Large Language Models

Introduction to deep learning

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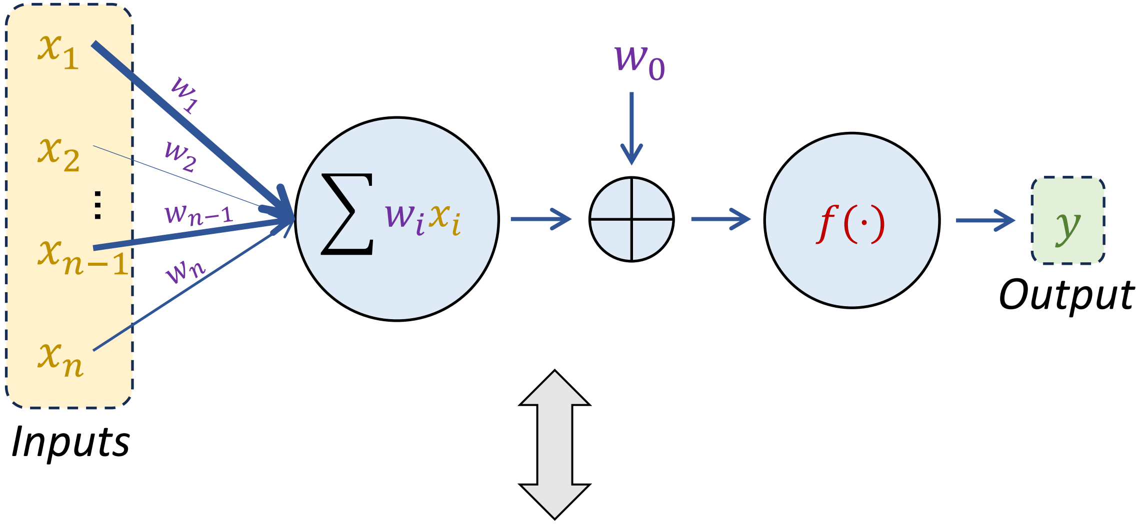
The perceptron

- The perceptron is the simplest unit of neural networks
- It takes an input with *multiple features*, and does the following:
  - It weights each input feature with a given *weight*,
  - It produces a weighted sum of the inputs, and
  - It applies a *function* to the output
- $y = f(w_0 + w_1 x_1 + w_2 x_2 + \cdots + w_n x_n)$

The perceptron



Or, in other words, $y = f\left(\sum_{i=0}^{n} w_i x_i\right) = f\left(w^{\mathrm{T}} x\right)$ and $x_0 = 1$

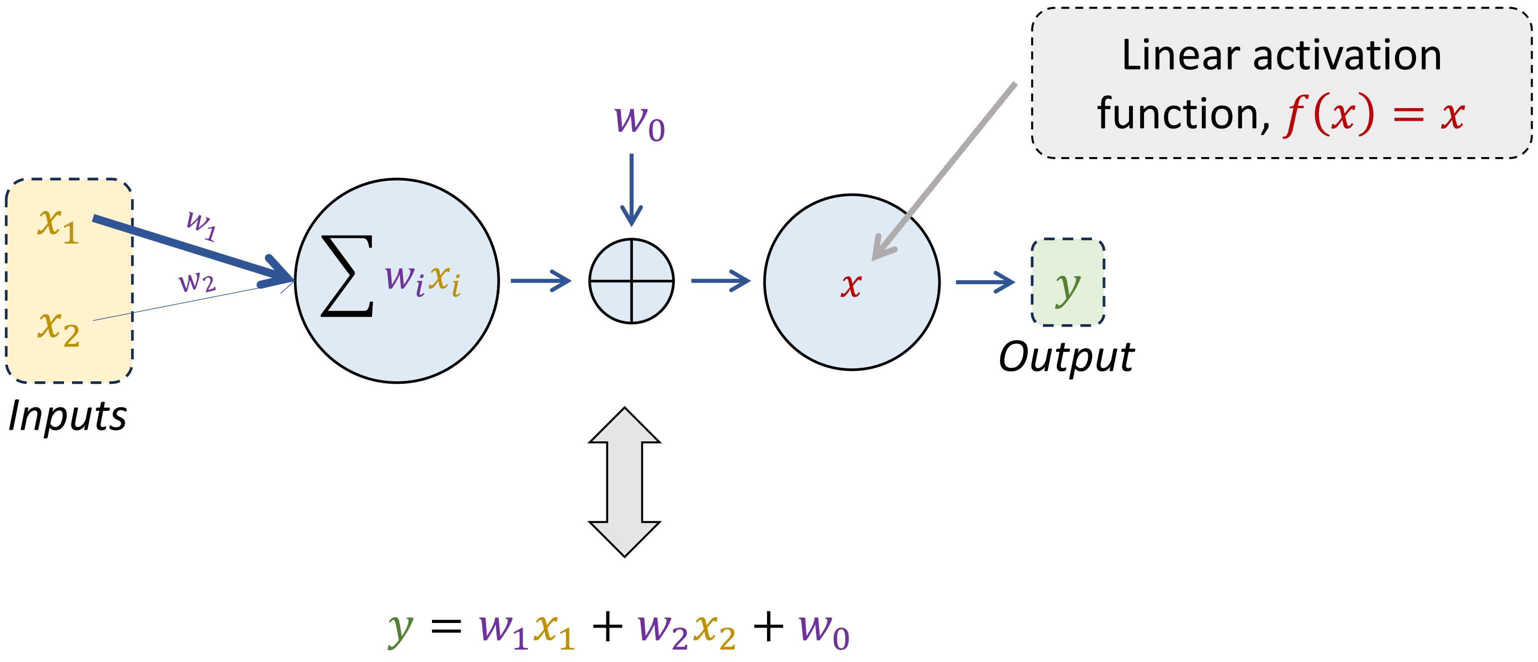
- $x = (x_1, x_2, \dots, x_n)$ is the input sample
- y represents the output of the perceptron.
- $f(\cdot)$ represents a non-linear "activation" function
- w_i (and w_0) are weights (and bias), which are "learned"

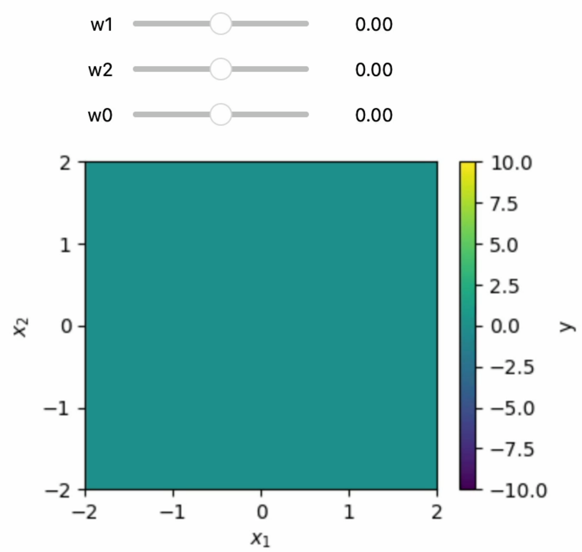
Note

With the exception of $f(\cdot)$, this looks like the classic *linear regression*

