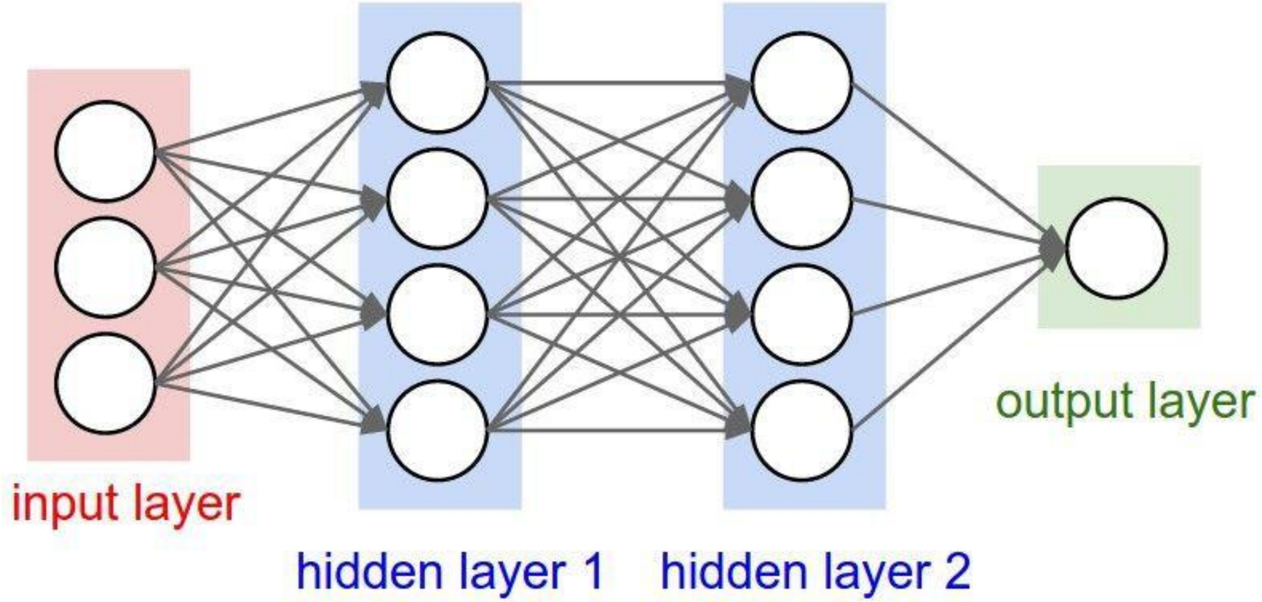
- Find parameters that **minimize the total error**
- **Loss** for a given sample is the total error in predictions made
- Going through the network, the predictions are dependent on the settings of the parameters
- We have a mathematical function representing the network
- A way of measuring how ”good” it is

The Metaphor Breaks Down

<u>Biological Neurons:</u>
Complex connectivity patterns



<u>Neurons in a neural network:</u>
Organized into regular layers for computational efficiency



The Metaphor Breaks Down

- Biological neurons are vastly more complex: they use a mixture of electrical and chemical signals, have complex temporal dynamics, and can restructure their own connections.
- The brain is not just a feed-forward network: it has many complex feedback loops, which are not typically found in artificial neural networks.
- The brain isn't easily divided into distinct layers, as we do in artificial neural networks.

The Metaphor Breaks Down

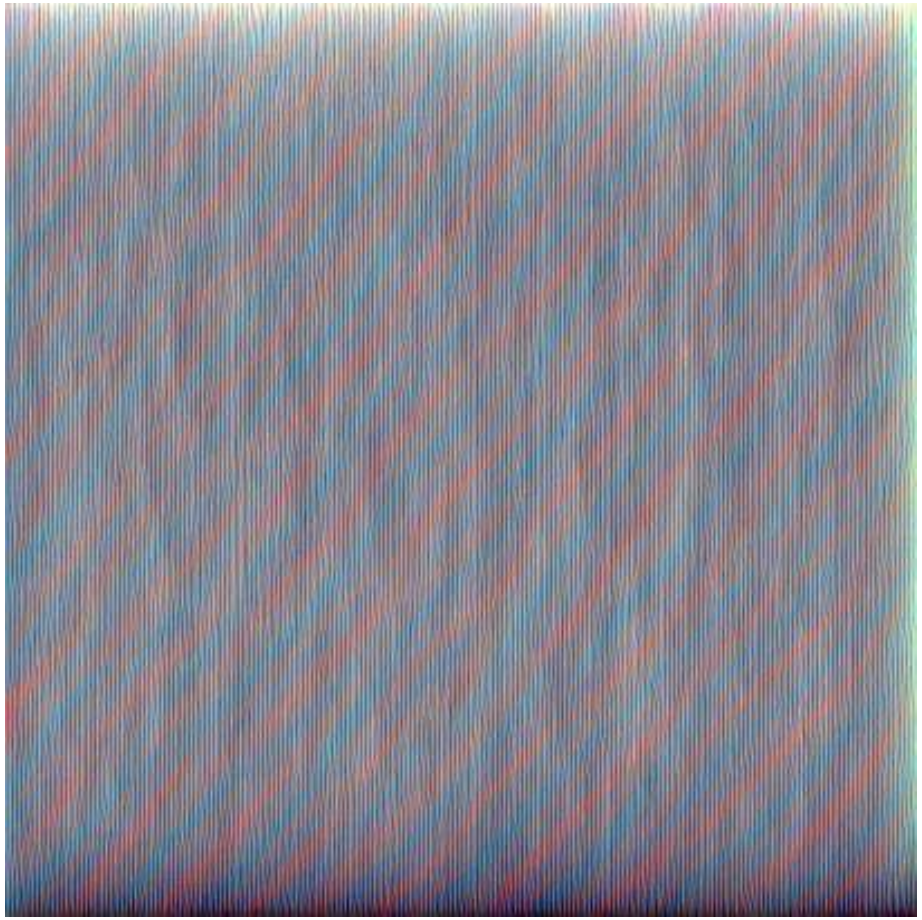
- Over-reliance on the analogy can lead to misunderstandings about how neural networks function and their capabilities.
- This can lead to unrealistic expectations about what neural networks can do, or to overgeneralizations about their functioning.
- For instance, claiming a neural network "thinks" or "understands" like a human brain is misleading.
- To further progress, it's important to view artificial neural networks as mathematical/statistical tools, and not overstate the comparison to the human brain.

