CS 190I Deep Learning Feedforward Network

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Acknowledgement: Slides borrowed from Bhiksha Raj's 11485 and Mu Li & Alex Smola's 157 courses on Deep Learning, with modification

Recap

- Logistic Regression for classification
  - single linear layer with Softmax output
- How to train LR
- Inference for LR
- How to evaluate LR model (validation/ testing)
- Kullback-Leibler Divergence

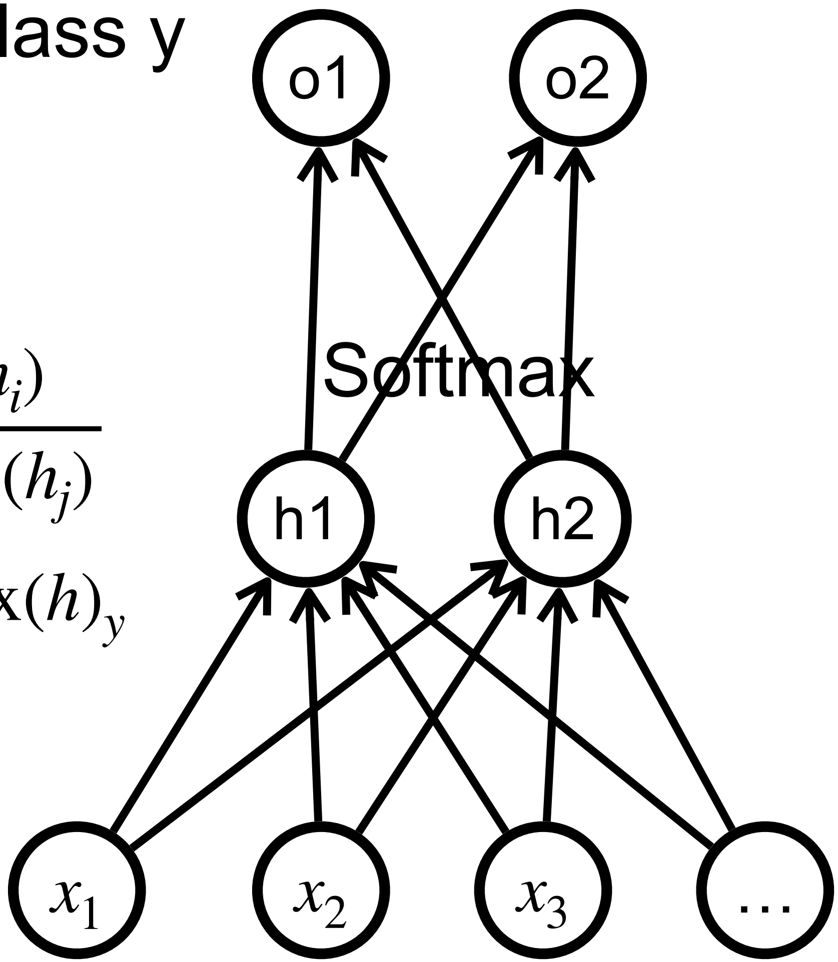
Logistic Regression

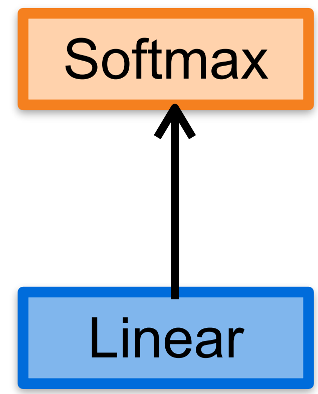
output: prob. of class y

$$h = \mathbf{W} \cdot \mathbf{x}$$

$$\text{softmax}(h)_i = \frac{\exp(h_i)}{\sum_j \exp(h_j)}$$

$$p(y \mid h) = \text{softmax}(h)_y$$



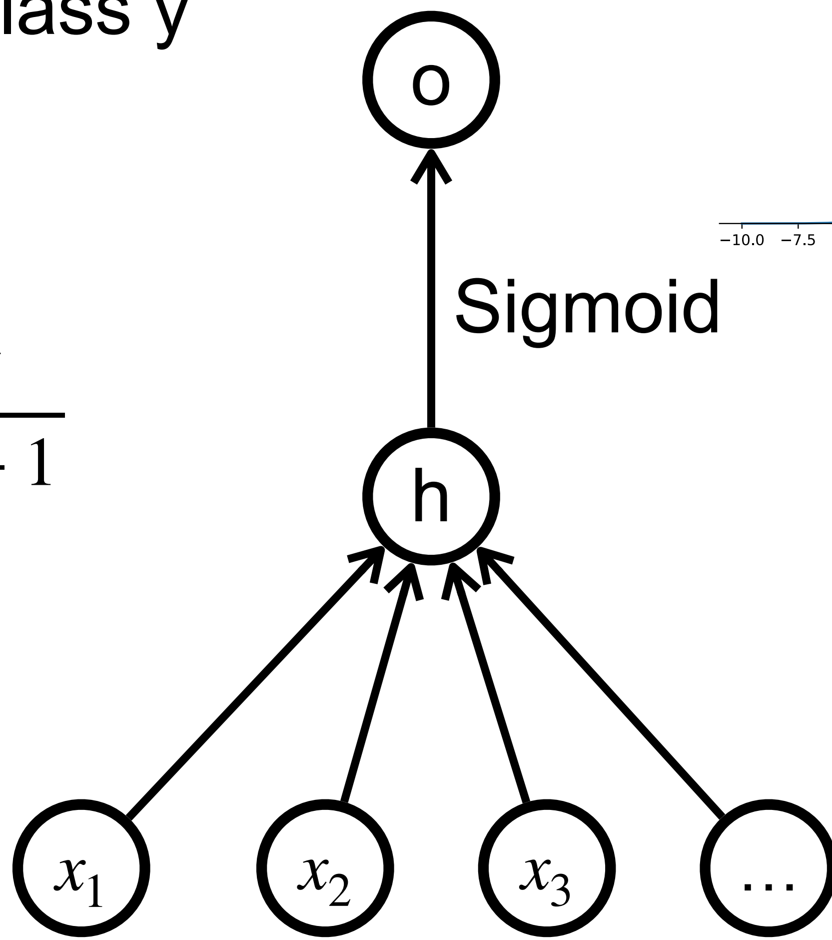


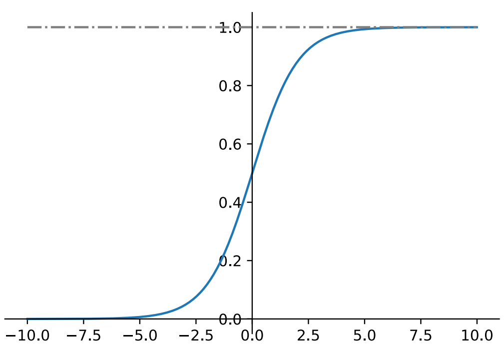
Logistic Regression for Binary Classification