And if $f(\cdot) = \sigma(\cdot)$ (sigmoid function), this looks like the (just as classic) *logistic regression*

The perceptron, in 2D





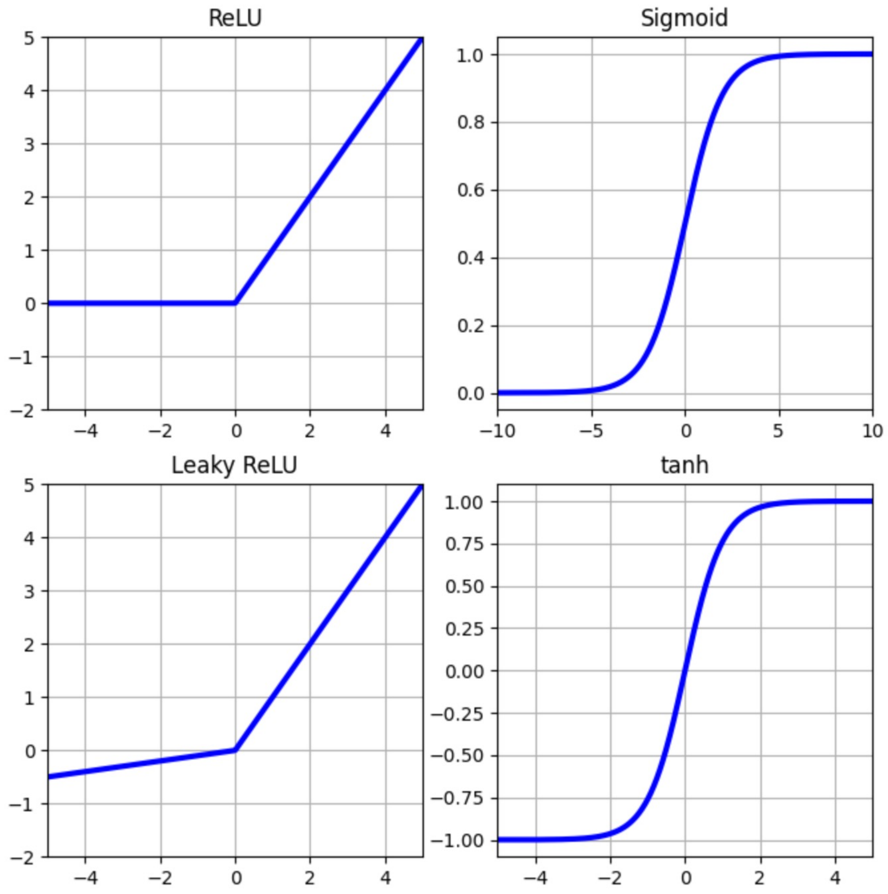
The perceptron can be used to represent a family of functions, $y = w_1 x_1 + w_2 x_2 + w_0$

Various values of w_0, w_1, w_2 define the different functions that can be learned by the perceptron.

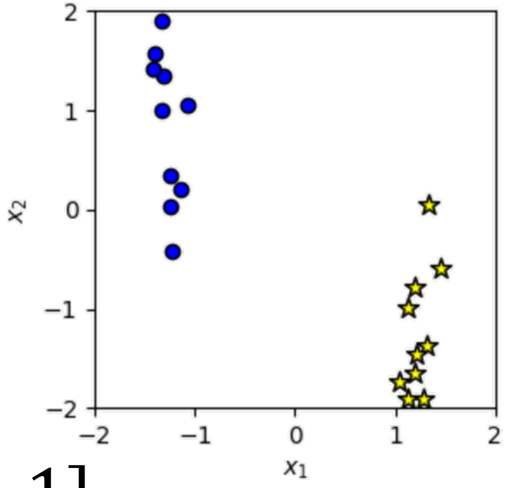
Activation functions

- Activation functions are used for two *main* reasons:
  1. Enforce *properties* on perceptron's output
     - E.g., sigmoid ➔ binds output to [0, 1] range
  2. Introduce *non-linearities* in the model

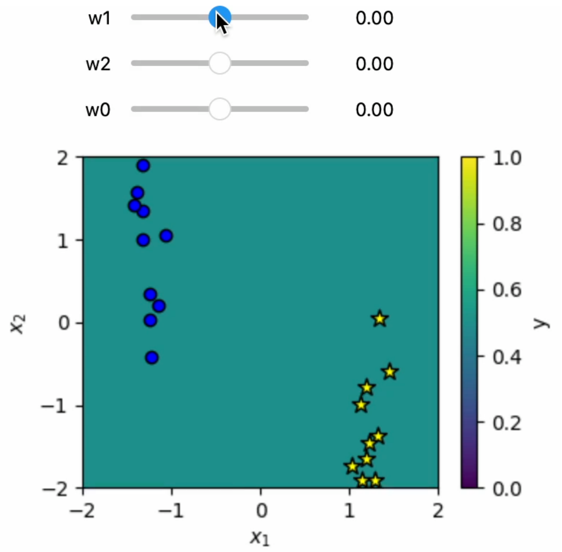
  \+ some others (faster convergence, sparsity, …)
- Commonly adopted functions:
  - ReLU
  - Sigmoid
  - Leaky ReLU
  - Tanh
  - Softmax
  - Linear
  - GeLU