Going past the fully connected network

- In many image tasks, we want to be able to recognize something regardless of where it is in the image
- For fully-connected networks, the order of the inputs is fixed
- No “shift invariance”

Going past the fully connected network

- In the 1950s and 60s, researchers showed that the brain contains neurons which respond to specific patterns, regardless of where they appear
- Combinations of very basic patterns can then be recognized as a more complicated one!



VGG-16, neuron in layer 7

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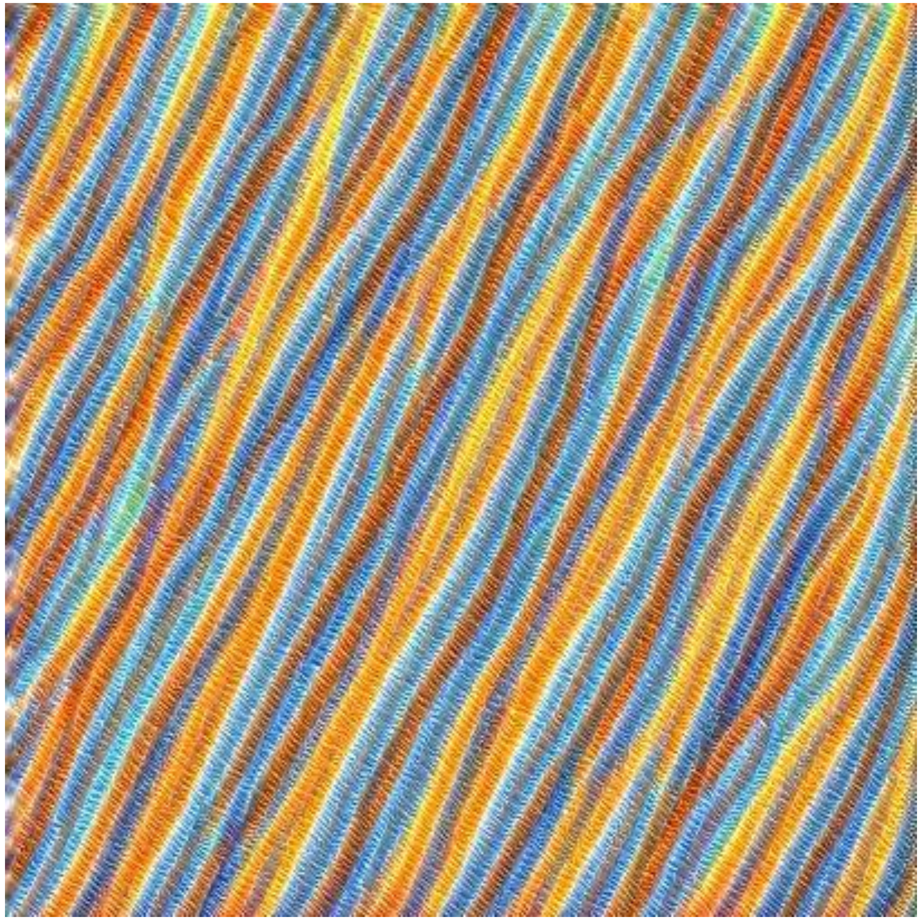

VGG-16, neuron in layer 14

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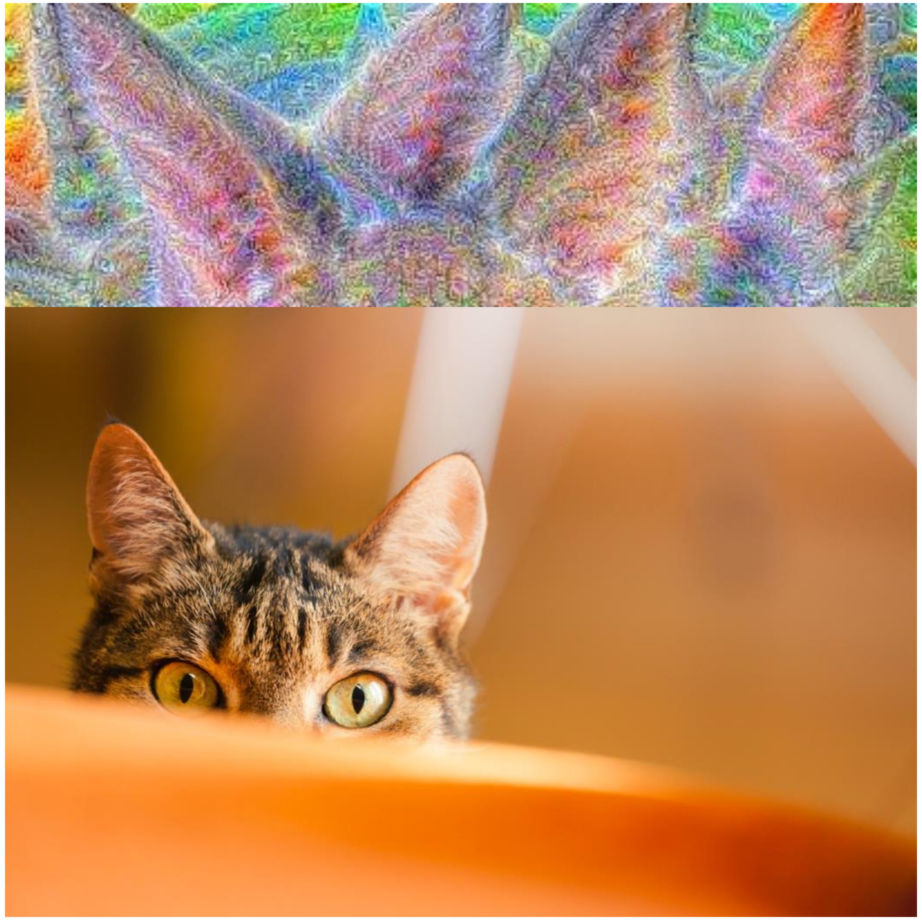
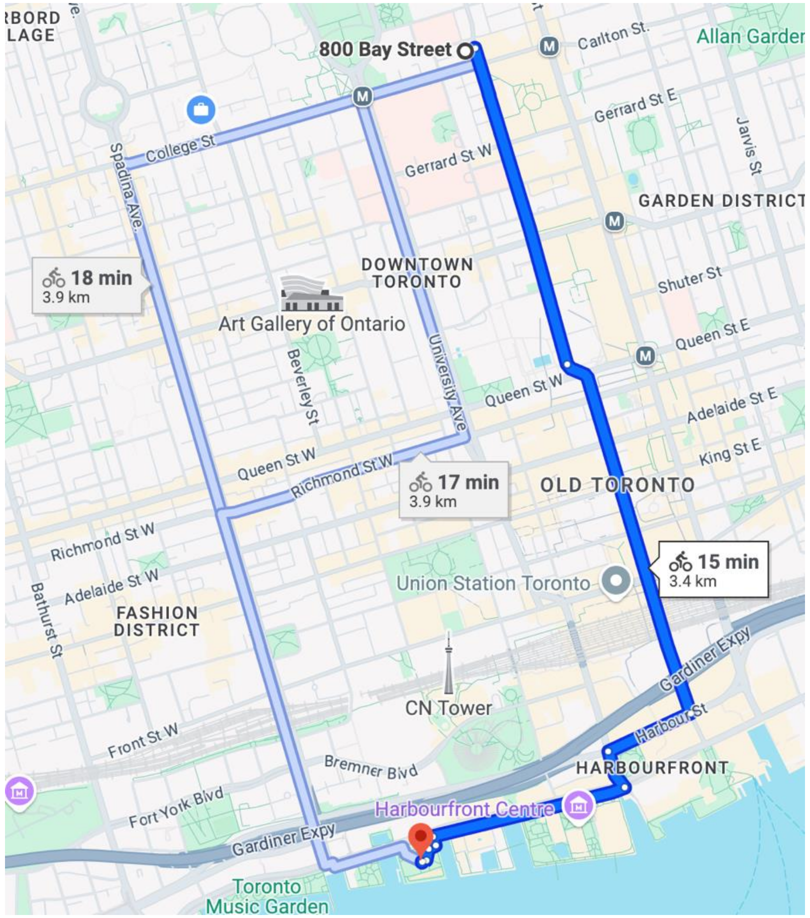