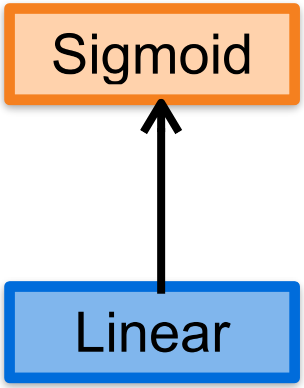
output: prob. of class y

$$h = \mathbf{w} \cdot \mathbf{x}$$

$$p(y \mid h) = \sigma(h) = \frac{e^h}{e^h + 1}$$







Cross-Entropy Loss for Classification

$$\boxed{\min \mathscr{L}(\theta) = \frac{1}{N}\sum_{n=1}^{N} H(y_n, f(x_n)) = \frac{1}{N}\sum_{n=1}^{N} -\log f(x_n)_{y_n}}$$

Spam Email Classification

Subject: Hello
Sender: Aisha Al-Gaddafi <aishaalgaddafi112@gmail.com>

Tue, Jan 10, 9:35 AM (12 days ago)

to bcc:

I am sorry to encroach into your privacy in this manner, There is absolutely going to be a great doubt and distrust in your heart in respect of this email, coupled with the fact that so many individuals have taken possession of the Internet to facilitate their nefarious deeds, thereby making it extremely difficult for genuine and legitimate business class persons to get attention and recognition.

I am seeking your assistance for the transfer of Twenty Seven Million Five Hundred Thousand United State Dollars ($27.500.000.00) to your account for private investment purpose.

I look forward to your response.
Mrs. Aisha Al-Gaddafi.

Feature

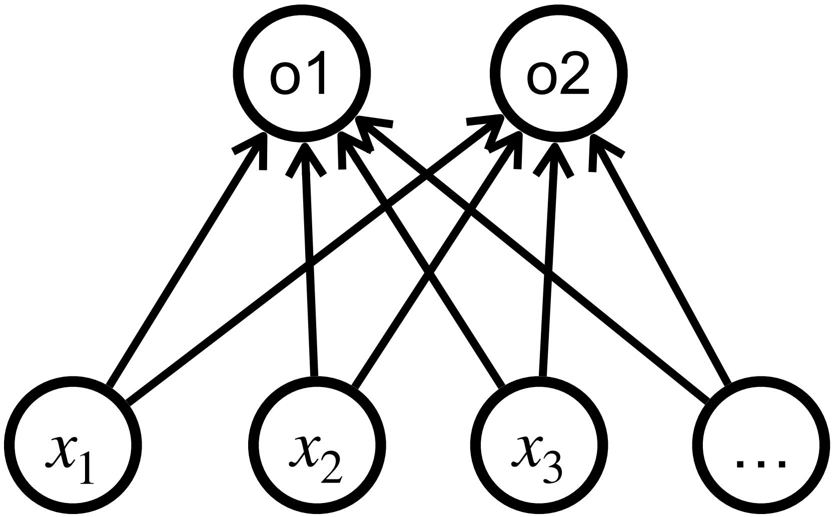
	dollor	$	money	account	…	sender		
x	1	1	0	1				

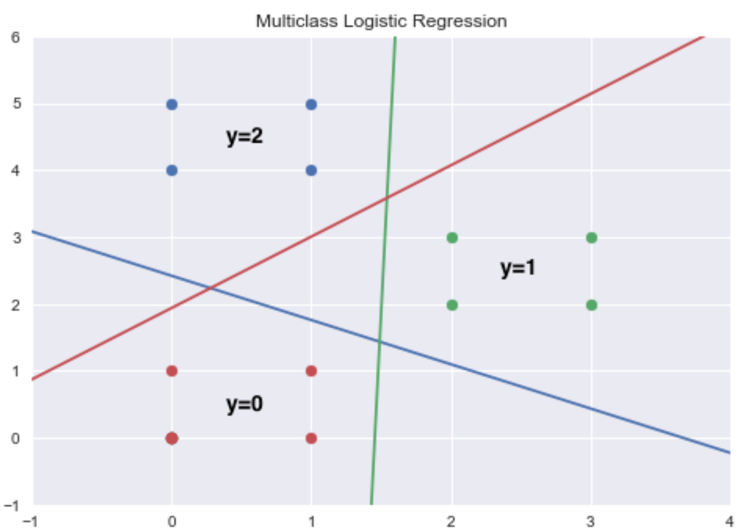
y: 0 or 1 (spam)

