Classification

CISC 7026: Introduction to Deep Learning

University of Macau

Admin

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I am still grading quiz 2, but I had a look at the responses to question 4

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Some requests from students:

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1. More coding, less theory

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1. More coding, less theory
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3. Too easy, go faster

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4. Speak slower

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There are conflicting student needs

Admin

https://github.com/smorad/um_cisc_7026

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2. Torch optimization coding
3. Classification task
4. Probability review
5. Define model f
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Review

Last time, we reviewed derivatives

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$$f'(x) = \frac{d}{dx} f = \frac{df}{dx} = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}$$

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and gradients

$$\nabla_{\boldsymbol{x}} f\left(\begin{bmatrix} x_1 & x_2 & \dots & x_n \end{bmatrix}^\top\right) = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} & \dots & \frac{\partial f}{\partial x_n} \end{bmatrix}^\top$$

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Gradients are important in deep learning for two reasons:

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$$\textbf{Reason 1}: f(\boldsymbol{x}) \text{ has critical points at } \nabla_{\boldsymbol{x}} f(\boldsymbol{x}) = 0$$

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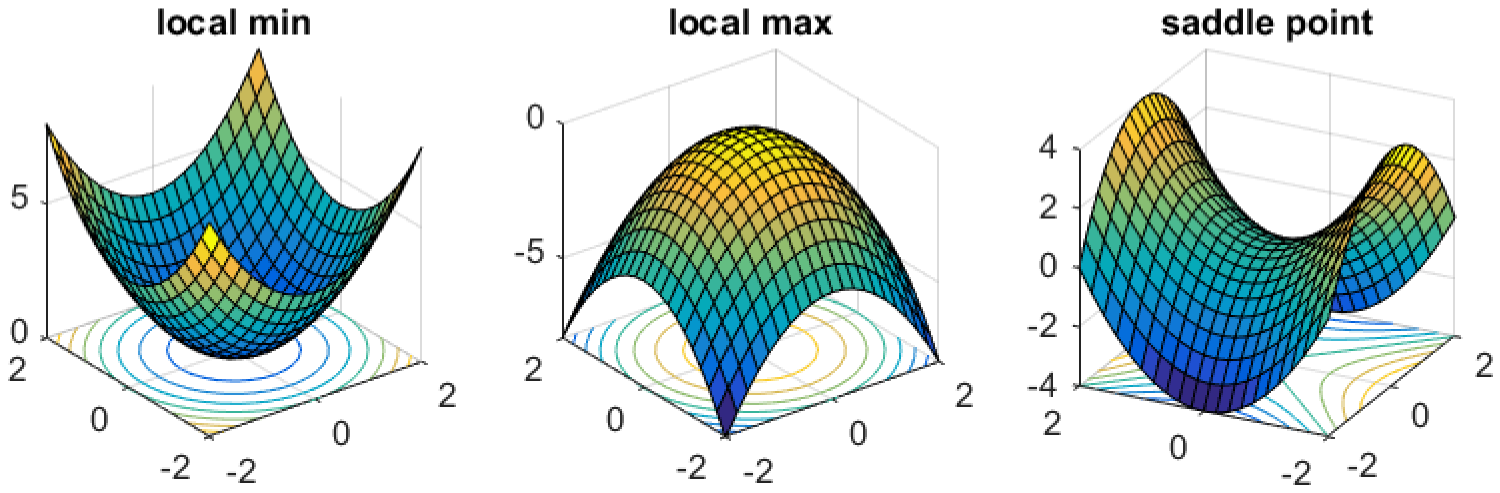

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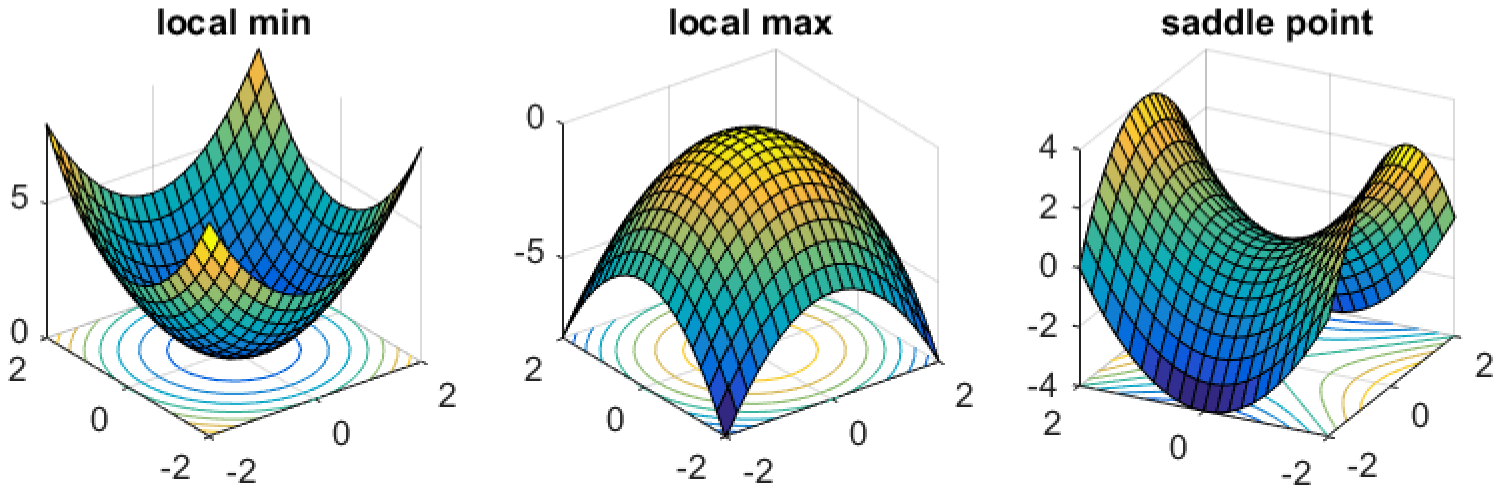

With optimization, we attempt to find minima of loss functions

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Reason 2: For problems without analytical solutions, the gradient (slope) is necessary for gradient descent