VGG-16, neuron in layer 40

What is Optimization?

- Major field within Data Analytics, Operations Research and Management Science
- Basic idea: find the values of the decision variables that maximize (or minimize) the objective value, while staying within the constraints
- How do I find the shortest route to bike to the harbourfront, without breaking traffic laws?



What is Optimization?

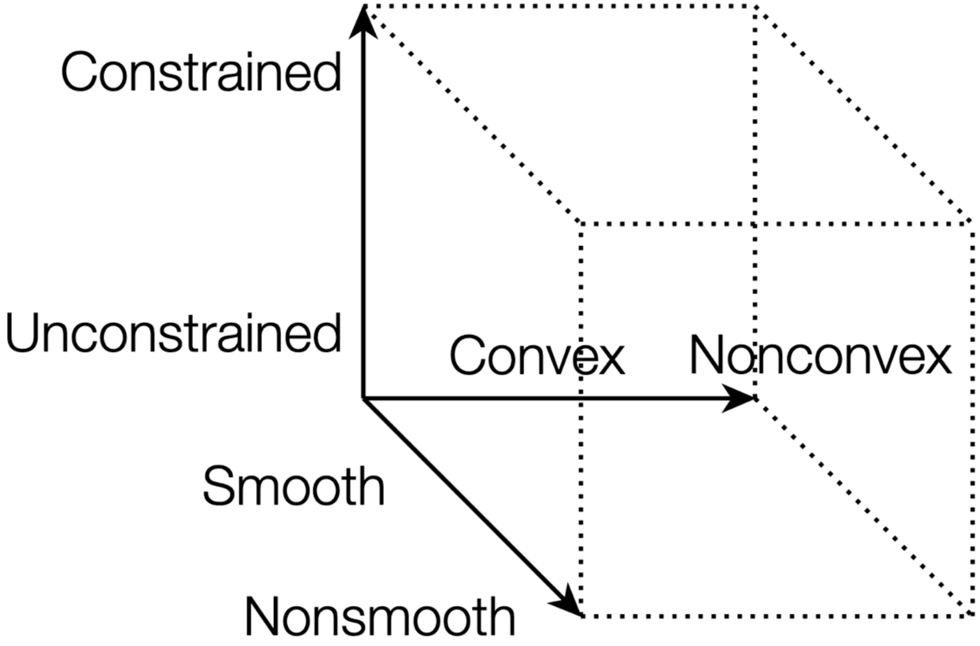
- In machine learning, we usually want to minimize the result of a loss function
- A huge number of ML problems can be solved using optimization
  - e.g. regression, classification, maximum likelihood
- If we can use optimization, we get access to powerful tools which can find our answer

GUROBI OPTIMIZATION

Google OR-Tools

Classes of optimization problem

- Many different types of problem can be framed as an optimization problem
- Three main distinctions help to define them
- Constrained vs Unconstrained
- Convex vs Nonconvex
- Smooth vs Nonsmooth (less important)



Constrained vs Unconstrained

- Constraints are conditions on what answers are acceptable
- When finding the shortest driving route, you are really finding the shortest *legal* driving route
- When scheduling employees, have to factor in their availability

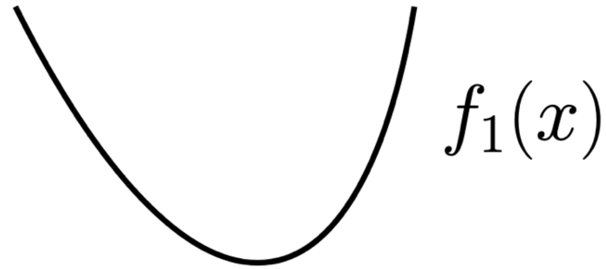
$$\underset{x}{\text{minimize}} \quad f(x)$$

vs

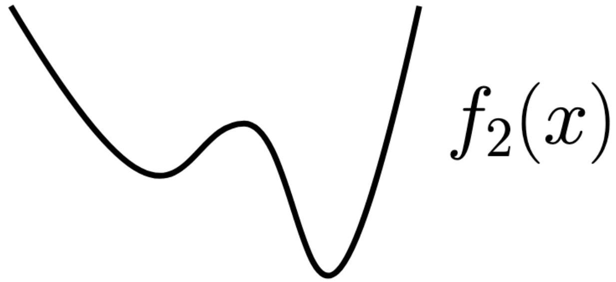
$$\begin{aligned} \underset{x}{\text{minimize}} \quad & f(x) \\ \text{subject to} \quad & g_i(x) \leq 0, \quad i = 1, \dots, m \\ & h_i(x) = 0, \quad i = 1, \dots, p \end{aligned}$$

Convex vs Nonconvex

- A function is convex if there is exactly one “bottom” point – the global minimum
- This makes the problem much easier to solve because as long as the error is decreasing, you are getting closer to the best answer
- If the function is nonconvex, you can be “tricked” by a local minimum