$$h = \mathbf{w} \cdot \mathbf{x}$$

$$p(y \mid h) = \sigma(h) = \frac{e^h}{e^h + 1}$$

Limitation of Logistic Regression

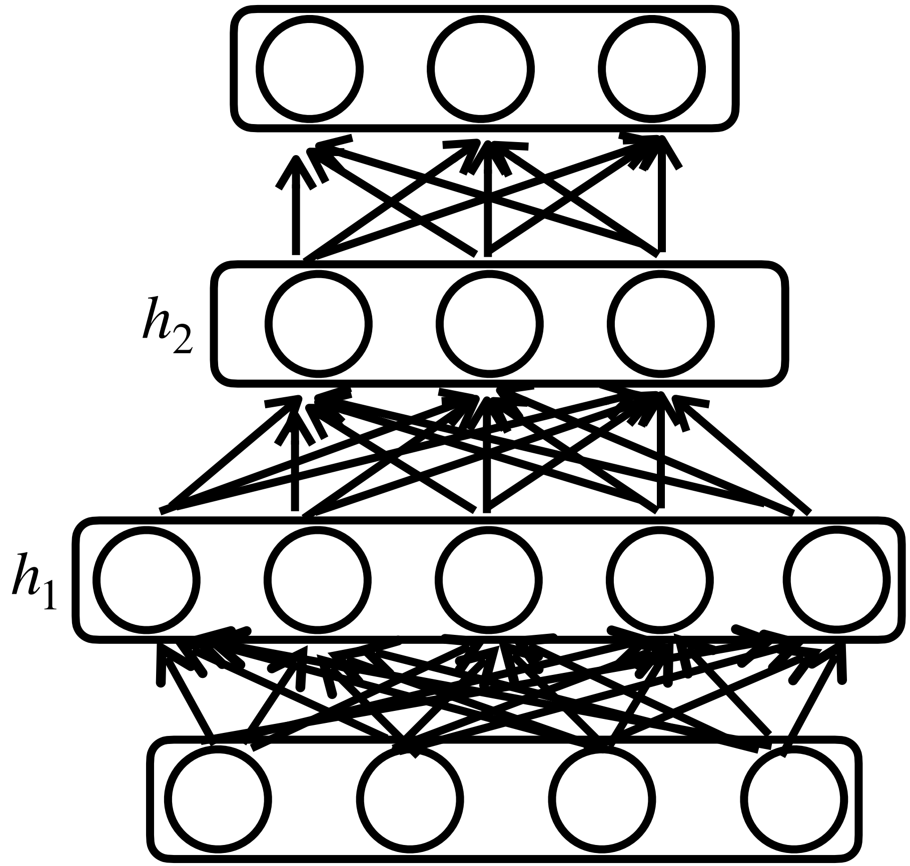




- Single layer has limited capability
  - cannot learn XOR
- The decision boundary is linear
  - cannot learn a nonlinear decision boundary
  - why?

Feedforward Neural Net (FFN)

- also known as multilayer perceptron (MLP)
- Layers are connected sequentially
- Each layer has full-connection (each unit is connected to all units of next layer)
  - Linear project followed by
  - an element-wise nonlinear activation function
- There is no connection from output to input



Feedforward Neural Net (FFN)

- also known as multilayer perceptron (MLP)

$$x \in \mathbb{R}^d$$

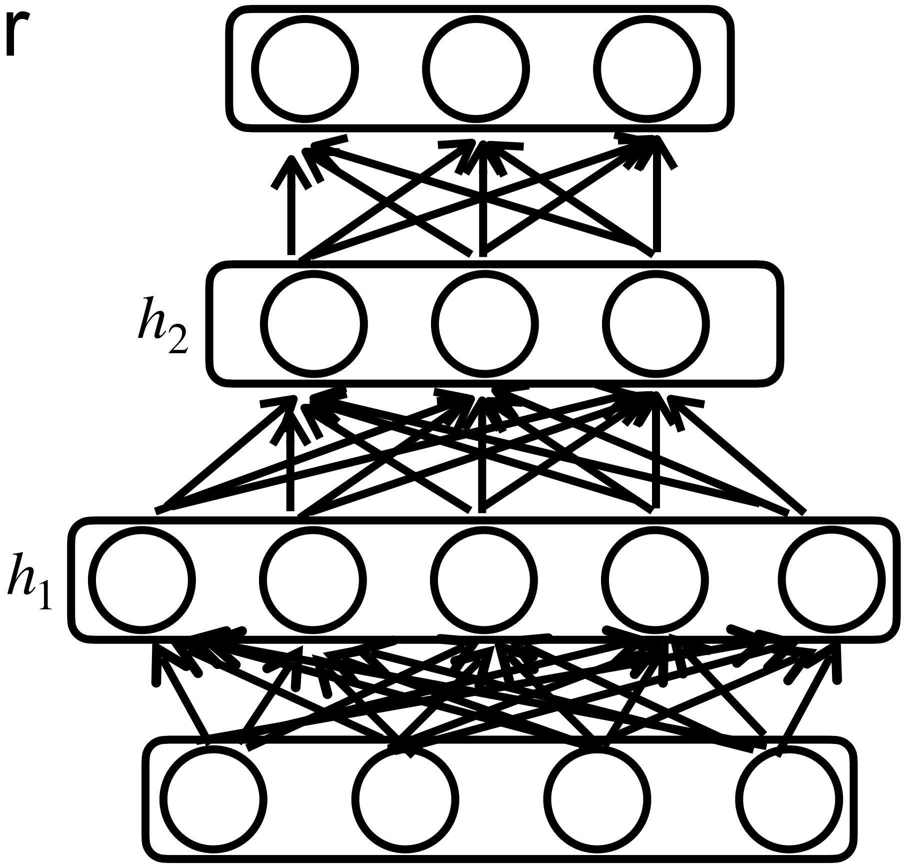
$$h_1 = \sigma(w_1 \cdot x + b_1) \in \mathbb{R}^{d_1}$$

$$h_l = \sigma(w_l \cdot h_{l-1} + b_l) \in \mathbb{R}^{d_l}$$

$$o = \text{Softmax}(w_L \cdot h_{L-1} + b_L)$$

Parameters

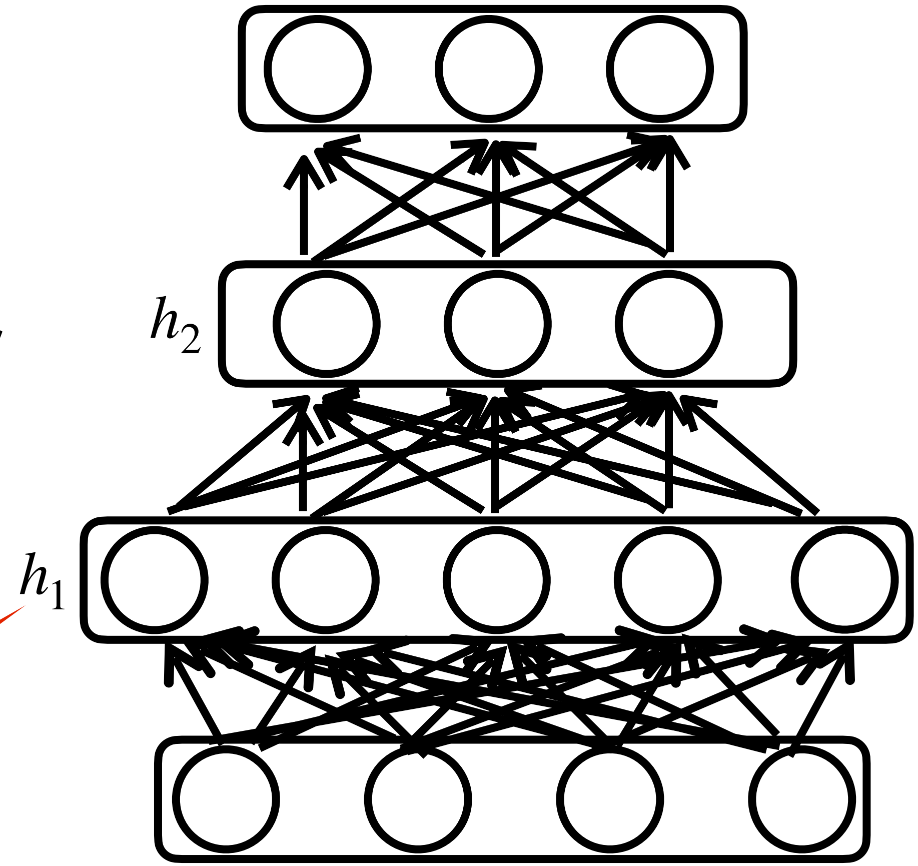
$$\theta = \{w_1, b_1, w_2, b_2, \ldots\}$$



Hidden layers

- $$h_1 = \sigma(w_1 \cdot x + b_1) \in \mathbb{R}^{d_1}$$
  $$h_l = \sigma(w_l \cdot h_{l-1} + b_l) \in \mathbb{R}^{d_l}$$

σ is element-wise nonlinear activation function



Why do we need an a nonlinear

What-if Layer with no activation?