1. Enforce *properties* on perceptron's output

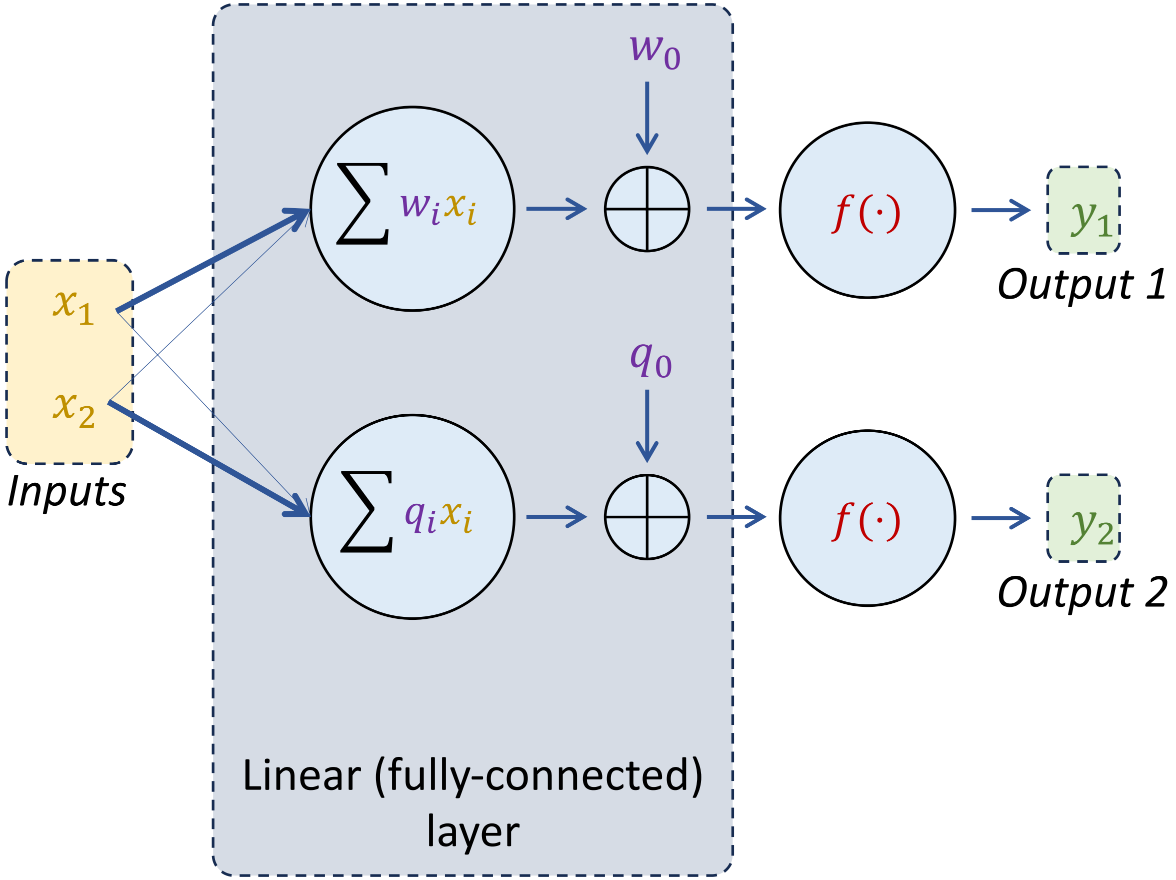


- Binary classification problem
  - Separate positive (★) and negative (●) samples
- For a point $x \in \mathbb{R}^2$, the perceptron can predict $p(\bigstar | x)$
  - For the binary case, this implies $p(\bullet | x) = 1 - p(\bigstar | x)$
- To get a valid probability, we must enforce $p(\bigstar|x) \in [0, 1]$
  - We already have $p(\bullet | x) + p(\bigstar | x) = 1$ by construction



- The Sigmoid maps any value in $\mathbb{R}$ to the range $[0, 1]$
  - i.e., the perceptron's output (in $\mathbb{R}$) is squashed to $[0, 1]$
  - $\sigma(x) = \frac{1}{1+e^{-x}}$

Adding some perceptrons



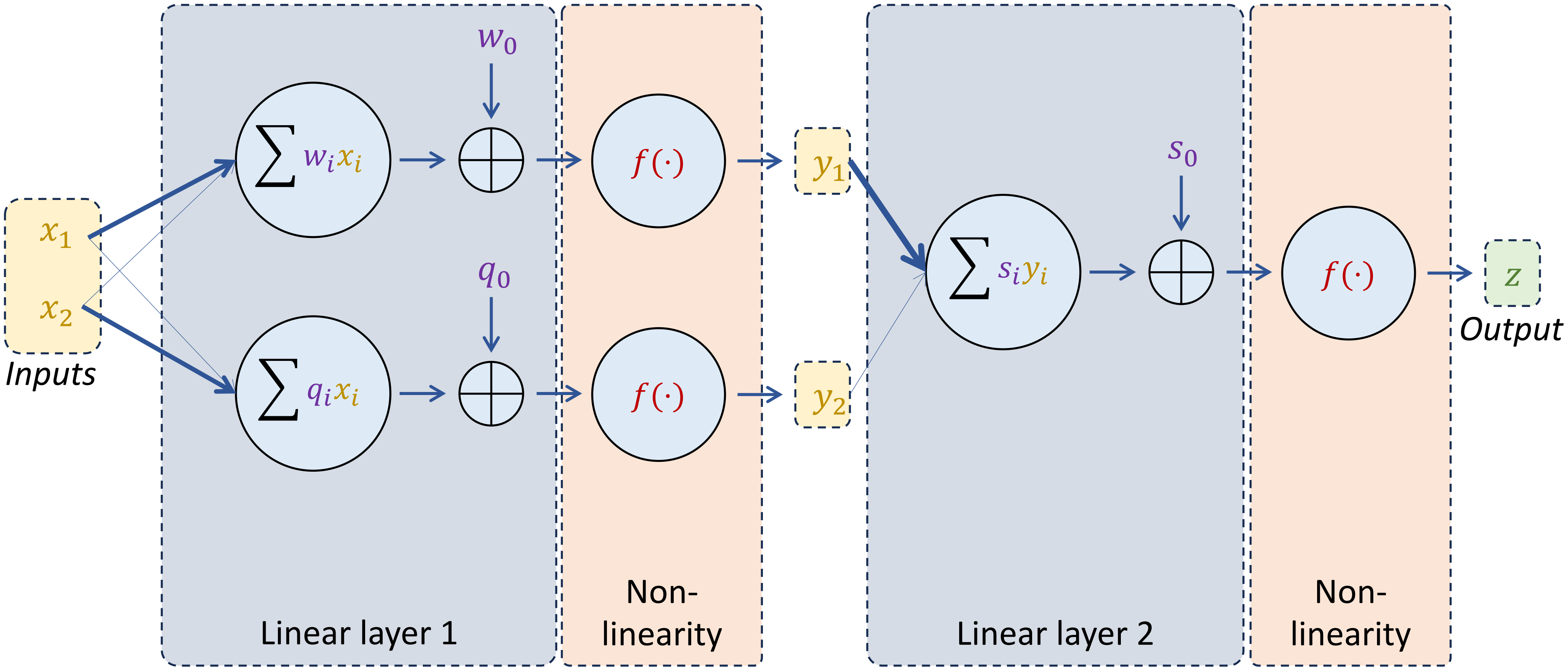
$$y_1 = f(w^{\mathrm{T}} x)$$

$$y_2 = f(q^{\mathrm{T}} x)$$

$$y = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = f\left(\begin{bmatrix} w_0 & w_1 & w_2 \\ q_0 & q_1 & q_2 \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ x_2 \end{bmatrix}\right) = f(W^{\mathrm{T}} x)$$

Note
When we refer to the "number of parameters" in a model, we refer to the total number of weights the model has. This is a "6 parameters" model!