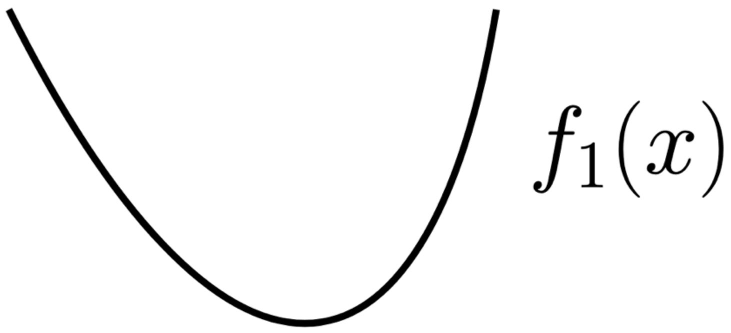
Convex function



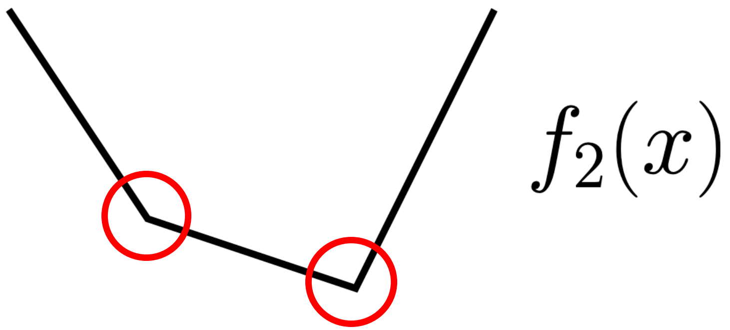
Nonconvex function

Smooth vs Nonsmooth

- Many modelling methods depend on calculating the derivative of the error – this tells us how to change our answer to get closer to the minimum
- If the function is nonsmooth, there are points (red) where it is not possible to differentiate



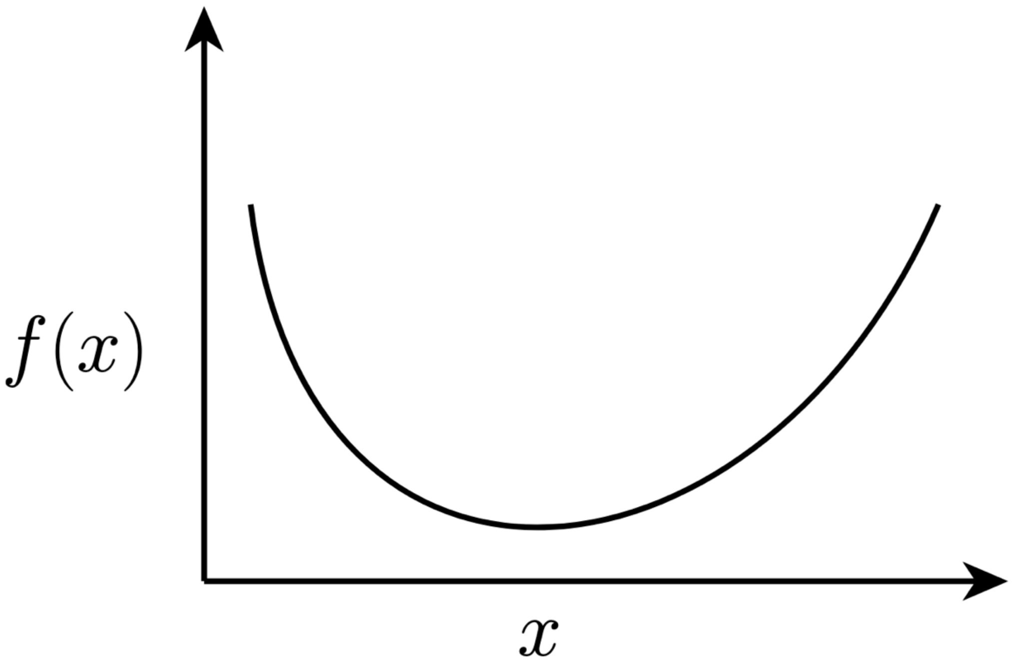
Smooth function



Nonsmooth function

Solving an optimization problem

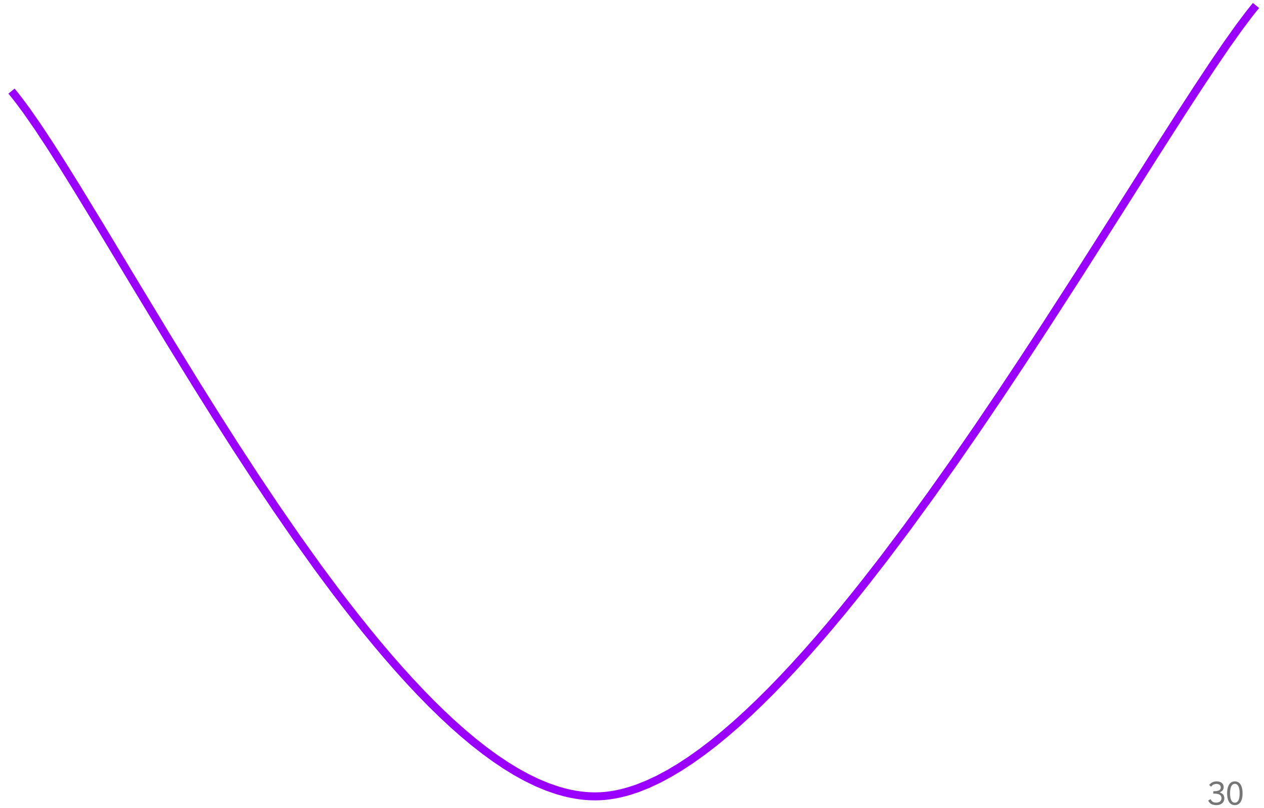
- Let's start with the simplest case: unconstrained, convex, smooth function
- We just need to find the point where the curve is flat (i.e. derivative is zero) - this is the minimum
- If the function is very simple, we can just calculate this value directly
- Otherwise, we can use gradient descent