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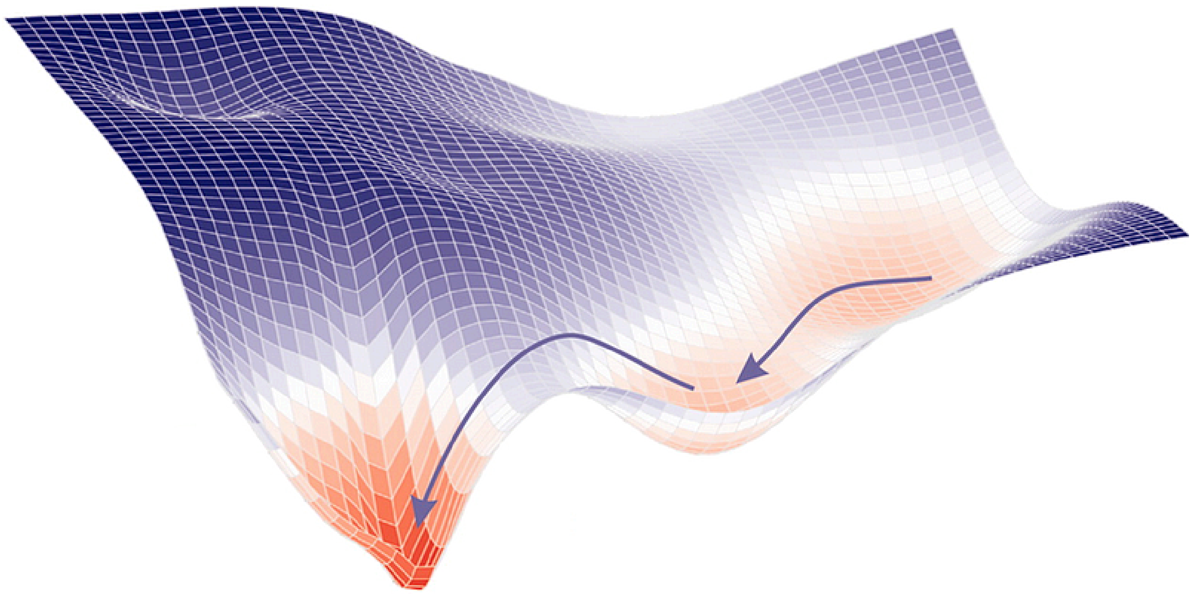

Review

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$$\mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta}) = \sum_{i=1}^{n} \left(f\left(\boldsymbol{x}_{[i]}, \boldsymbol{\theta}\right) - \boldsymbol{y}_{[i]} \right)^2$$

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$$\mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta}) = (\boldsymbol{Y} - \boldsymbol{X}_D \boldsymbol{\theta})^\top (\boldsymbol{Y} - \boldsymbol{X}_D \boldsymbol{\theta})$$

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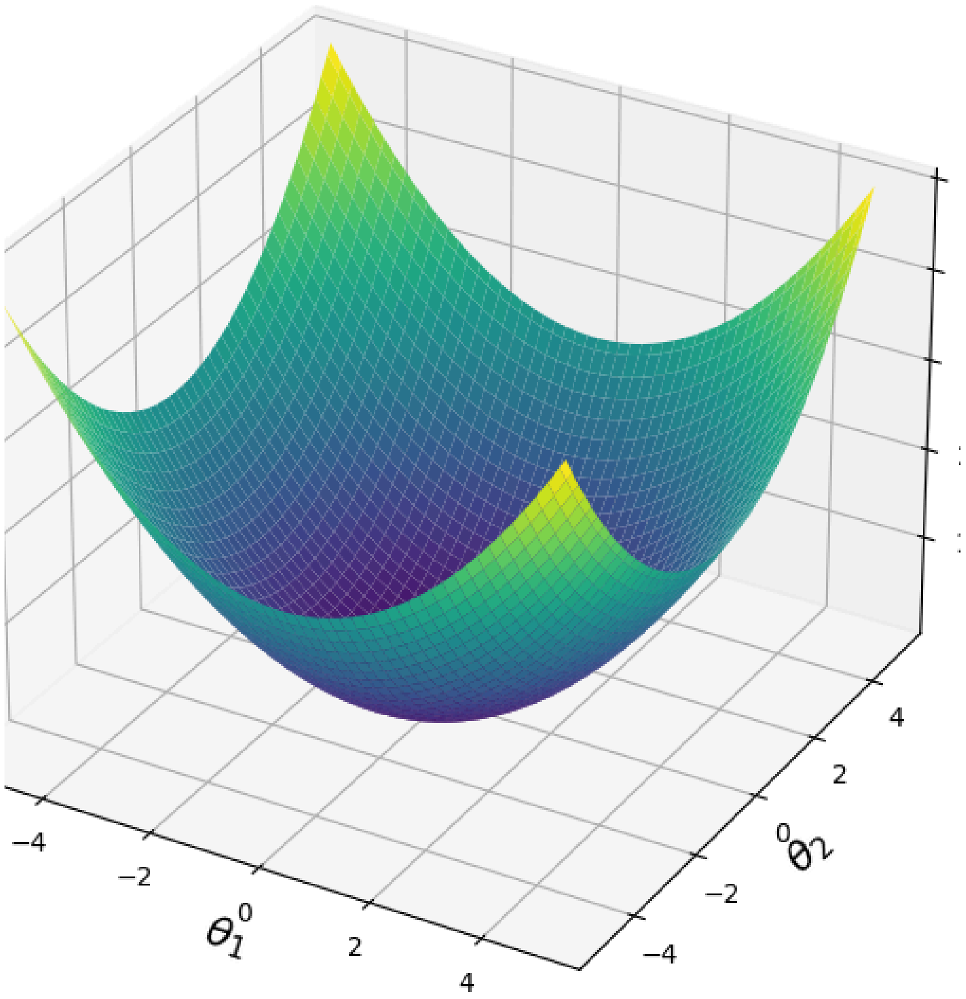
$$\mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta}) = \underbrace{\underbrace{(\boldsymbol{Y} - \boldsymbol{X}_D \boldsymbol{\theta})^\top}_{\text{Linear function of } \theta} \underbrace{(\boldsymbol{Y} - \boldsymbol{X}_D \boldsymbol{\theta})}_{\text{Linear function of } \theta}}_{\text{Quadratic function of } \theta}$$

Review

A quadratic function has a single critical point, which must be a global minimum



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We found the analytical solution for linear regression by finding where the gradient was zero and solving for $\boldsymbol{\theta}$