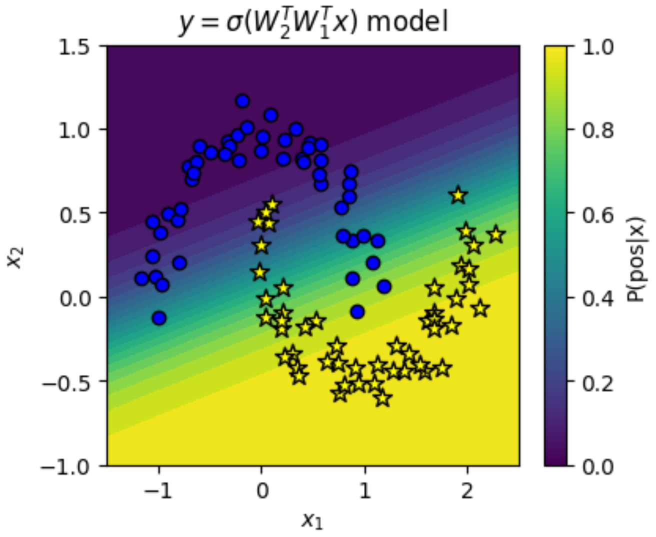
and adding other layers!

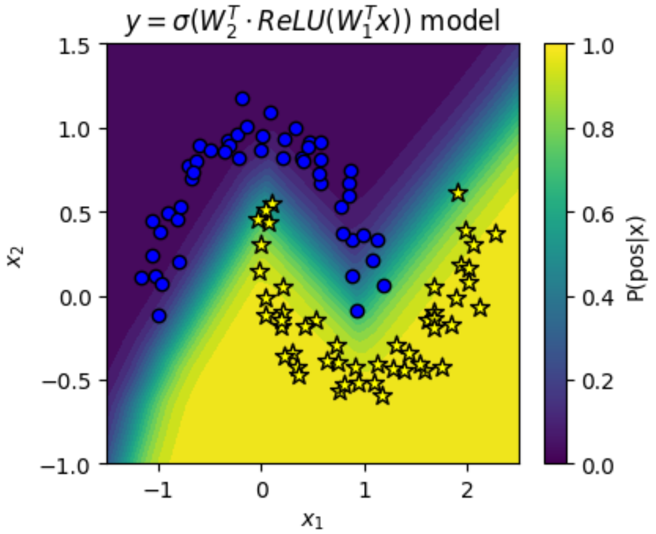


$$z = f\left(s^{\mathrm{T}} f\left(W^{\mathrm{T}} x\right)\right)$$

2. Introduce *non-linearities* in the model

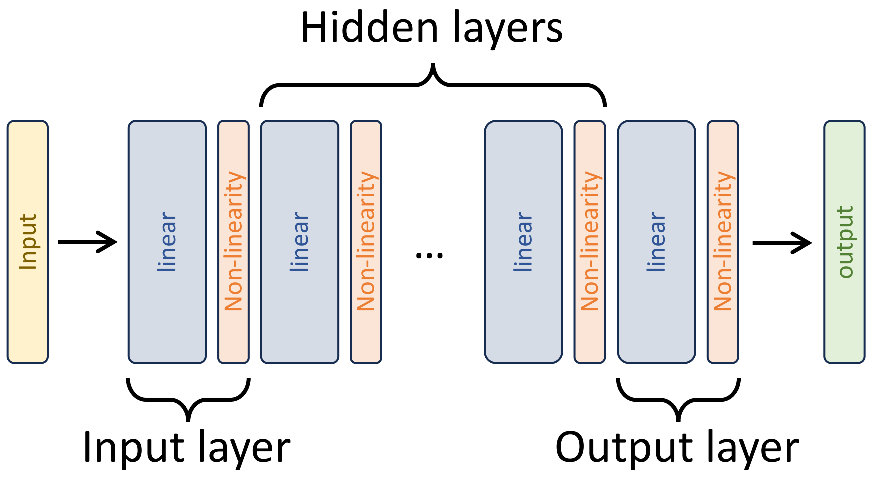
- if $f(x) = x$ (i.e., no non-linearity is added), we get $z = s^{T}W^{T}x$
- This implies:
  1. We could have used $W' = Ws$ and get the same output
  2. We wouldn't have needed a second layer!
  3. But our model is still linear
- So, we use non-linear activation functions to model more complex functions





Multi-layer perceptron models

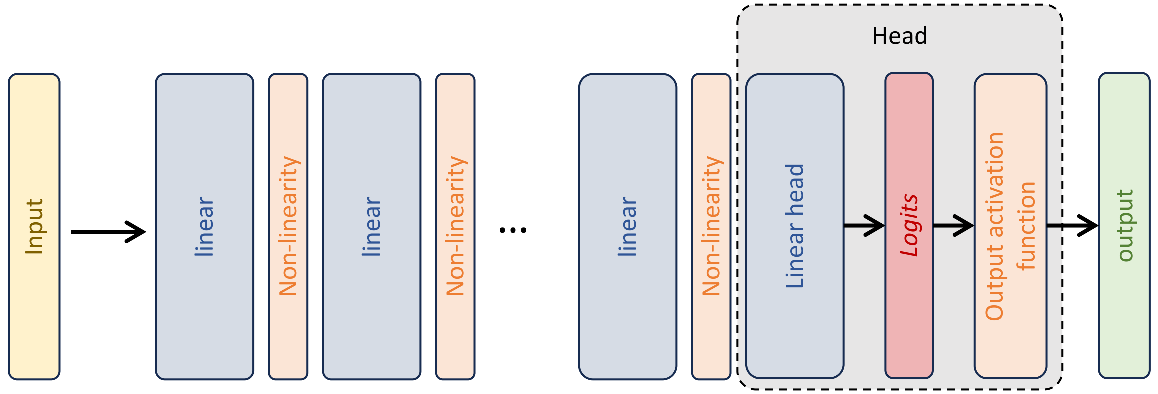
- We can stack additional *layers*
  - separated by *non-linearities* (activation functions) to prevent collapses
- *Universal Approximation Theorem* tells us that we can approximate "any" function with MLPs
  - "For any continuous function g defined on a compact subset of $\mathbb{R}^n$ and for any $\epsilon > 0$, there exists a feedforward neural network with a single hidden layer and a finite number of neurons that can approximate g to within an arbitrary degree of accuracy ϵ"
  - A single-layer MLP works … but no information on the number of neurons, or the weights' values!
  - *Deeper*, *narrower* networks are generally used



Cybenko, George. "Approximation by superpositions of a sigmoidal function." *Mathematics of control, signals and systems* 2.4 (1989): 303-314.
Hornik, Kurt, Maxwell Stinchcombe, and Halbert White. "Multilayer feedforward networks are universal approximators." *Neural networks* 2, no. 5 (1989): 359-366.