Gradient descent

For some loss function $L(\mathbf{w})$, gradient $\nabla L(\mathbf{w})$ points towards in direction of steepest ascent.

In 1d, either points left or right



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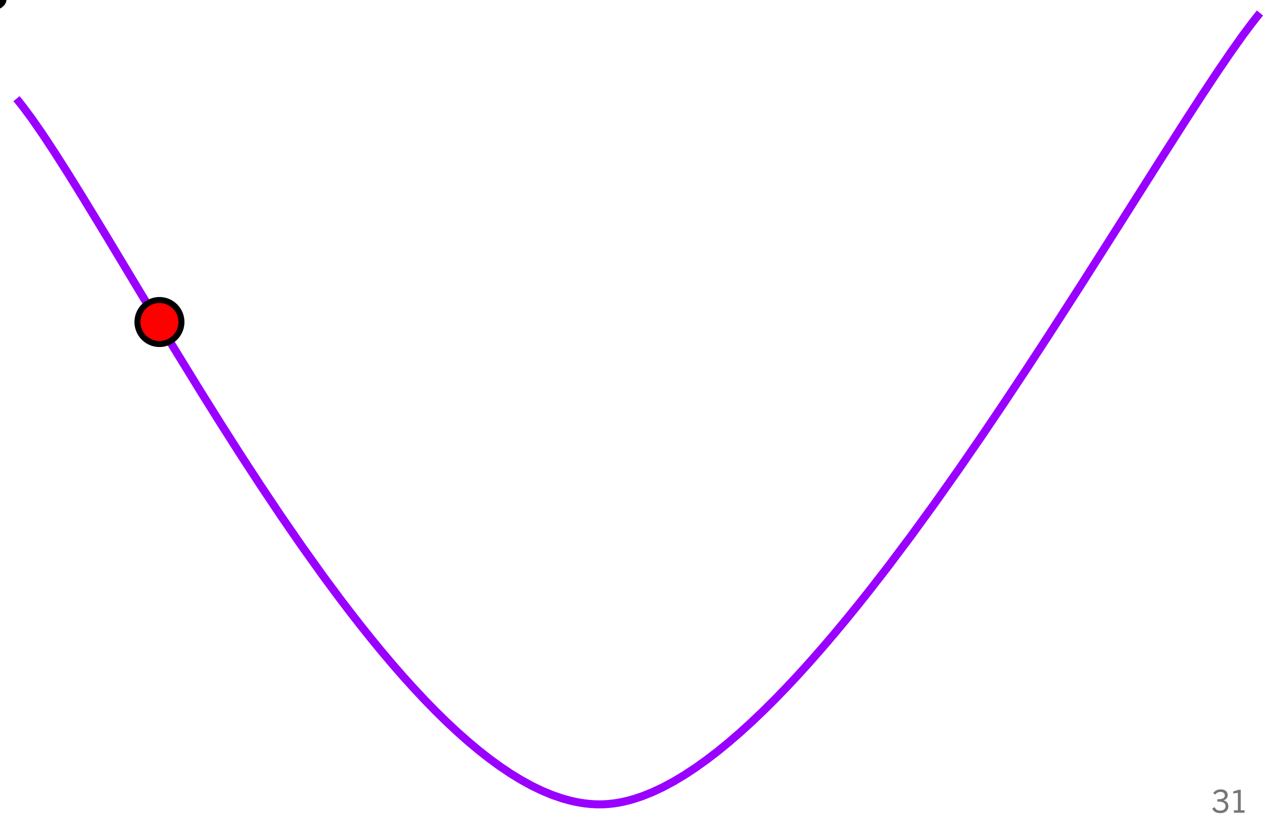