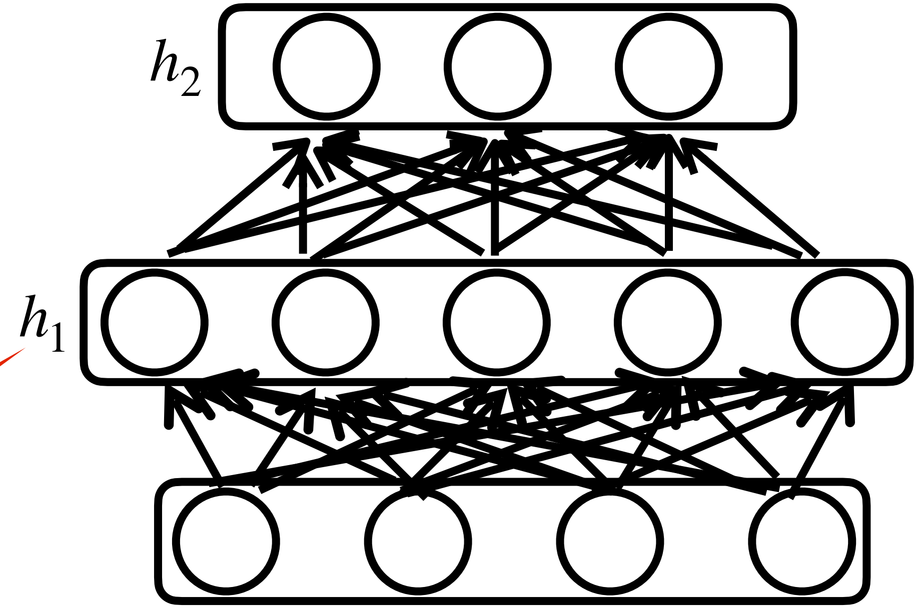
Linear ...

$$\mathbf{h}_1 = \mathbf{W}_1\mathbf{x} + \mathbf{b}_1$$

$$\mathbf{h}_2 = \mathbf{w}_2^T\mathbf{h}_1 + b_2$$

hence $h_2 = \mathbf{w}_2^\top\mathbf{W}_1\mathbf{x} + b'$

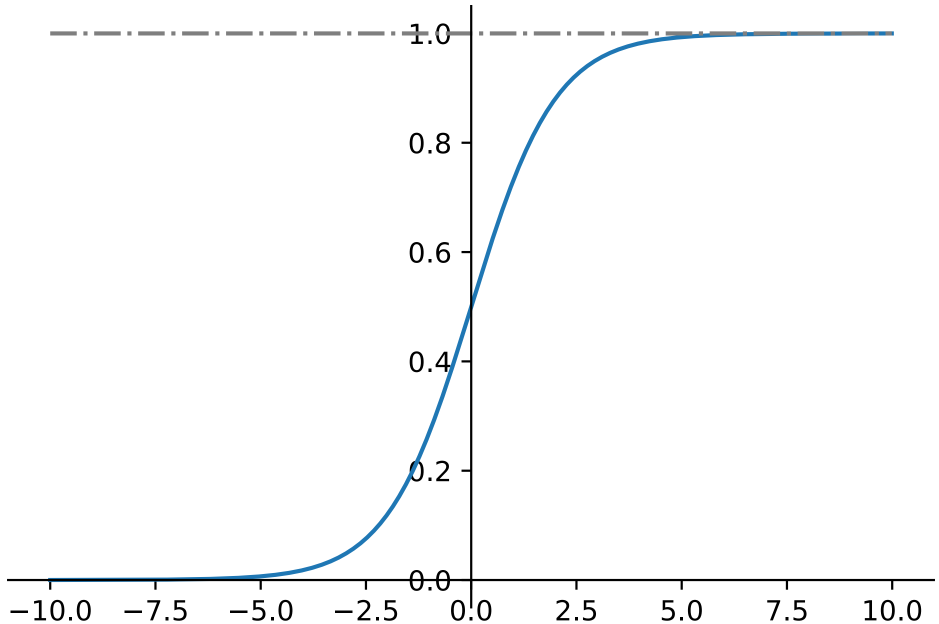
Why do we need an a nonlinear



Sigmoid Activation

Map input into (0, 1), a soft version of $\sigma(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{otherwise} \end{cases}$

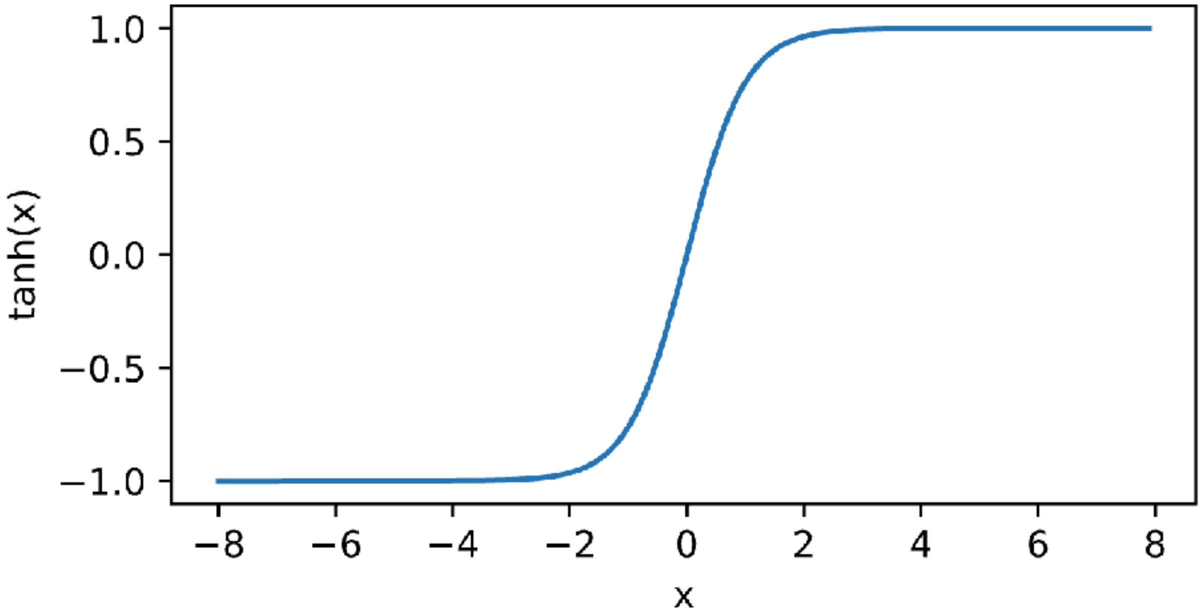
$$\text{sigmoid}(x) = \frac{1}{1 + \exp(-x)}$$