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Which solves

$$\arg \min_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$$

Review

For neural networks, the square error loss is no longer quadratic

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$$\mathcal{L}(x, y, \boldsymbol{\theta}) = (f(x, \boldsymbol{\theta}) - y)^2 \qquad \text{Loss function}$$

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$$\mathcal{L}(x, y, \boldsymbol{\theta}) = (f(x, \boldsymbol{\theta}) - y)^2$$ Loss function

$$f(x, \boldsymbol{\theta}) = \sigma(\theta_0 + \theta_1 x)$$ Neural network model

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$$\mathcal{L}(x, y, \boldsymbol{\theta}) = \underbrace{(\sigma(\theta_0 + \theta_1 x) - y)}_{\text{Nonlinear function of } \theta}\underbrace{(\sigma(\theta_0 + \theta_1 x) - y)}_{\text{Nonlinear function of } \theta}$$

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There is no analytical solution for $\boldsymbol{\theta}$

Review

Instead, we found the parameters of a neural network through gradient descent

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Gradient descent is an optimization method for differentiable functions

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Gradient descent is an optimization method for differentiable functions

We went over both the intuition and mathematical definitions

Review

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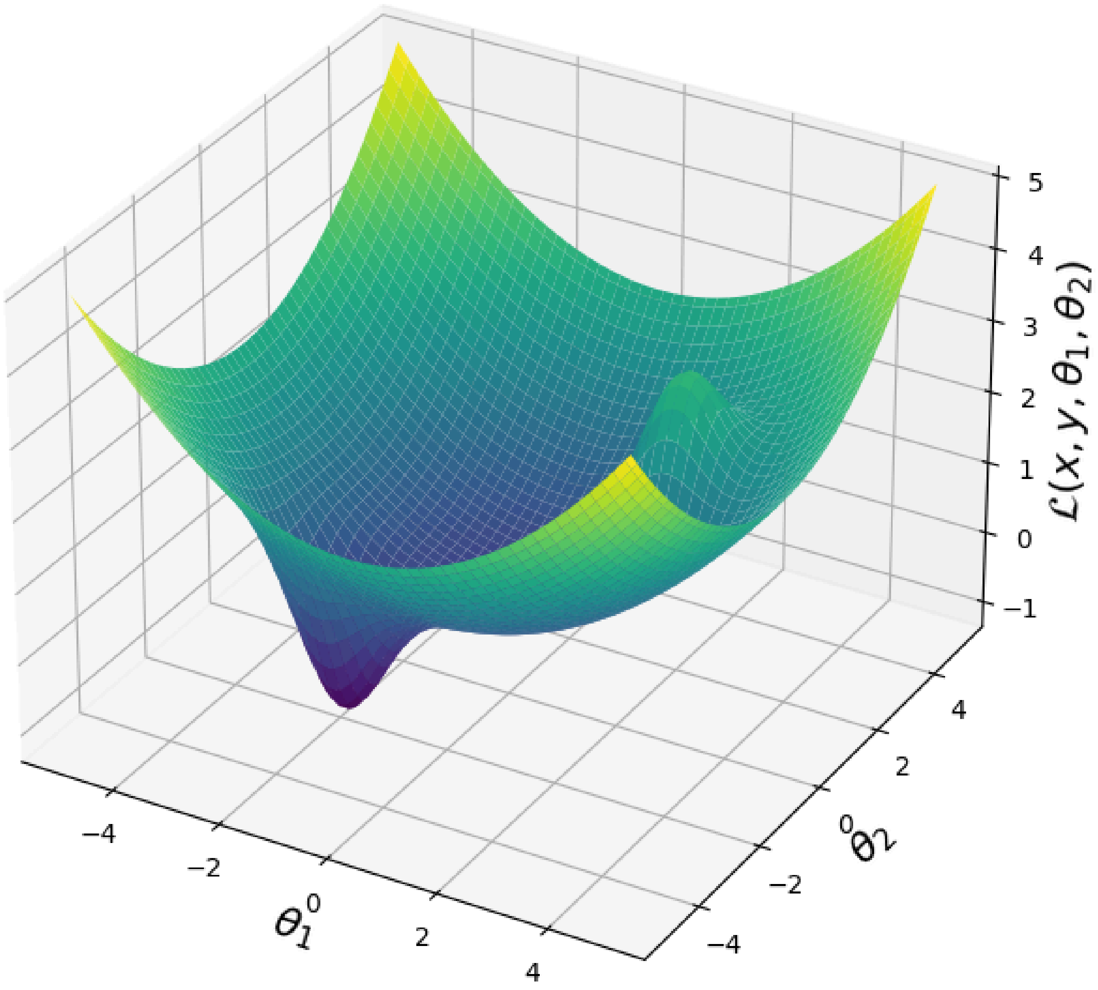

$\mathcal{L}(x, y, \theta_1, \theta_2)$
5
4
3
2
1
0
−1
θ_1
−4
−2
0
2
4
θ_2
4
2
0
−2
−4

Review

The gradient descent algorithm:

```
function GRADIENT DESCENT(X, Y, ℒ, t, α)
    ▷ Randomly initialize parameters
    θ ← 𝒩(0, 1)
    for i ∈ 1...t do
        ▷ Compute the gradient of the loss
        J ← ∇_θ ℒ(X, Y, θ)
        ▷ Update the parameters using the negative gradient
        θ ← θ − αJ
    return θ
```

$$\textbf{function}\ \textsc{Gradient Descent}(\boldsymbol{X}, \boldsymbol{Y}, \mathcal{L}, t, \alpha)$$

$$\boldsymbol{\theta} \leftarrow \mathcal{N}(0, 1)$$

$$\boldsymbol{J} \leftarrow \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$$

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \boldsymbol{J}$$

Review

We derived the $\nabla_{\boldsymbol{\theta}} \mathcal{L}$ for deep neural networks using the chain rule

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$$\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta}) = \sum_{i=1}^{n} 2\left(f\left(\boldsymbol{x}_{[i]}, \boldsymbol{\theta}\right) - \boldsymbol{y}_{[i]}\right) \color{red}{\nabla_{\boldsymbol{\theta}} f\left(\boldsymbol{x}_{[i]}, \boldsymbol{\theta}\right)}$$