Gradient descent

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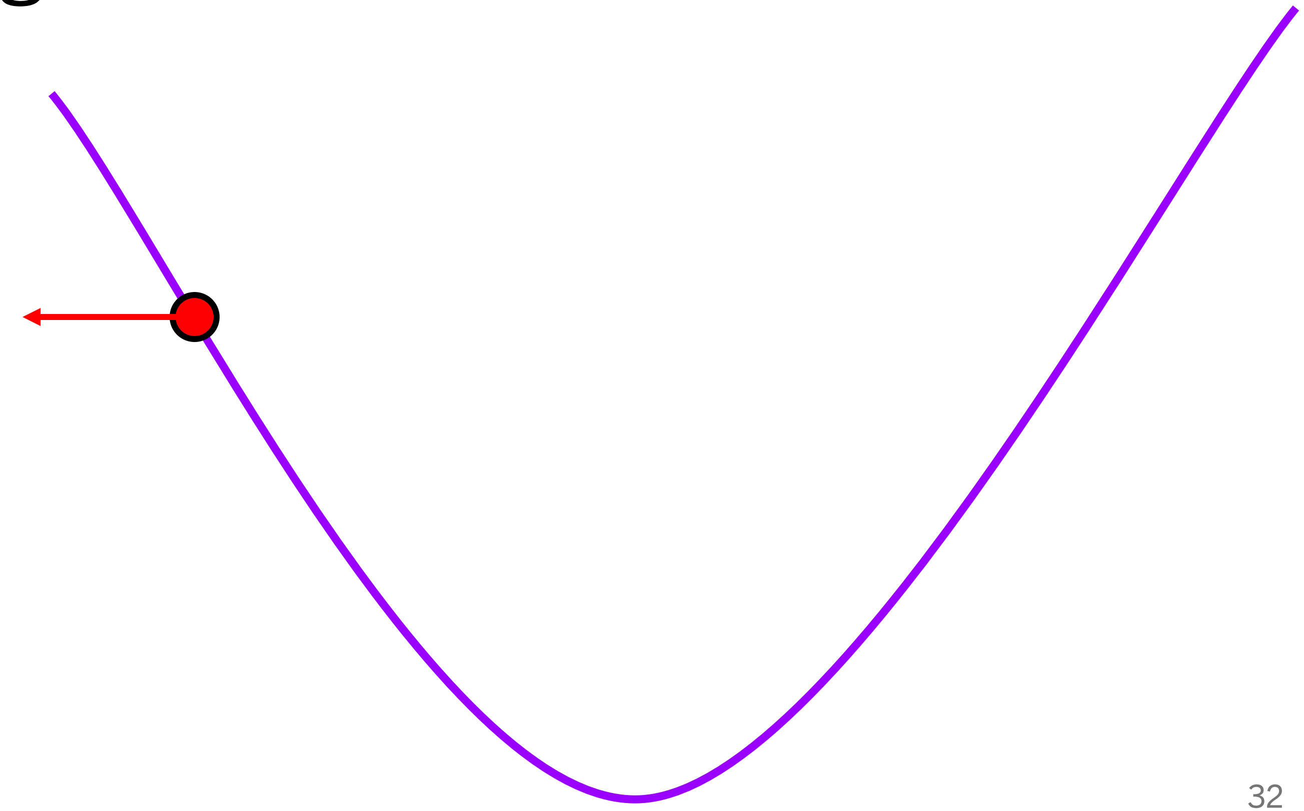

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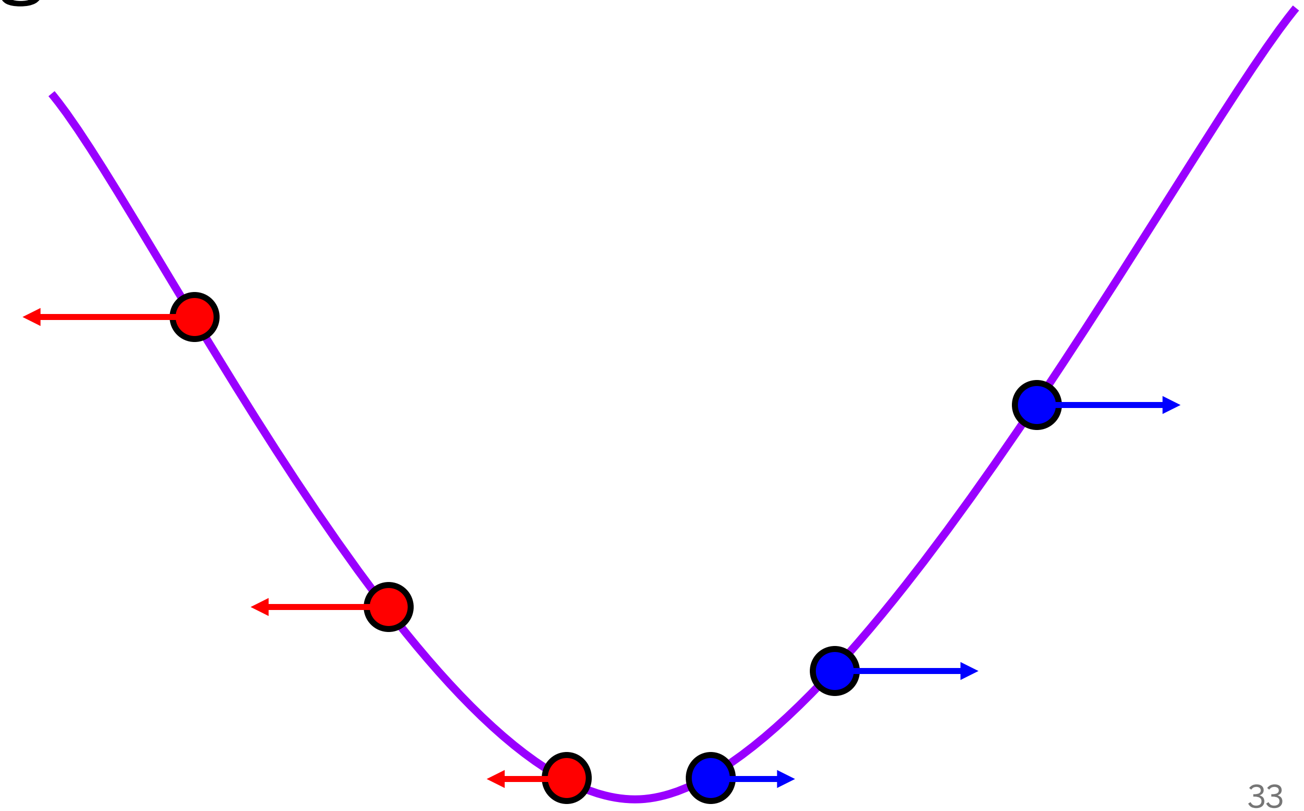

Gradient descent

For some loss function L(**w**), gradient ∇L(**w**) points towards in direction of steepest ascent.