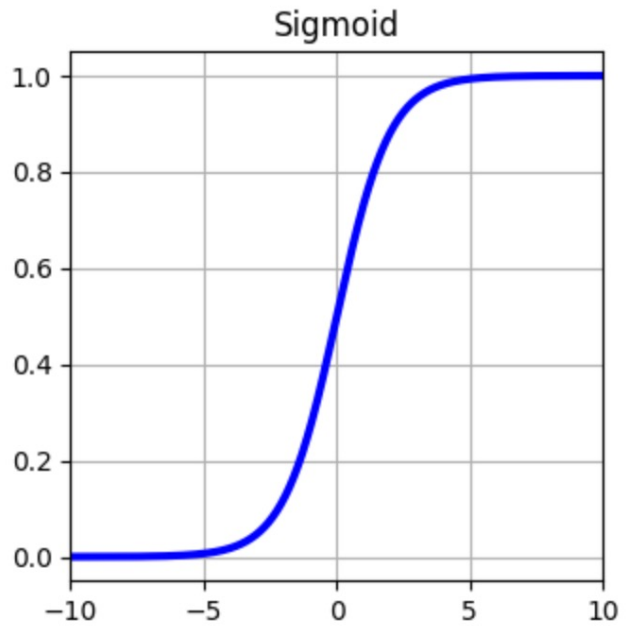
Activation functions for classification models

- As argued, activation functions can be used to enforce properties on the model's output
- In classification problems, the output *before* the final activation is treated as *unnormalized probabilities* (*logits*)
- We still need a step to convert *logits* into *valid* probabilities
  - i.e., all probabilities should sum to 1, and be in [0, 1]



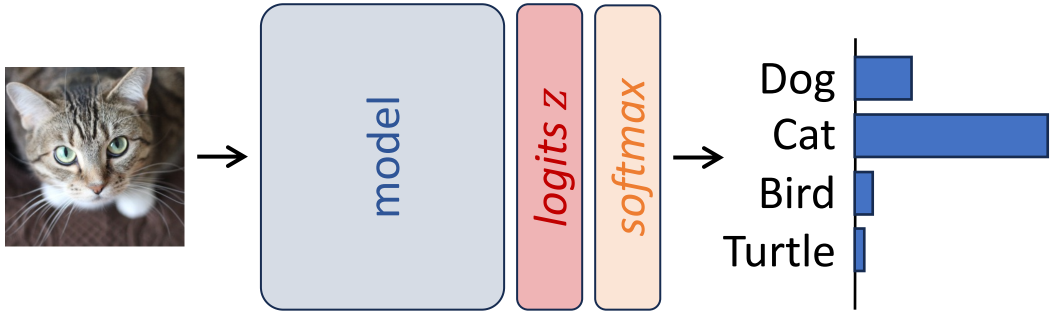
Binary classification

- The model predicts the probability of a single class for point x
  - As a convention, the *positive* one $P(pos|x)$
- The model produces a logit $z = model(x)$
- We use the *sigmoid function* on the output logit z
  - $\sigma(z) = \frac{1}{1+e^{-z}}$
  - This guarantees $P(pos|x) \in [0, 1]$ ✅
- We work out the probability of the negative class
  - $P(neg|x) = 1 - P(pos|x)$
  - We can easily show that $P(neg|x) \in [0,1]$ ✅
- By construction, $P(pos|x) + P(neg|x) = 1$ ✅



Multi-class classification

- The output class is one of many $(c_1, c_2, \dots, c_n)$
- The model produces n logits for a point x
  - (i.e., the last layer will have n perceptrons)
  - $z = (z_1, z_2, \dots, z_n) = model(x)$
- We need to obtain, from the logits, valid probabilities
  - $P(c_1|x), P(c_2|x), \dots, P(c_n|x)$
- The *softmax* function is applied:
  - $P(c_i|x) = \frac{e^{z_i}}{\sum_j e^{z_j}}$
- It can be easily shown that:
  - $P(c_i|x) \in [0,1]$ ✅
  - $\sum_i P(c_i|x) = 1$ ✅



Activation functions for regression models

- In regression, models generally predict real numbers
- Typically, there is no need to enforce properties
- Output activation function can be the identity function
  - $f(x) = x$
  - Generally the only situation where it makes sense to use it!

Defining weights (parameters)

- So far, we assumed all weights and biases (let's call them θ) to be known
  - *But, we still need to figure out how we find them!*

- We pick a function (objective, or loss), $\mathcal{L}(\theta)$, that we want to minimize
  - e.g., in Linear Regression we minimize the Mean Squared Error
    - $\mathcal{L}(\theta) = MSE(\theta) = \frac{1}{n}\sum(y_i - \theta^T x_i)^2$
  - Then, we pick θ that minimizes it

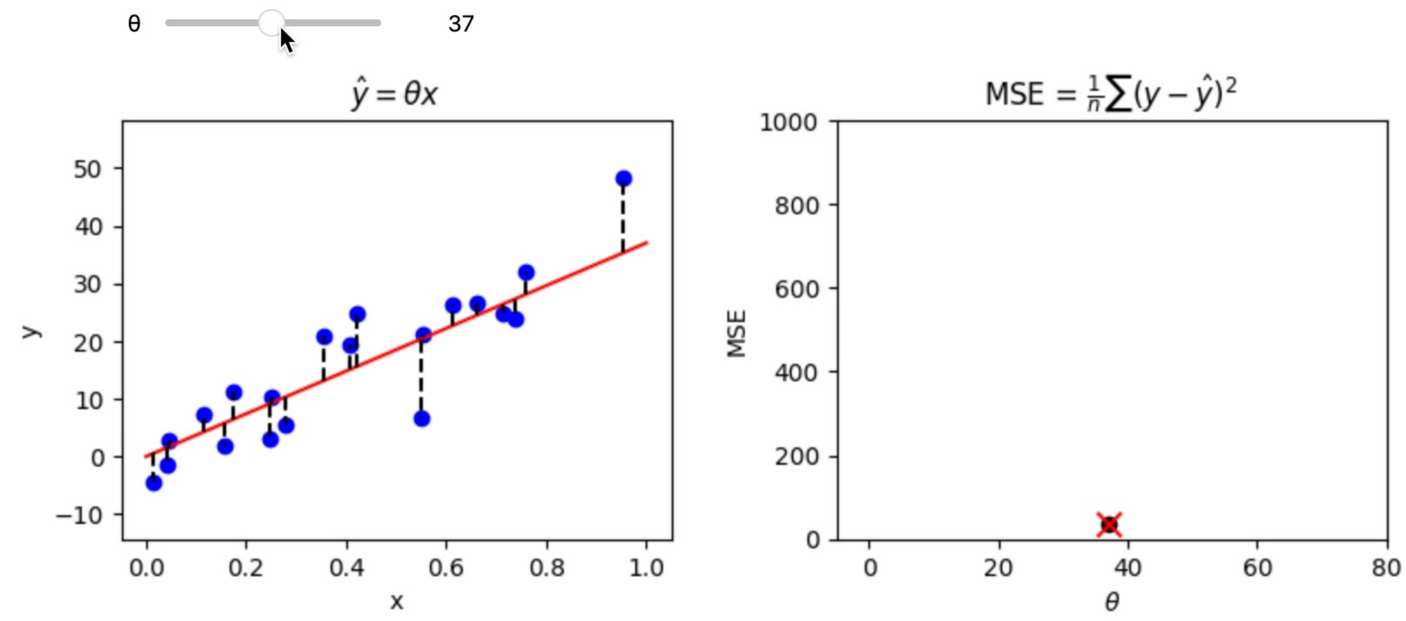
Note

$\mathcal{L}$ also depends on the training points x_i, y_i, so we should refer to it as $\mathcal{L}(\theta, X, y)$.