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$$\nabla_{\boldsymbol{\theta}} f(\boldsymbol{x}, \boldsymbol{\theta}) = \nabla_{\boldsymbol{\varphi}, \boldsymbol{\psi}, \ldots, \boldsymbol{\xi}} f\left(\boldsymbol{x}, [\boldsymbol{\varphi} \ \ \boldsymbol{\psi} \ \ \ldots \ \ \boldsymbol{\xi}]^\top\right) = \begin{bmatrix} \nabla_{\boldsymbol{\varphi}} f_1(\boldsymbol{x}, \boldsymbol{\varphi}) \\ \nabla_{\boldsymbol{\psi}} f_2(\boldsymbol{z}_1, \boldsymbol{\psi}) \\ \vdots \\ \nabla_{\boldsymbol{\xi}} f_\ell(\boldsymbol{z}_{\ell-1}, \boldsymbol{\xi}) \end{bmatrix}$$

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$$\nabla_{\boldsymbol{\theta}} f(\boldsymbol{x}, \boldsymbol{\theta}) = \nabla_{\boldsymbol{\varphi}, \boldsymbol{\psi}, \ldots, \boldsymbol{\xi}} f\left(\boldsymbol{x}, \begin{bmatrix} \boldsymbol{\varphi} & \boldsymbol{\psi} & \ldots & \boldsymbol{\xi} \end{bmatrix}^\top\right) = \begin{bmatrix} \nabla_{\boldsymbol{\varphi}} f_1(\boldsymbol{x}, \boldsymbol{\varphi}) \\ \nabla_{\boldsymbol{\psi}} f_2(\boldsymbol{z}_1, \boldsymbol{\psi}) \\ \vdots \\ \nabla_{\boldsymbol{\xi}} f_\ell(\boldsymbol{z}_{\ell-1}, \boldsymbol{\xi}) \end{bmatrix}$$

$$\nabla_{\boldsymbol{\xi}} f_\ell(\boldsymbol{z}_{\ell-1}, \boldsymbol{\xi}) = \left(\sigma\left(\boldsymbol{\xi}^\top \overline{\boldsymbol{z}}_{\ell-1}\right) \odot \left(1 - \sigma\left(\boldsymbol{\xi}^\top \overline{\boldsymbol{z}}_{\ell-1}\right)\right)\right) \overline{\boldsymbol{z}}_{\ell-1}^\top$$

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We ran into issues computing the gradient of a layer because of the Heaviside step function

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We replaced it with a differentiable (soft) approximation called the sigmoid function

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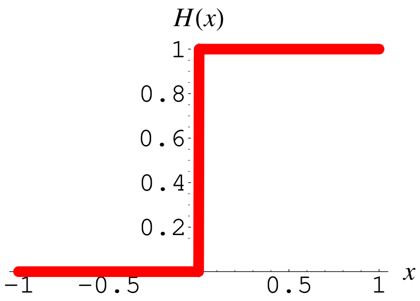

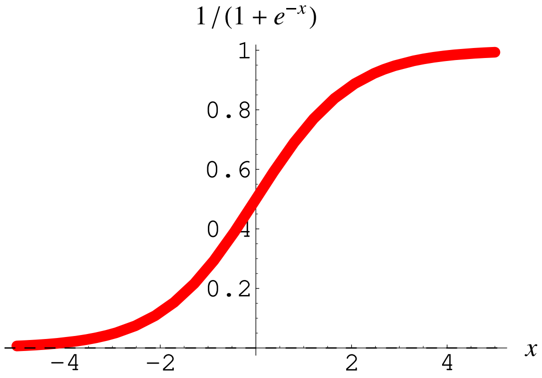

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

Review

In `jax`, we compute the gradient using the `jax.grad` function

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```
import jax

def L(theta, X, Y):
   ...

# Create a new function that is the gradient of L
# Then compute gradient of L for given inputs
J = jax.grad(L)(X, Y, theta)
# Update parameters
alpha = 0.0001
theta = theta - alpha * J
```

Review

In `torch`, we backpropagate through a graph of operations

```
import torch
optimizer = torch.optim.SGD(lr=0.0001)