Tanh Activation

Map inputs into (-1, 1)

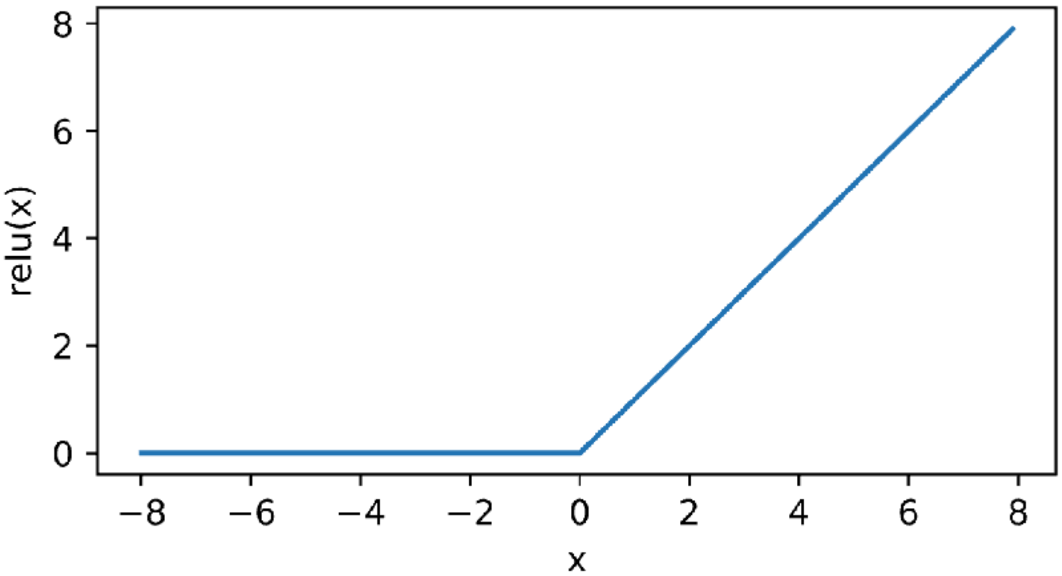
$$\tanh(x) = \frac{1 - \exp(-2x)}{1 + \exp(-2x)}$$



ReLU Activation

ReLU: rectified linear unit

$$\mathrm{ReLU}(x) = \max(x, 0)$$

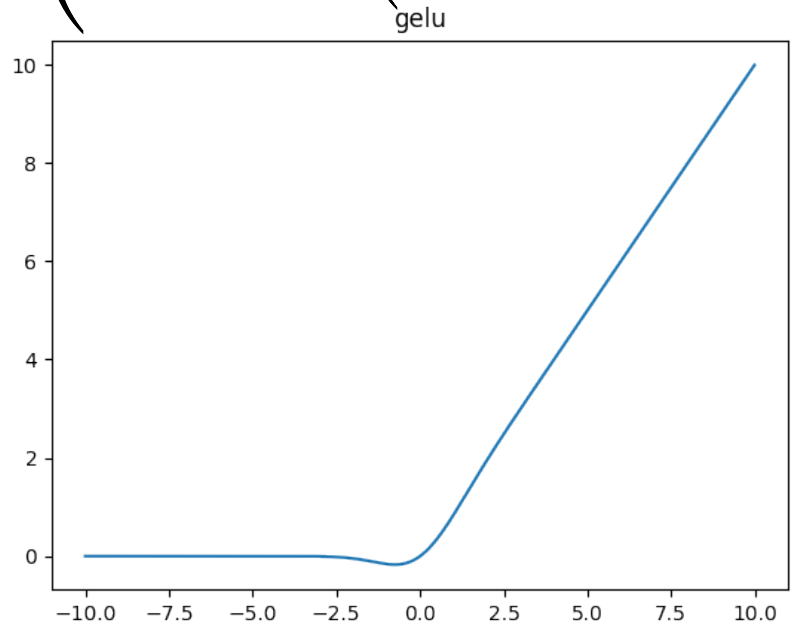


Gaussian Error Linear Units (GELU)

smoothed version of RELU

$$\text{GELU}(x) = xP(X \leq x) = x\Phi(x) = x \cdot \frac{1}{2}\left[1 + \text{erf}(x/\sqrt{2})\right]$$

$$\text{GELU}(x) \approx 0.5x\left(1 + \tanh\left(\sqrt{2/\pi}(x + 0.044715x^3)\right)\right)$$



Feedforward Network for Classification

Softmax as the final
output layer.