However, the training set X, y is generally fixed. Thus, we only have control over θ, so we use the notation $\mathcal{L}(\theta)$.

Linear regression

- For *simple* models, we can find the optimal weights in closed form
  - $\frac{\partial \mathcal{L}(\theta)}{\partial \theta} = \frac{\partial MSE(\theta)}{\partial \theta} = 0$
  - Quadratic in θ, can be solved easily!
- Or, we can evaluate the loss function for a bunch of θ's, and find the "best" one

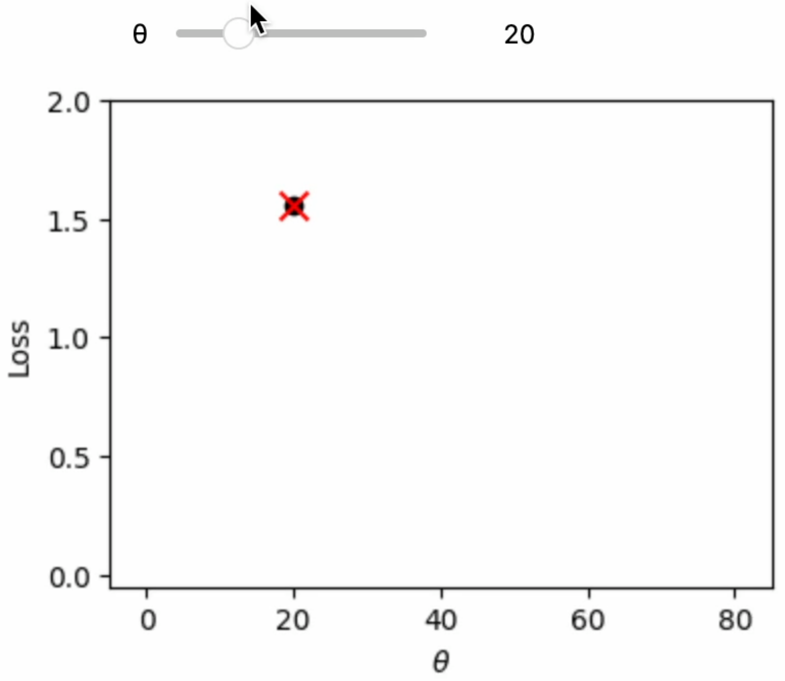


Note
For linear regression, we don't try a bunch of θ since we can easily find the best value in closed form.

However, this provides the intuition for what we will do next with more complex loss functions/models.

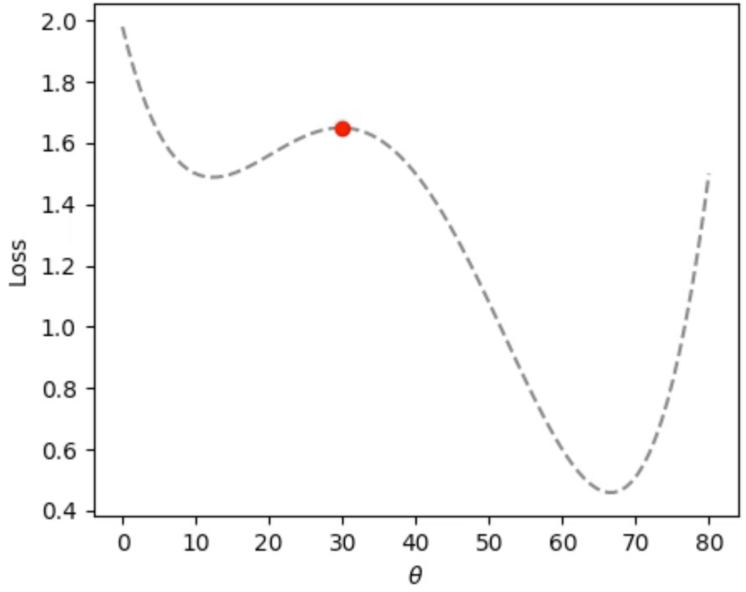
More complex losses/models

- For *more complex* loss functions/models, we may not be able to solve the problem in closed form
  - But we can evaluate $\mathcal{L}(\theta)$ for various values of θ
- We can iteratively update θ to reach a local minimum:
  - We start from a random value θ, then
  - we "move around" according to "some policy"



We "move around" according to "some policy"

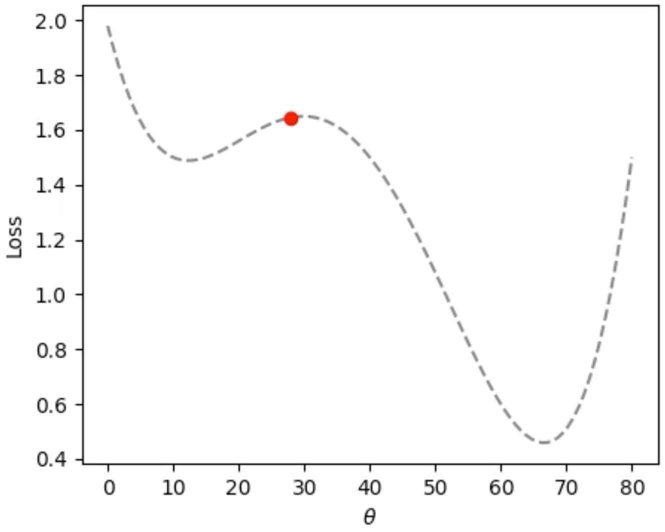
- Move around = update θ incrementally, based on its current value
  - The new value of θ at any step depends on the previous step's value
  - $\theta_{t+1} := \theta_t + update$
- Some policy = we take a small step in the direction where the function decreases locally
  - i.e. in the *opposite* direction of the gradient
  - $\theta_{t+1} := \theta_t - \alpha \nabla_\theta \mathcal{L}(\theta_t)$
    - for 1-dimensional θ, we have $\theta_{t+1} = \theta_t - \alpha \frac{\partial \mathcal{L}(\theta)}{\partial \theta}$
    - α: learning rate, controls the "size" of the step
- Gradient Descent!