def L(model, X, Y):
  ...
# Pytorch will record a graph of all operations
# Everytime you do theta @ x, it stores inputs and outputs
loss = L(X, Y, model) # compute loss
# Traverse the graph backward and compute the gradient
loss.backward() # Sets .grad attribute on each parameter
optimizer.step() # Update the parameters using .grad
optimizer.zero_grad() # Set .grad to zero, DO NOT FORGET!!
```

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2. Torch optimization coding
3. Classification task
4. Probability review
5. Define model f
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8. Coding

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First, a video of one application of gradient descent

https://youtu.be/kGDO2e_qiyI?si=ZopZKy-6WQ4B0csX

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Time for some interactive coding

https://colab.research.google.com/drive/1W8WVZ8n_9yJCcOqkPVURp_wJUx3EQc5w

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So far, we only looked at regression. Now, let us look at classification

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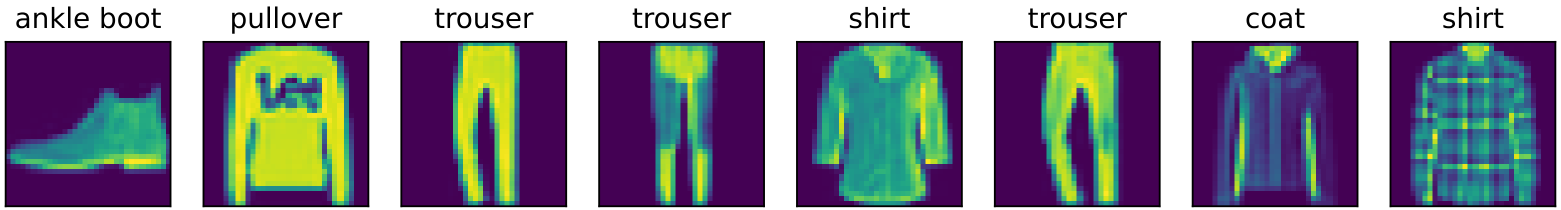
$X : \mathbb{Z}_{0,255}^{32 \times 32}$



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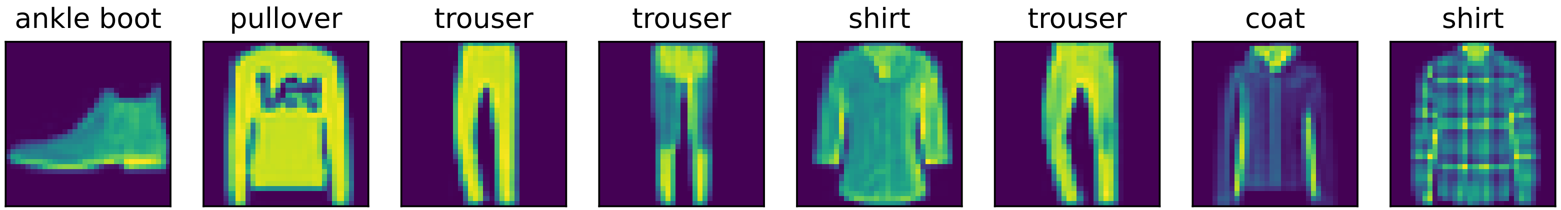

Y : {T-shirt, Trouser, Pullover, Dress, Coat, Sandal, Shirt, Sneaker, Bag, Ankle boot}

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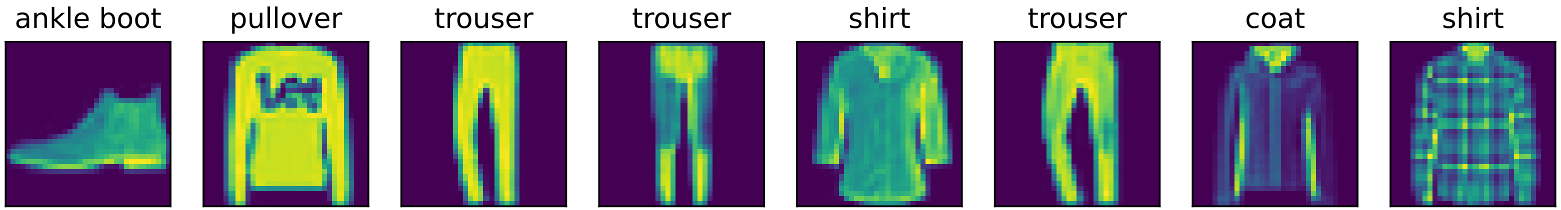

$Y : \{\text{T-shirt, Trouser, Pullover, Dress, Coat,}$
$\text{Sandal, Shirt, Sneaker, Bag, Ankle boot}\}$

Approach: Learn $\boldsymbol{\theta}$ that produce **conditional probabilities**

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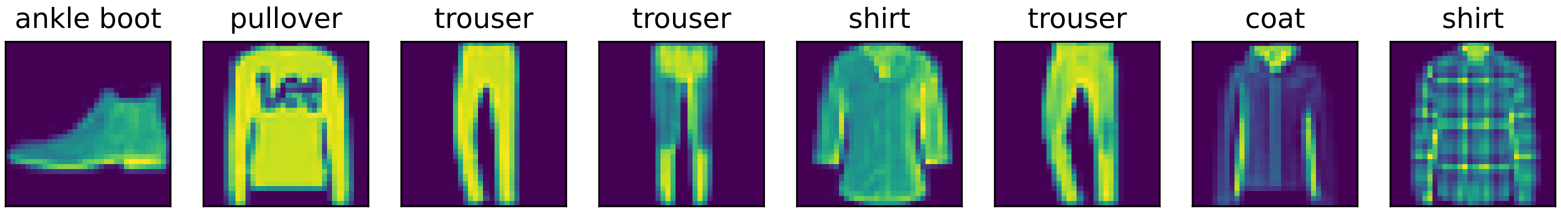

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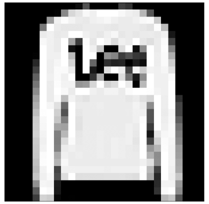
Sandal, Shirt, Sneaker, Bag, Ankle boot}

Approach: Learn $\boldsymbol{\theta}$ that produce **conditional probabilities**

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = P(\boldsymbol{y} \mid \boldsymbol{x}) = P\left(\begin{bmatrix} \text{T-Shirt} \\ \text{Trouser} \\ \vdots \end{bmatrix} \middle| \right.$$



$$\left. \right) = \begin{bmatrix} 0.2 \\ 0.01 \\ \vdots \end{bmatrix}$$