$x \in \mathbb{R}^d$

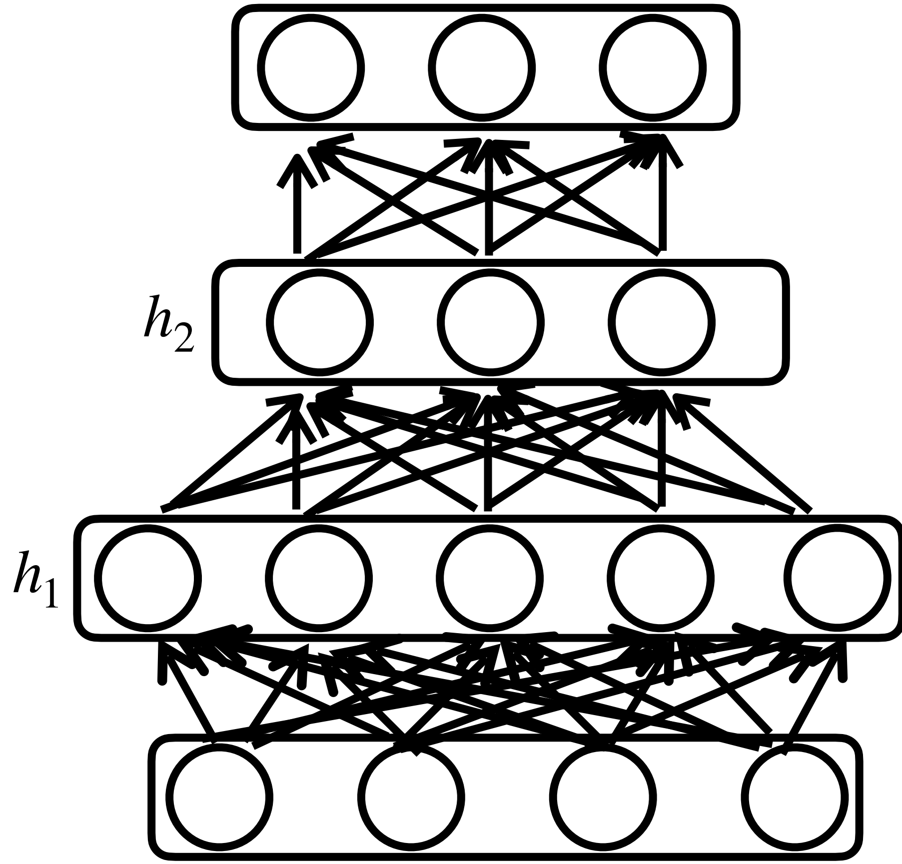
$h_1 = \sigma(w_1 \cdot x + b_1) \in \mathbb{R}^{d_1}$

$h_l = \sigma(w_l \cdot h_{l-1} + b_l) \in \mathbb{R}^{d_l}$

$o = \mathrm{Softmax}(w_L \cdot h_{L-1} + b_L)$

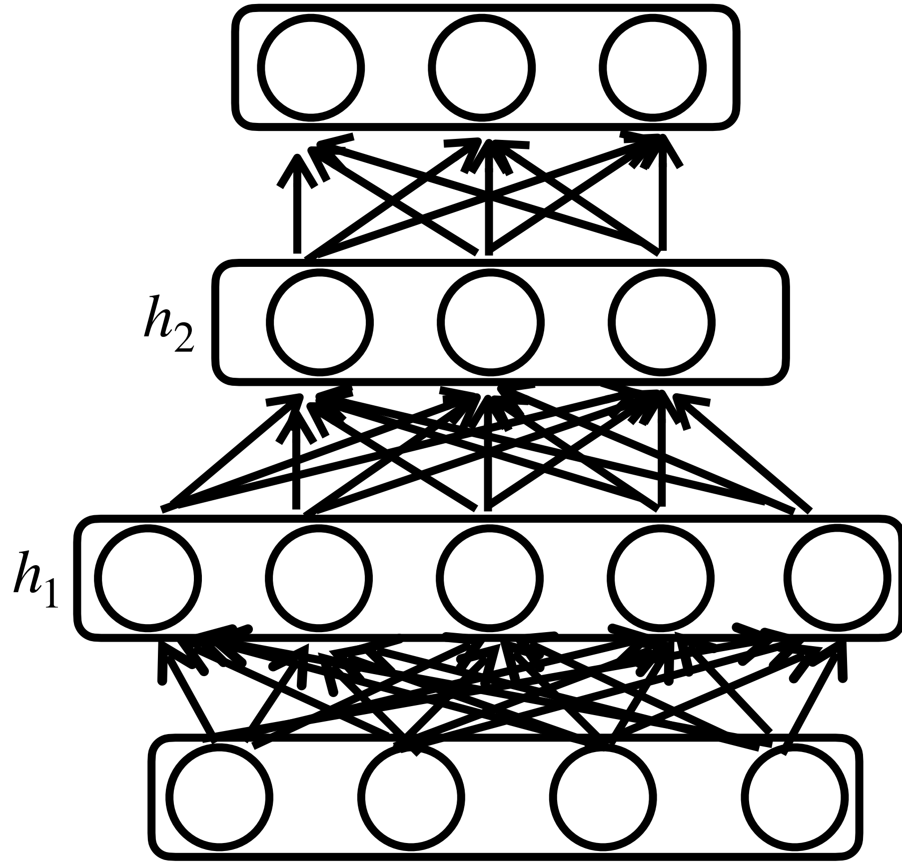
Parameters

$\theta = \{w_1, b_1, w_2, b_2, \ldots\}$



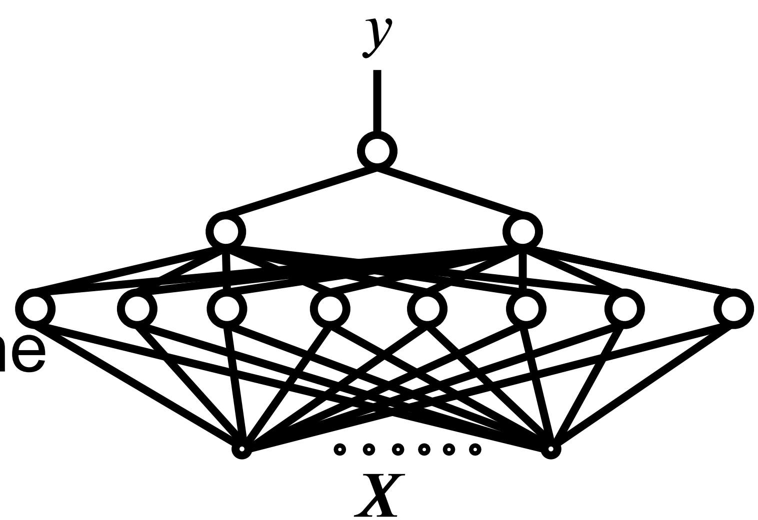
Hyperparameters for FFN

- Number of layers
- Number of hidden dimension for each layer



The Learning Problem

- Given a training set of input-output pairs $D = \{(x_n, y_n)\}_{n=1}^{N}$
  - x_n and y_n may both be vectors
- To find the model parameters such that the model produces the most accurate output for each training input
  - Or a close approximation of it
- Learning the parameter of a neural network is an instance!
  - The network architecture is given



Risk

- The expected risk is the average risk (loss) over the entire (x, y) data space

$$R(\theta) = E_{\langle x,y \rangle \in P}\left[\ell(y, f(x;\theta))\right] = \int \ell(y, f(x;\theta))dP(x,y)$$

The general learning framework: Empirical Risk Minimization (ERM)

- Ideally, we want to minimize the expected risk
  - but, unknown data distribution …
- Instead, given a training set of empirical data $D = \{(x_n, y_n)\}_{n=1}^{N}$
- Minimize the empirical risk over training data

$$\hat{\theta} \leftarrow \arg\min_{\theta} L(\theta) = \frac{1}{N} \sum_{n} \ell(y_n, f(x_n; \theta))$$