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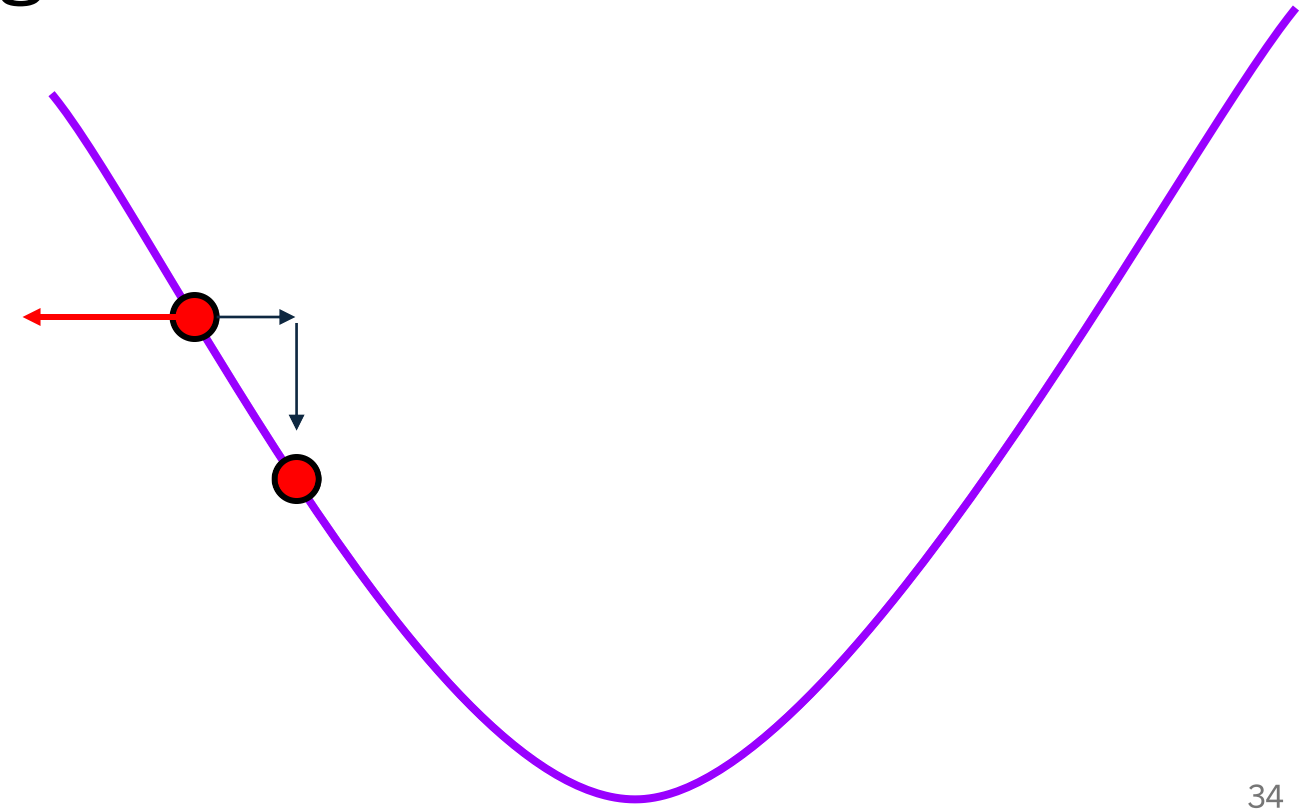
Algorithm:

Take derivative

Move slightly in other direction

Repeat



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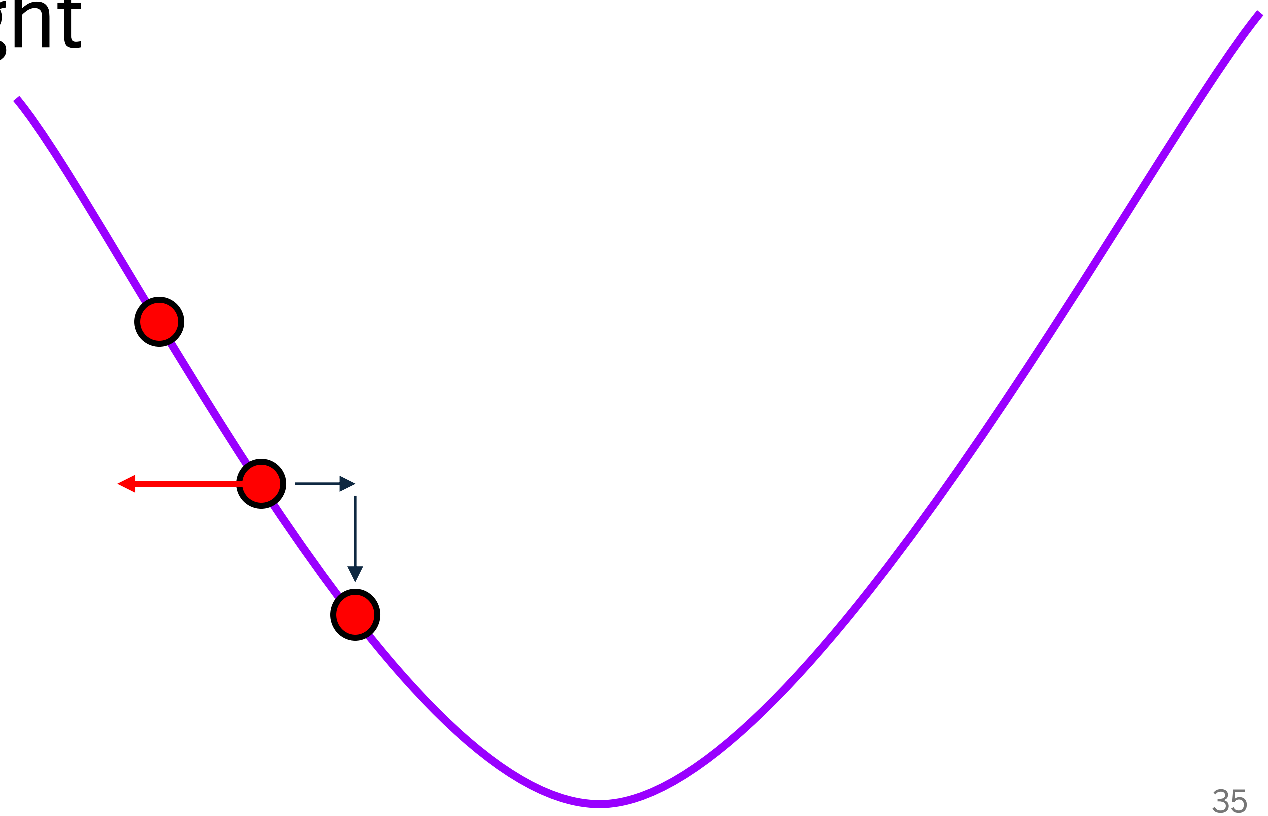