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Experiment	Outcome

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Experiment	Outcome
Flip a coin	Heads

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Experiment	Outcome
Flip a coin	Heads
Walk outside	Rain

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Experiment	Outcome
Flip a coin	Heads
Walk outside	Rain
Grab clothing from closest	Coat

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An experiment yields one of many possible outcomes

Experiment	Outcome
Flip a coin	Heads
Walk outside	Rain
Grab clothing from closest	Coat

The **sample space** S defines all possible outcomes for an experiment

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Flip a coin	$S = \{\text{heads}, \text{tails}\}$
Walk outside	$S = \{\text{rain}, \text{sun}, \text{wind}, \text{cloud}\}$
Take clothing from closet	$S = \{\text{T-shirt}, \text{Trouser}, \text{Pullover}, \text{Dress}, \text{Coat}, \text{Sandal}, \text{Shirt}, \text{Sneaker}, \text{Bag}, \text{Ankle boot}\}$

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Take from closet	$\{\text{T-shirt}, \text{Trouser}, \text{Pullover}, \text{Dress}, \text{Coat}, \text{Sandal}, \text{Shirt}, \text{Sneaker}, \text{Bag}, \text{Ankle boot}\}$	$E = \{\text{Shirt}, \text{T-Shirt}, \text{Coat}\}$

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Experiment Probabilities

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Experiment	Probabilities
Flip a coin	$P(\text{heads}) = 0.5$
Walk outside	$P(\text{rain}) = 0.15$
Take from closet	$P(\text{Shirt}) = 0.1$

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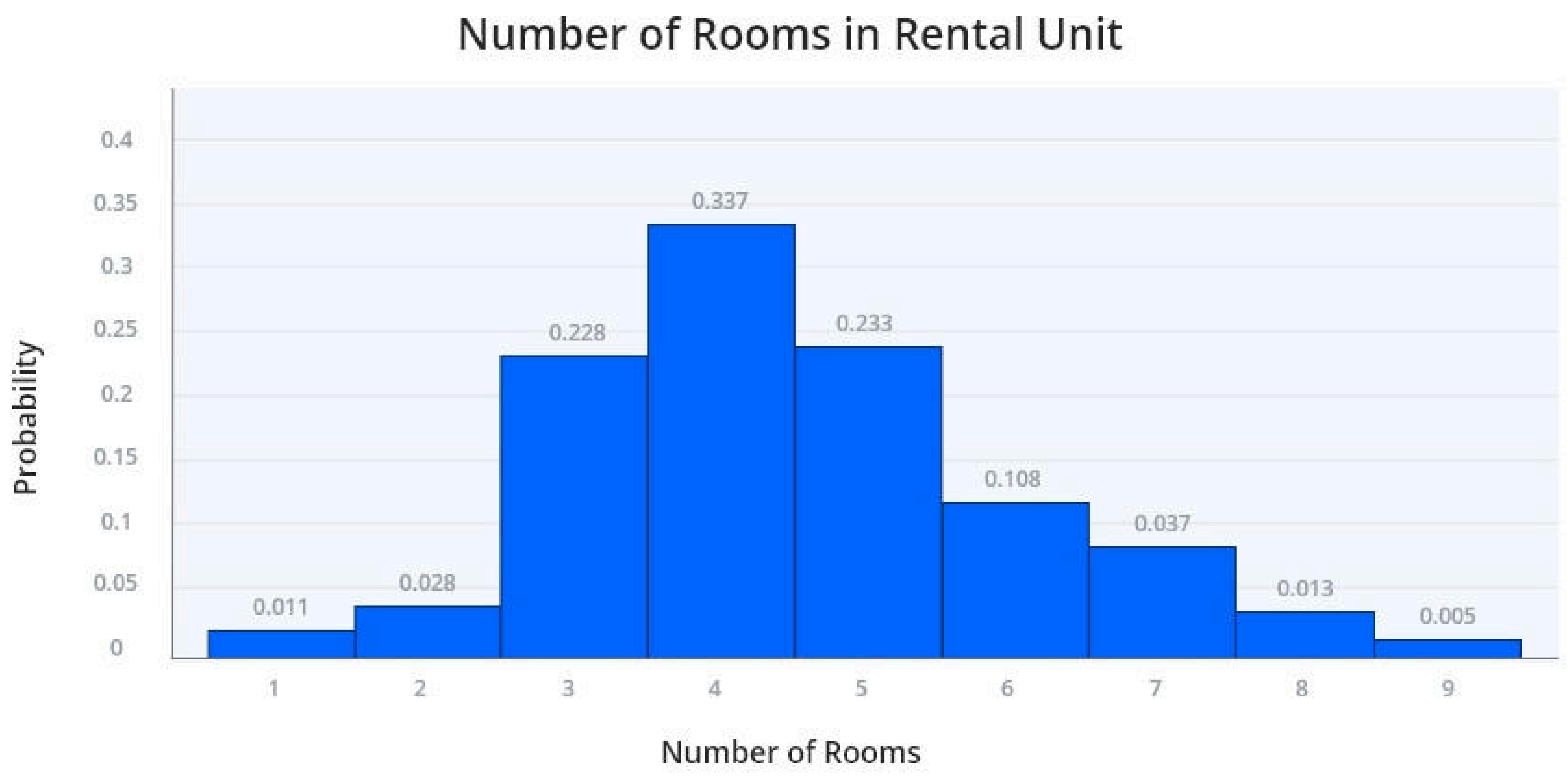
Flip a coin $$\{P(\text{heads}) = 0.5, P(\text{tails}) = 0.5\}$$

Take clothing from closet $$\{P(\text{T-shirt}) = 0.1, P(\text{Trouser}) = 0.08, P(\text{Pullover}) = 0.12, ...\}$$

The distribution is a function, so we can plot it


Number of Rooms in Rental Unit
Probability
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0.011
0.028
0.228
0.337
0.233
0.108
0.037
0.013
0.005
1
2
3
4
5
6
7
8
9
Number of Rooms

Events can overlap with each other

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- Disjoint events