The general learning framework: Empirical Risk Minimization (ERM)

- Ideally, we want to minimize the expected

Note : Its really a measure of error, but using standard terminology, we will call it a "Loss"

Note 2: The empirical risk $L(\theta)$ is only an empirical approximation to the true risk $R(\theta) = E_{\langle x,y \rangle \in P}\left[\ell(y, f(x;\theta))\right]$, which is our ultimate optimization objective

Note 3: For a given training set the loss is only a function of θ

$$\theta^* \leftarrow \arg\min_{\theta} L(\theta) = \frac{1}{N}\sum_{n} \ell(y_n, f(x_n; \theta))$$

Loss function

- The empirical risk (loss) is determined by the loss function
- Ideal loss for classification: 0-1 loss

$$l(y, f(x)) = \begin{cases} 0 & \text{if } y = \arg\max_k f(x)_k \\ 1 & \text{otherwise} \end{cases}$$

- Cross entropy loss is one common loss for classification

$$\min \mathscr{L}(\theta) = \frac{1}{N} \sum_{n=1}^{N} H(y_n, f(x_n)) = \frac{1}{N} \sum_{n=1}^{N} -y_n \cdot \log f(x_n)$$

Other Loss for Classification

- Hinge loss

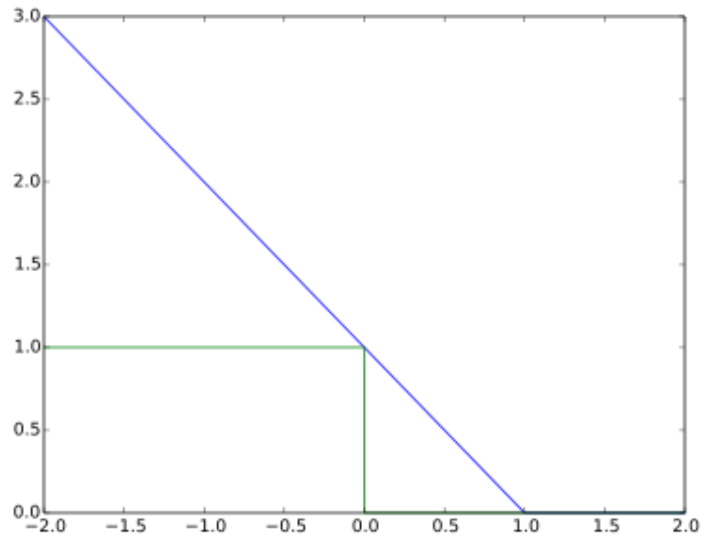
  - Binary classification:

$$\ell(y, \hat{y}) = \max(0, 1 - y\hat{y})$$

When ground-truth y is +1, prediction $\hat{y}$<0 lead to larger penalty

  - Multi-class

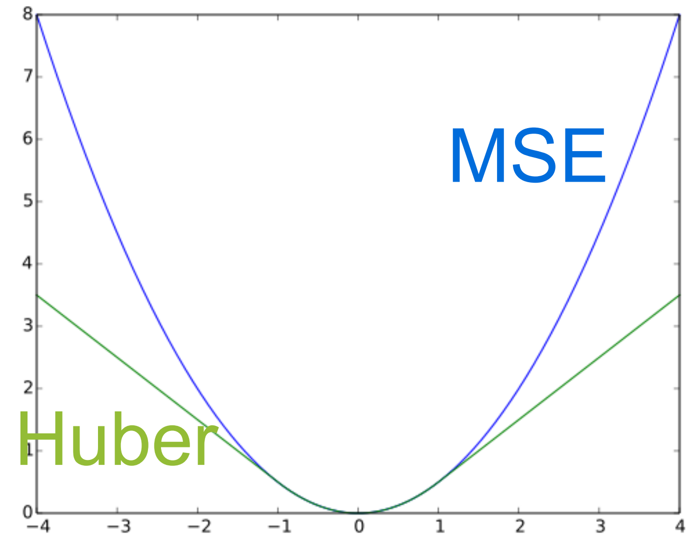
$$\ell(y, \hat{y}) = \sum_{k \neq y} \max(0, 1 - \hat{y}_y + \hat{y}_k)$$



Loss for Regression

- Continuous outcome

$$\mathcal{L}(\theta) = \frac{1}{N}\sum_{n=1}^{N} \ell(y_n, f(x_n))$$



- squared loss: $\ell(y, f) = \frac{1}{2} | f - y |_2^2$
- L1 loss: $\ell(y, f) = \frac{1}{2} | f - y |$
- Huber loss: $\ell(y, f) = \begin{cases} \frac{1}{2} | f - y |_2^2 & \text{if } | f - y |_2 \leq \delta \\ \delta(| f - y | - \frac{\delta}{2}) & \text{otherwise} \end{cases}$

Recap

- General framework to formulate a learning task is through empirical risk minimization (ERM)
- Minimizing cross-entropy is a realization of ERM

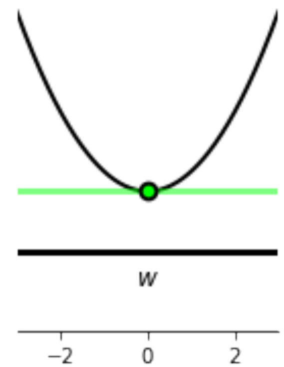
Learning the Model

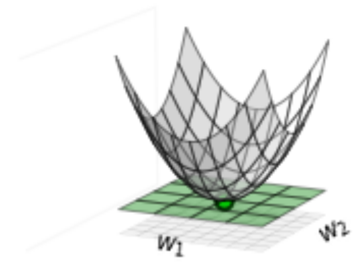
- Finding the parameter θ to minimize the empirical risk over training data
  $D = \{(x_n, y_n)\}_{n=1}^{N}$
  $$\hat{\theta} \leftarrow \arg\min_{\theta} L(\theta) = \frac{1}{N} \sum_{n} \ell(y_n, f(x_n; \theta))$$
- This is an instance of function optimization problem
  - Many algorithms exist (following lectures)

Optimization

- Consider a generic function minimization problem

$$\min_x f(x) \text{ where } f : \mathbb{R}^d \to \mathbb{R}$$





- Optimality condition:

$$\nabla f|_x = 0, \text{ where i-th element of } \nabla f|_x \text{ is } \frac{\partial f}{\partial x_i}$$

- Linear regression has closed-form solution
- In general, no closed-form solution for the equation.