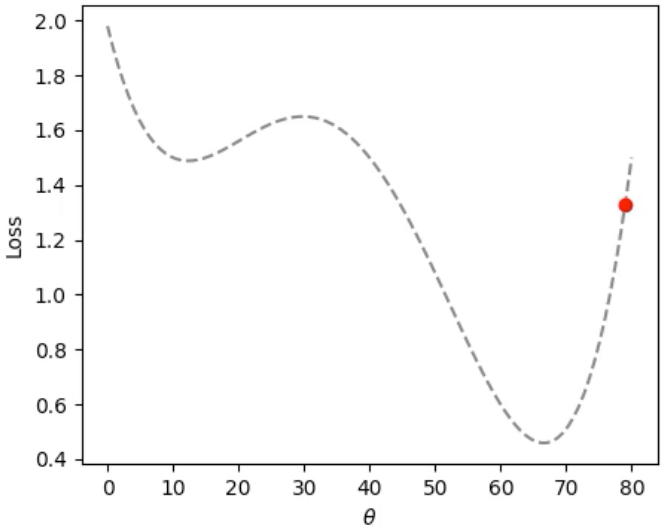
Some limitations of GD

Note
Different initializations will lead to the global minimum for convex loss functions. However, that represents a trivial situation we typically do not encounter.

- GD is sensitive to weight initialization
  - Different initializations can lead to different solutions!
  - GD can get stuck in local minima



- Various solutions to help prevent local minima:
  - Adding momentum
  - Adaptive learning rates
  - Learning rate schedules



Backpropagation

- So far, we assumed we were able to compute $\nabla_\theta \mathcal{L}(\theta)$
- However, any loss/model combination would need a different gradient computation!
- We can use backpropagation to compute the gradient of the loss w.r.t. any weight!
  - Backpropagation is just a fancy word for “using the chain rule”

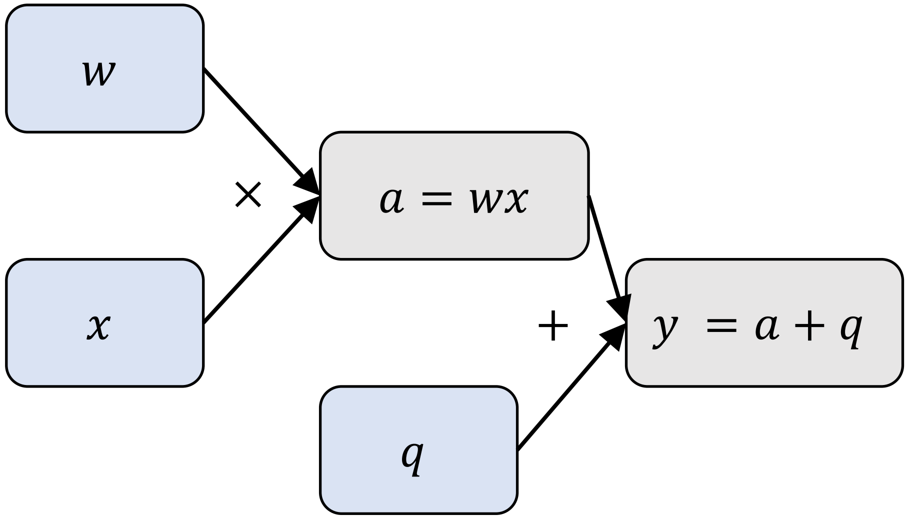
Using the chain rule

- We use the chain rule from calculus, $\frac{\partial f}{\partial x} = \frac{\partial f}{\partial g}\frac{\partial g}{\partial x}$
  - Sometimes known as $f\big(g(x)\big)' = f'\big(g(x)\big) \cdot g'(x)$

- And apply it from the end of the computational graph, backwards
  - (hence the name, backpropagation)

Computational graph

- A computational graph is a directed graph
  - Each node corresponds to an operation
  - Each edge represents the flow of data between nodes
- For instance, we may want to compute $y = wx + q$
  - We start from three variables, w, x and y
  - The computational graph performs one operation at a time
    - First, compute the intermediate variable $a = wx$
    - Then, compute the output variable $z = a + y = wx + y$



Backpropagation example

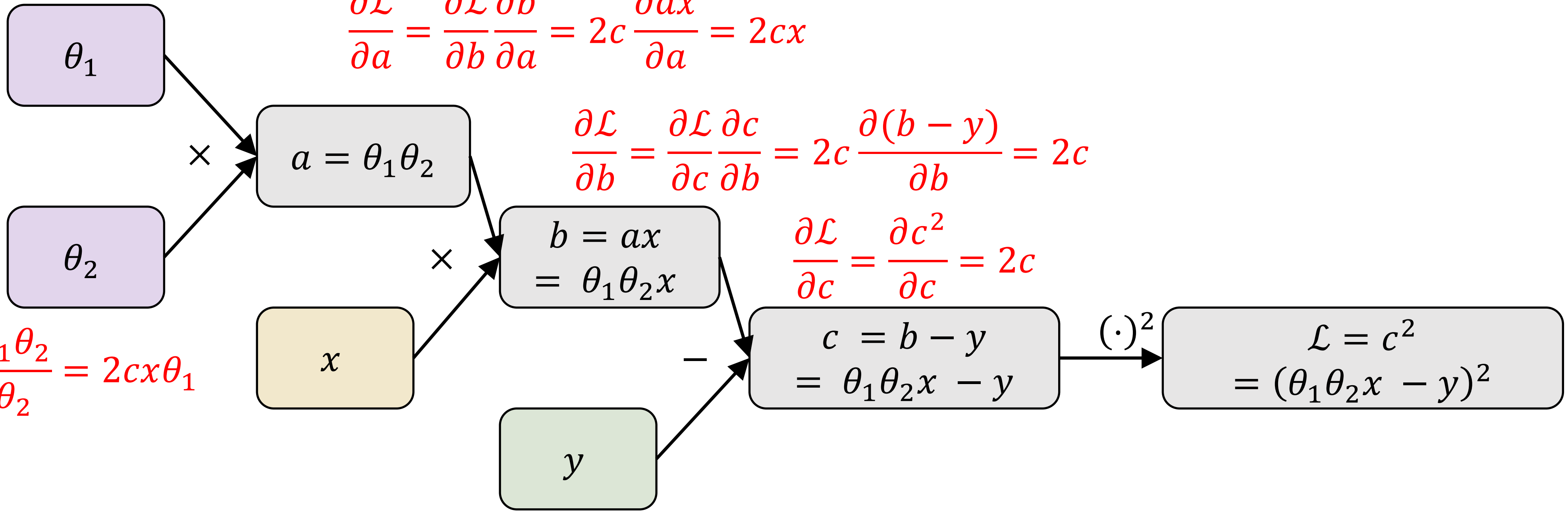
- Let's say:
  - Our dataset has one point, (x, y)
  - Our (weird) model has two parameters, θ_1 and θ_2, and predicts $\theta_1\theta_2 x$
  - Our loss function will be $\mathcal{L} = (\theta_1\theta_2 x - y)^2$
- We build a computational graph with all operations and intermediate variables
  - $a = \theta_1\theta_2$
  - $b = ax = \theta_1\theta_2 x$
  - $c = b - y = ax - y = \theta_1\theta_2 x - y$
  - $\mathcal{L} = c^2 = (b - y)^2 = (ax - y)^2 = (\theta_1\theta_2 x - y)^2$