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- Conditionally dependent events

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$$P(\text{Heads}) = 0.5, P(\text{Tails}) = 0.5$$
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Be careful!

Walk outside

$$P(\text{Rain}) = 0.05, P(\text{Sun}) = 0.4$$
$$P(\text{Rain} \cap \text{Sun}) \neq 0$$

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$$P(\text{Rain} \cap \text{Cloud}) = 0.2$$

Walk outside

$$P(\text{Cloud}) = 0.4$$

$$P(\text{Rain} \mid \text{Cloud}) = \frac{0.2}{0.4} = 0.5$$

Task: Given a picture of clothes, predict the text description

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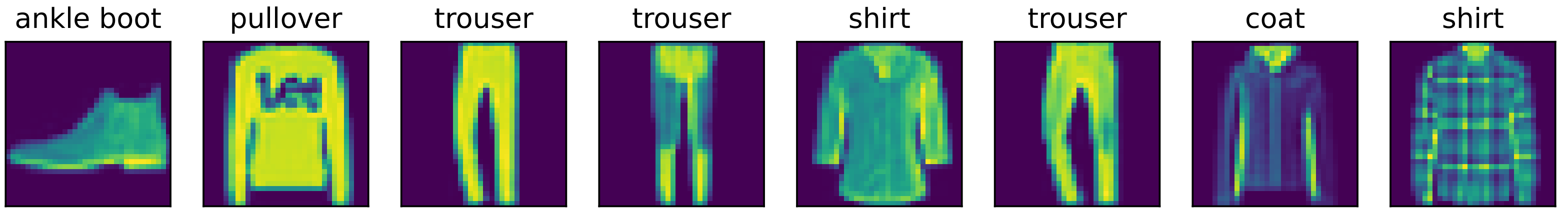
$X : \mathbb{Z}_{0,255}^{32 \times 32}$



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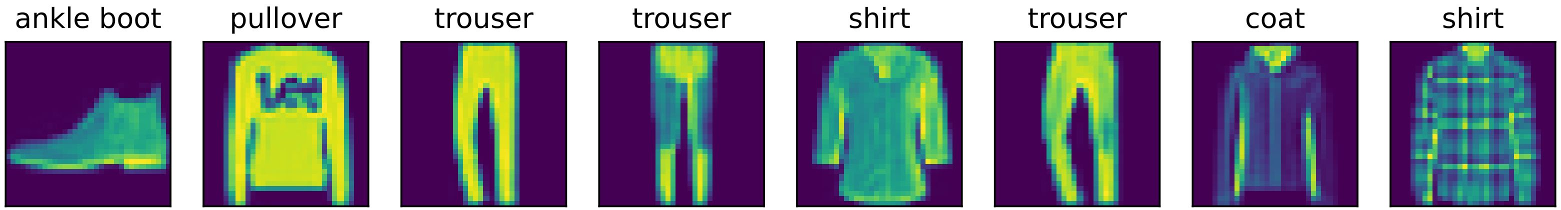
$X : \mathbb{Z}_{0,255}^{32 \times 32}$ 

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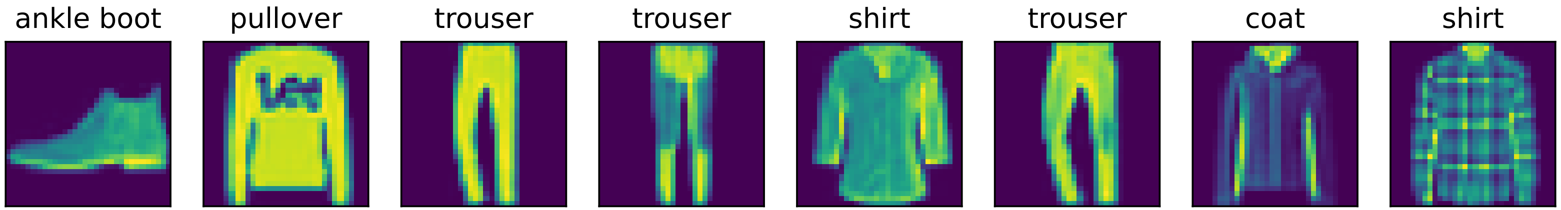

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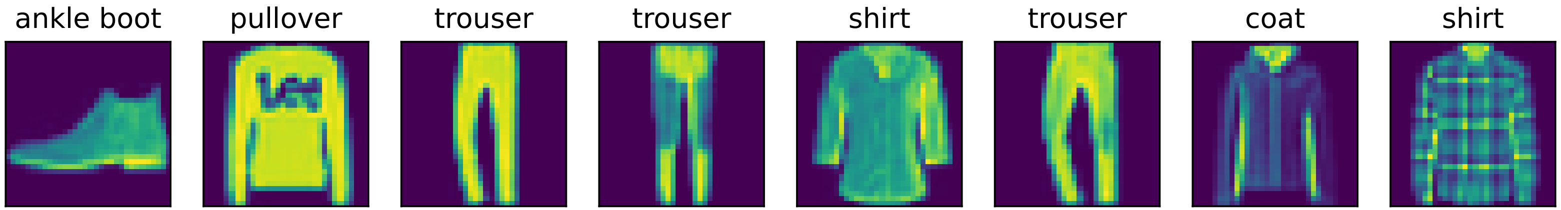

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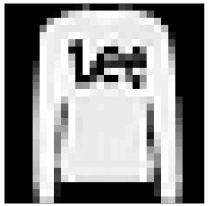
$$f(\boldsymbol{x}, \boldsymbol{\theta}) = P(\boldsymbol{y} \mid \boldsymbol{x}) = P\left(\begin{bmatrix} \text{T-Shirt} \\ \text{Trouser} \\ \vdots \end{bmatrix} \middle| \right.$$



$$\left. \right) = \begin{bmatrix} 0.2 \\ 0.01 \\ \vdots \end{bmatrix}$$

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1. Review
2. Torch optimization coding
3. Classification task
4. **Probability review**
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Answer: No! Because probabilities must sum to one

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$$\boldsymbol{v} = \left\{ \begin{bmatrix} v_1 \\ \vdots \\ v_{d_y} \end{bmatrix} \middle| \quad \sum_{i=1}^{d_y} v_i = 1 \right\}$$

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$$\Delta^{d_y - 1}$$

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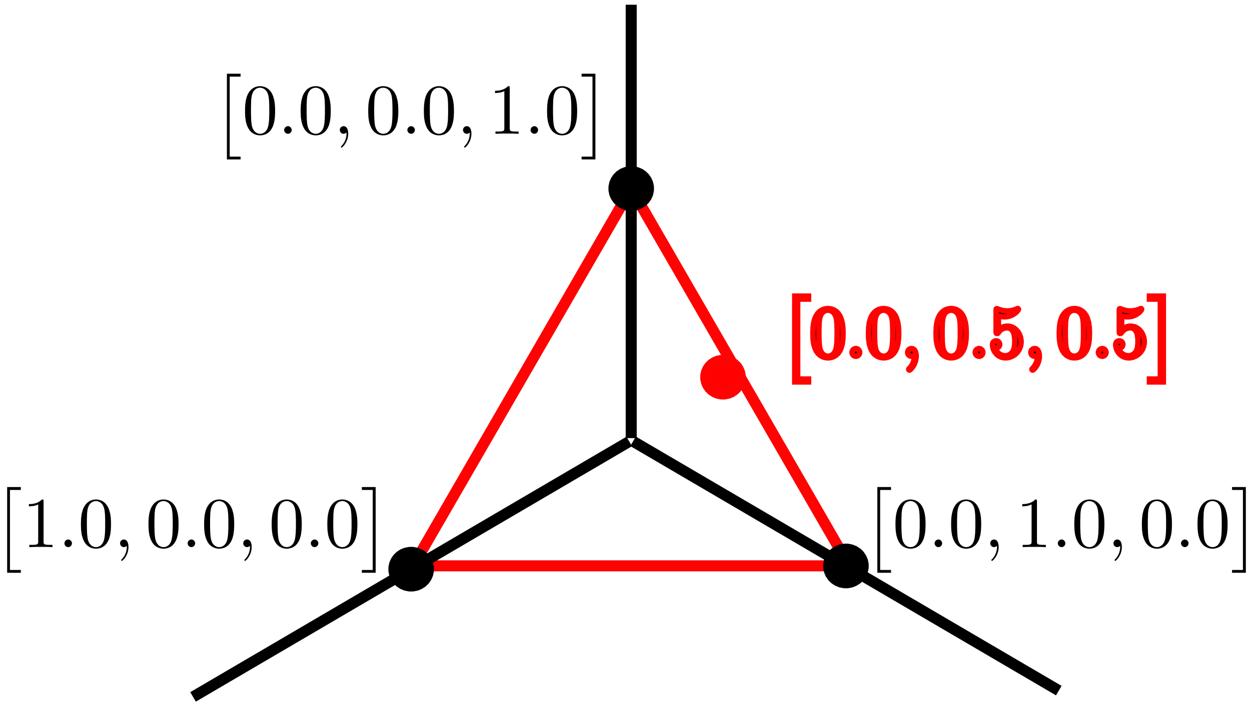

It has only $k-1$ free variables, because $x_k = 1 - \sum_{i=1}^{k-1} x_i$