Generic Iterative Algorithm

- Consider a generic function minimization problem, where x is unknown variable

$$\min_x f(x) \text{ where } f : \mathbb{R}^d \to \mathbb{R}$$

- Iterative update algorithm

$$x_{t+1} \leftarrow x_t + \Delta$$

- so that $f(x_{t+1}) \ll f(x_t)$
- How to find Δ

Taylor approximation

- $f(x+\Delta x) = f(x) + \Delta x^T \nabla f|_x + \frac{1}{2}\Delta x^T \nabla^2 f|_x \Delta x + \cdots$
- Theorem: if f is twice-differentiable and has continuous derivatives around x, for any small-enough Δx, there is $f(x+\Delta x) = f(x) + \Delta x^T \nabla f|_x + \frac{1}{2}\Delta x^T \nabla^2 f|_z \Delta x,$ where $\nabla^2 f|_z$ is the Hessian at z which lies on the line connecting x and $x + \Delta x$
- First-order and second-order Taylor approximation result in gradient descent and Newton's method

Gradient Descent

- $f(x_t + \Delta x) \approx f(x_t) + \Delta x^T \nabla f|_{x_t}$
- To make $\Delta x^T \nabla f|_{x_t}$ smallest
- $\Rightarrow \Delta x$ in the opposite direction of $\nabla f|_{x_t}$ i.e. $\Delta x = -\nabla f|_{x_t}$
- Update rule: $x_{t+1} = x_t - \eta \nabla f|_{x_t}$
- η is a hyper-parameter to control the learning rate

Gradient Descent Algorithm

```
learning rate eta.
1.set initial parameter θ ← θ_0
2.for epoch = 1 to maxEpoch or until
  converg:
3.  for each data (x, y) in D:
4.      compute error err(f(x; θ) - y)
5.      compute gradient g = ∂err(θ)/∂θ
6.      total_g += g
7.  update θ = θ - eta * total_g / N
```

learning rate eta.

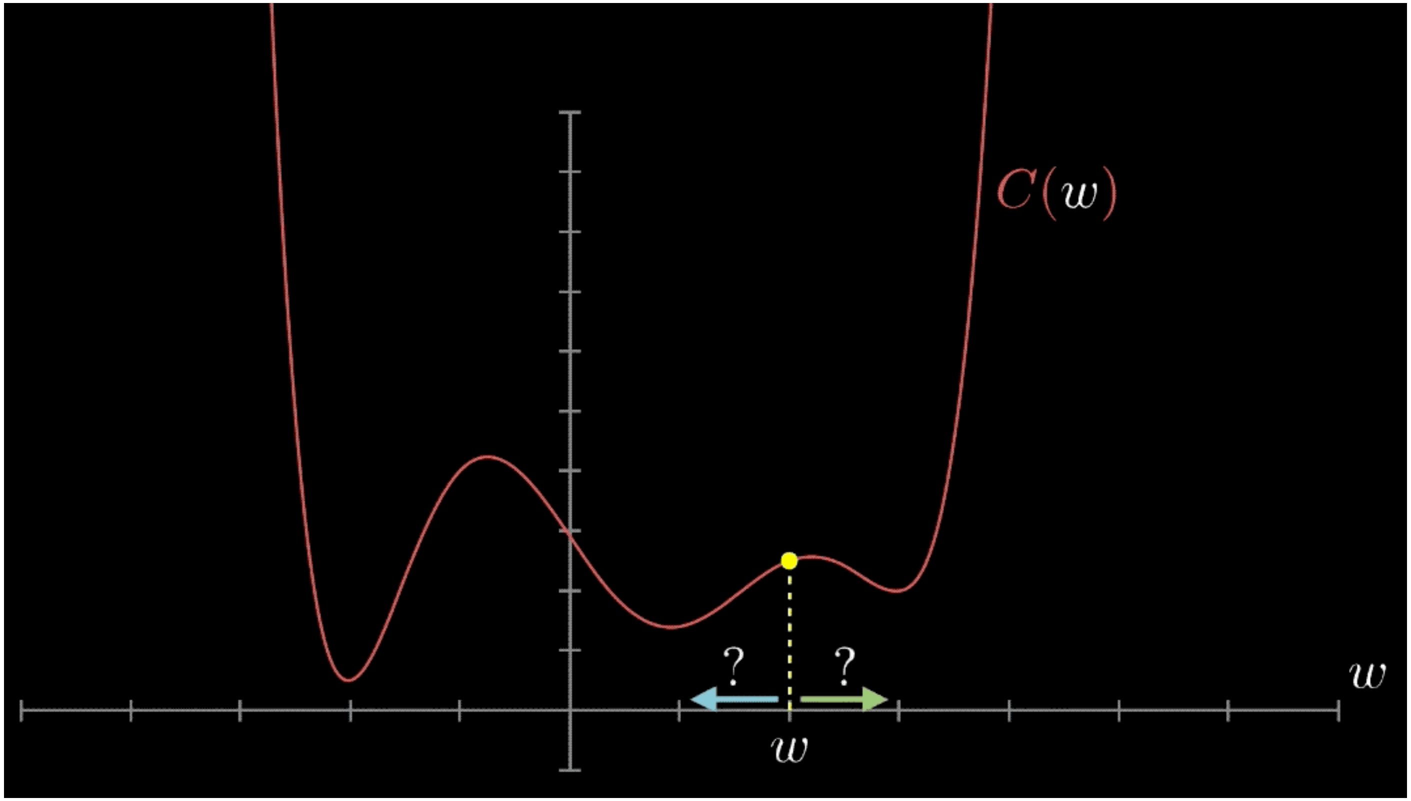
1. set initial parameter $\theta \leftarrow \theta_0$
2. for epoch = 1 to maxEpoch or until converg:
3. for each data (x, y) in D:
4. compute error err(f(x; θ) - y)
5. compute gradient $g = \dfrac{\partial \mathrm{err}(\theta)}{\partial \theta}$
6. total_g += g
7. update θ = θ - eta * total_g / N

Understand GD

- Surrogate function

$$\tilde{f}(x_t) = f(x_t) + \Delta x^T \nabla f|_{x_t} + \frac{1}{2}\|\Delta x\|_2^2$$

GD: Illustration



[credit: gif from 3blue1brown]

Does gradient descent guarantee finding the optimal solution?

- Depends
- Convex and smooth function: yes!
- Non-convex? local optimal

Recap

- First-order optimality condition: gradient=0
- Gradient descent is an iterative algorithm to update the parameter towards the opposite direction of gradient

Next Up

- Gradient calculation using Back-propagation
- More on optimization
- Generalization problem
- Regularization tricks