Gradient descent

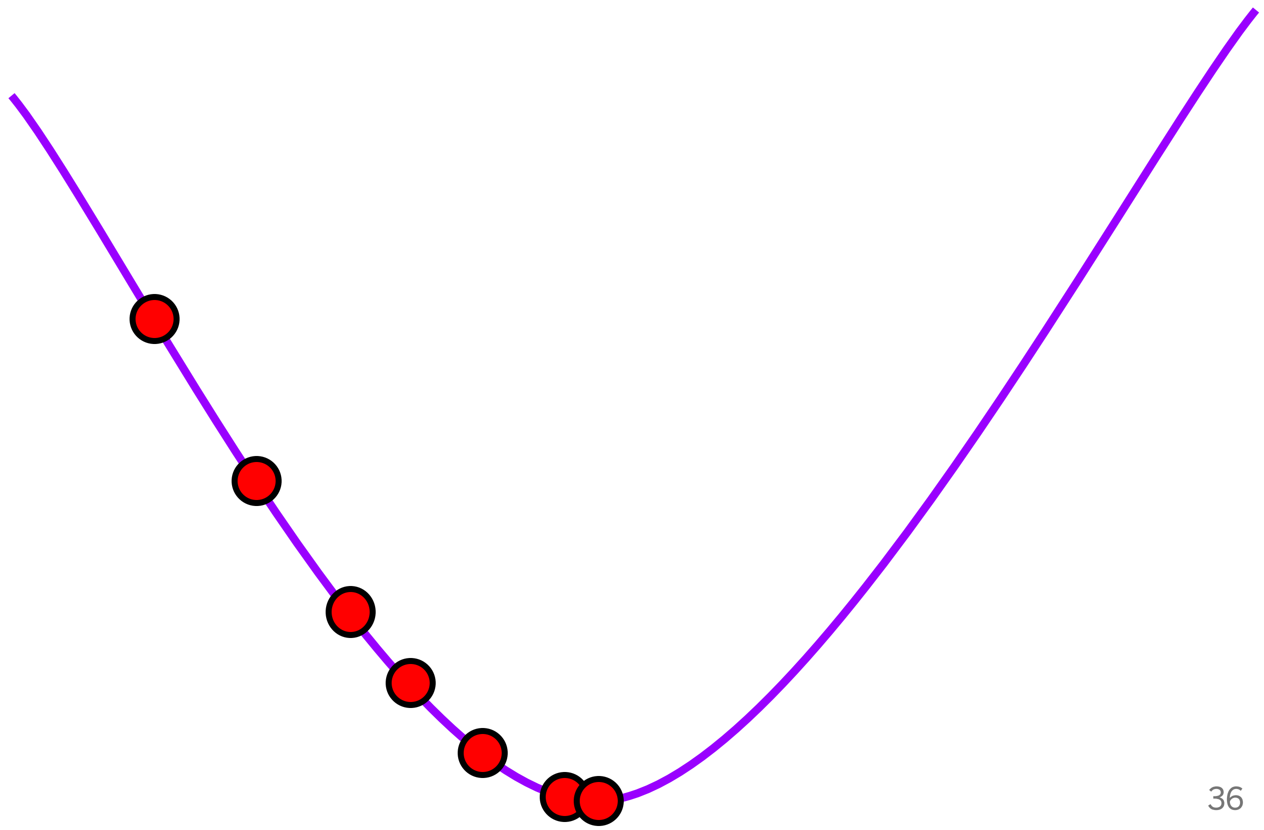
Algorithm:

Take derivative

Move slightly in other direction

Repeat

End up at local optima

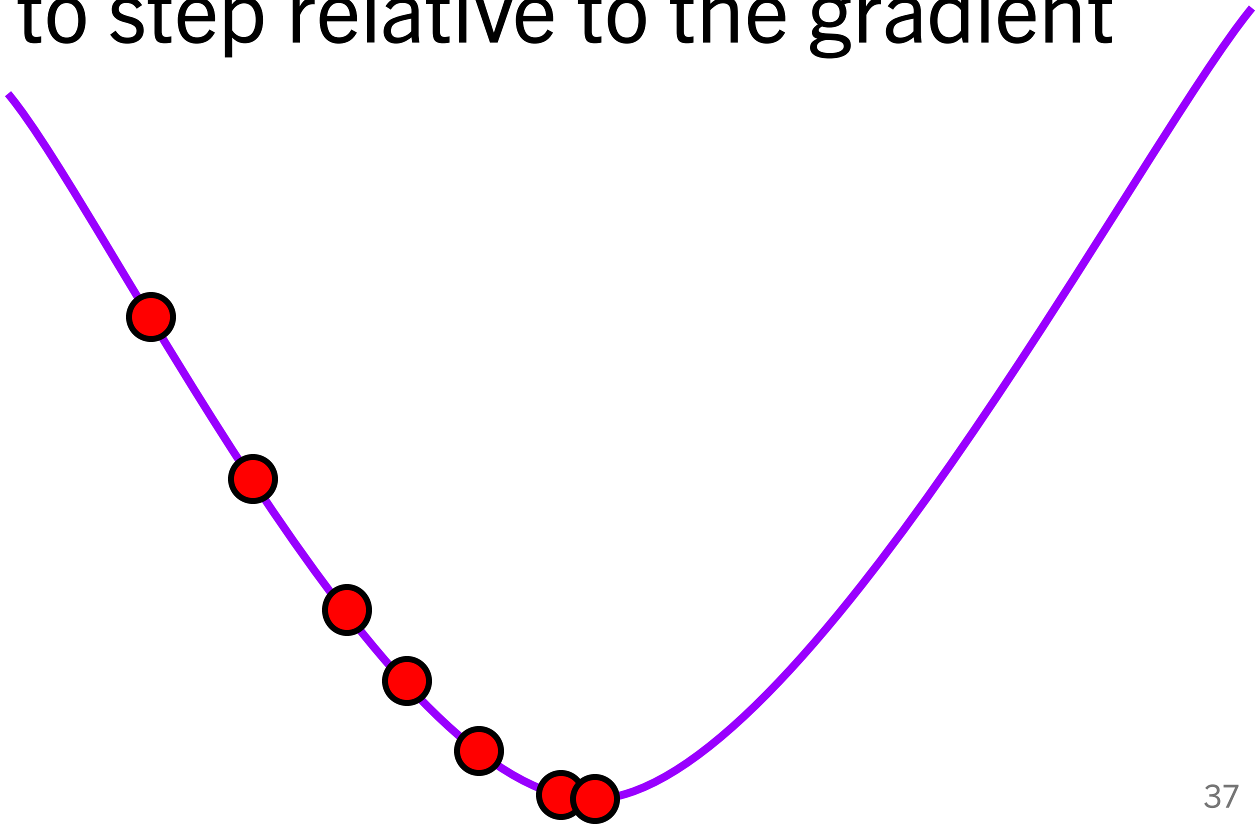


Gradient descent

Formally:

$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \nabla L(\mathbf{w})$

Where η is *step size*, how far to step relative to the gradient



Gradient Descent Visualization

https://gradient.carte.training/