$$\frac{\partial \mathcal{L}}{\partial \theta_1} = \frac{\partial \mathcal{L}}{\partial a}\frac{\partial a}{\partial \theta_1} = 2cx\frac{\partial \theta_1\theta_2}{\partial \theta_1} = 2cx\theta_2$$

$$\frac{\partial \mathcal{L}}{\partial a} = \frac{\partial \mathcal{L}}{\partial b}\frac{\partial b}{\partial a} = 2c\frac{\partial ax}{\partial a} = 2cx$$

$$\frac{\partial \mathcal{L}}{\partial b} = \frac{\partial \mathcal{L}}{\partial c}\frac{\partial c}{\partial b} = 2c\frac{\partial (b-y)}{\partial b} = 2c$$

$$\frac{\partial \mathcal{L}}{\partial c} = \frac{\partial c^2}{\partial c} = 2c$$



$$\frac{\partial \mathcal{L}}{\partial \theta_2} = \frac{\partial \mathcal{L}}{\partial a}\frac{\partial a}{\partial \theta_2} = 2cx\frac{\partial \theta_1\theta_2}{\partial \theta_2} = 2cx\theta_1$$

Forward step

- The loss $\mathcal{L}$ is computed starting from the "inputs" θ_1, θ_2, x, y

Backward step (backpropagation)

- The loss $\mathcal{L}$ is used to compute the derivative w.r.t. c ➔ $\frac{\partial \mathcal{L}}{\partial c}$
- The derivative $\frac{\partial \mathcal{L}}{\partial c}$ is used to compute the derivative w.r.t. b ➔ $\frac{\partial \mathcal{L}}{\partial b}$
- The derivative $\frac{\partial \mathcal{L}}{\partial b}$ is used to compute the derivative w.r.t. a ➔ $\frac{\partial \mathcal{L}}{\partial a}$
- The derivative $\frac{\partial \mathcal{L}}{\partial a}$ is used to compute the derivative w.r.t. θ_1, θ_2 ➔ $\frac{\partial \mathcal{L}}{\partial \theta_1}, \frac{\partial \mathcal{L}}{\partial \theta_2}$

$$\frac{\partial \mathcal{L}}{\partial \theta_1} = 2(\theta_1\theta_2 x - y)x\theta_2$$

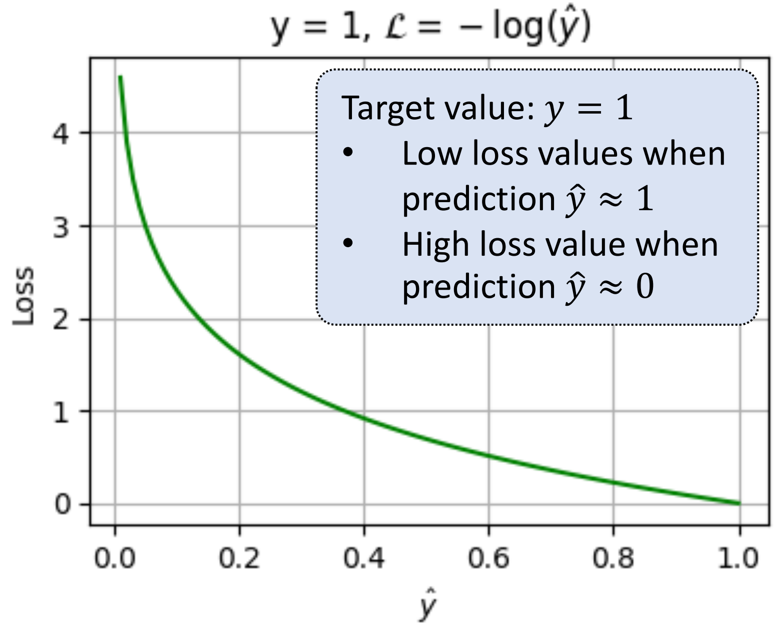
$$\frac{\partial \mathcal{L}}{\partial \theta_2} = 2(\theta_1\theta_2 x - y)x\theta_1$$

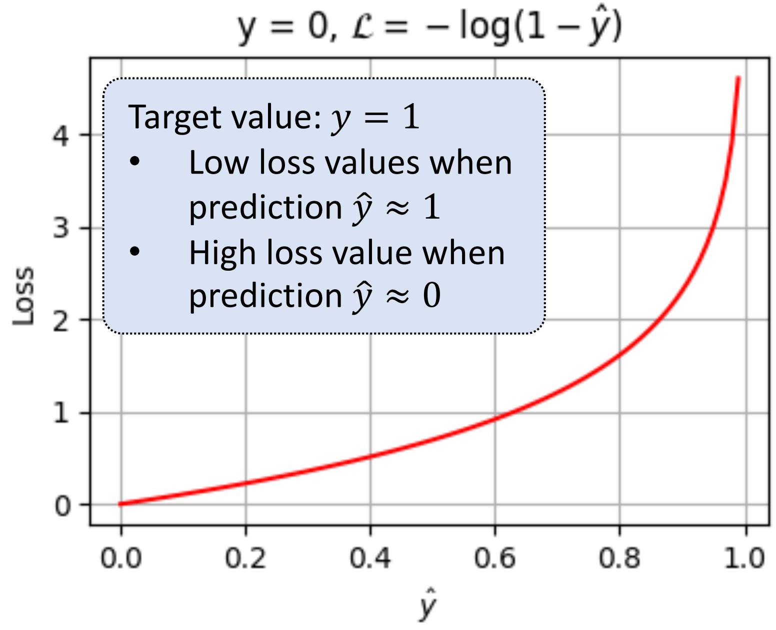
Loss functions

- Regression
  - *Mean Squared Error, Mean Absolute Error*
- Binary
  - *Binary Cross-Entropy* (*BCE*)
  - $y = \{0, 1\}$ ➔ ground truth
  - $\hat{y} = model(x) \in [0,1]$ ➔ predicted value

$$\mathcal{L} = -y log(\hat{y}) - (1 - y) log(1 - \hat{y})$$

  - y (ground truth) acts as a "selector" of the loss term to be applied
    - $y = 1$ ➔ $\mathcal{L} = -log(\hat{y})$
    - $y = 0$ ➔ $\mathcal{L} = -log(1 - \hat{y})$





Loss functions

- Multi-class classification
  - Cross-Entropy
  - Generalization to multiple classes of BCE
  - $y_i = 1$ when ground truth is the ith class, 0 otherwise
  - y_i plays the same “selector” mechanism as in BCE

$$\mathcal{L} = -\sum_i y_i \log(\hat{y}_i)$$