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In deep learning we often use the **softmax** function. When combined with the classification loss the gradient is linear, making learning faster

The softmax function maps real numbers to the simplex (probabilities)

$$\text{softmax} : \mathbb{R}^k \mapsto \Delta^{k-1}$$

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$$\text{softmax}\left(\begin{bmatrix} x_1 \\ \vdots \\ x_k \end{bmatrix} \right) = \frac{e^{\boldsymbol{x}}}{\sum_{i=1}^{k} e^{x_i}} = \begin{bmatrix} \frac{e^{x_1}}{e^{x_1} + e^{x_2} + \ldots e^{x_k}} \\ \frac{e^{x_2}}{e^{x_1} + e^{x_2} + \ldots e^{x_k}} \\ \vdots \\ \frac{e^{x_k}}{e^{x_1} + e^{x_2} + \ldots e^{x_k}} \end{bmatrix}$$

If we attach it to our linear model, we can output probabilities!

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \text{softmax}(\boldsymbol{\theta}^\top \boldsymbol{x})$$

And naturally, we can use the same method for a deep neural network

$$f_1(\boldsymbol{x}, \boldsymbol{\varphi}) = \sigma(\boldsymbol{\varphi}^\top \boldsymbol{x})$$

$$\vdots$$

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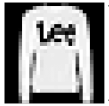
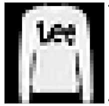
Now, our neural network can output probabilities

$f(\boldsymbol{x}, \boldsymbol{\theta}) =$

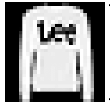
$P\Big(\text{Ankle boot} \mid$  $\Big)$

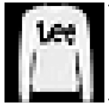
$P\Big(\text{Bag} \mid$  $\Big)$

$\vdots$

Question: Why do we output probabilities instead of a binary values

$f(\boldsymbol{x}, \boldsymbol{\theta}) =$

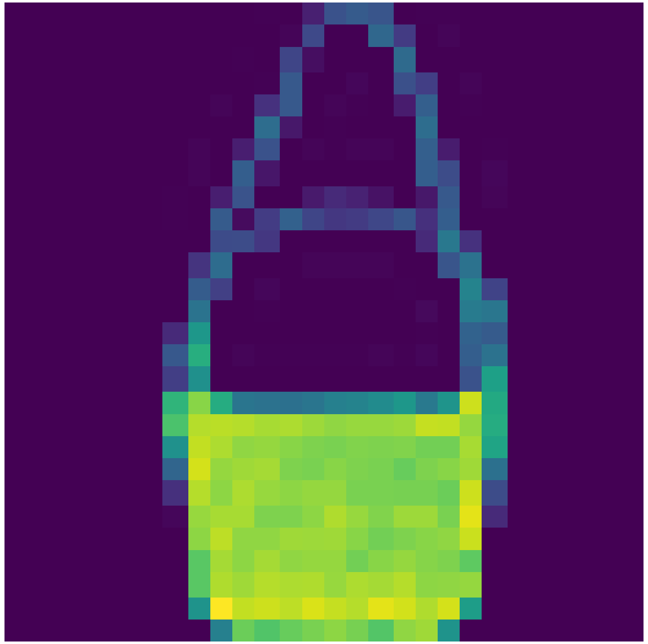
$P(\text{Shirt} \mid$  $)$

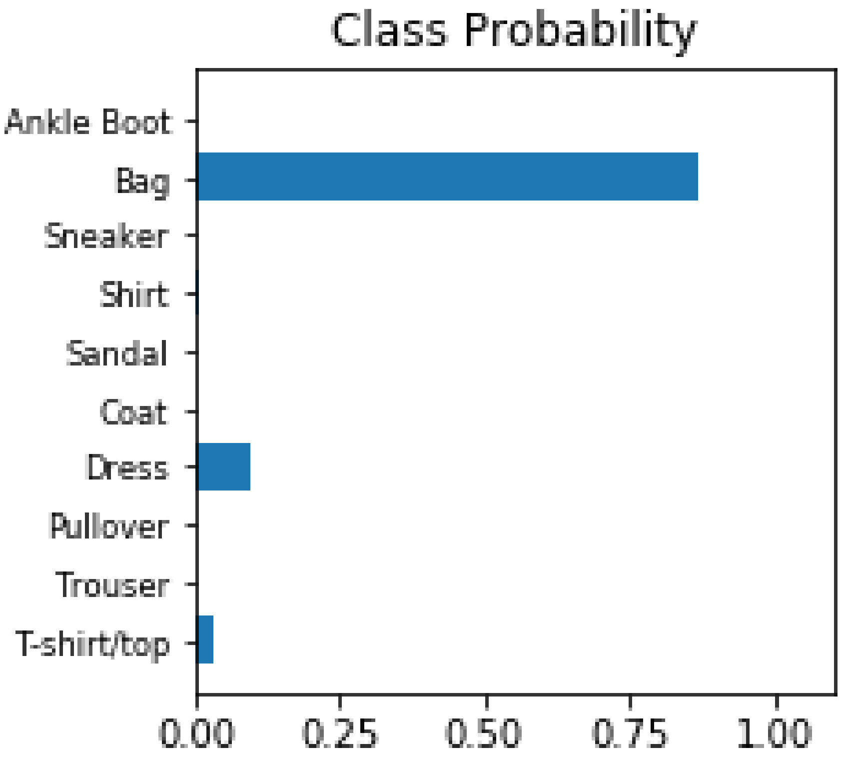
$P(\text{Bag} \mid$  $)$

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Answer 1: Outputting probabilities results in differentiable functions

Answer 2: We report uncertainty, which is useful in many applications




Class Probability
Ankle Boot
Bag
Sneaker
Shirt
Sandal
Coat
Dress
Pullover
Trouser
T-shirt/top
0.00
0.25
0.50
0.75
1.00

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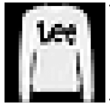
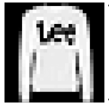
Consider the following prediction and truth

$$f\left(\boldsymbol{x}_{[i]}, \boldsymbol{\theta}\right) = \begin{bmatrix} P\left(\text{Shirt} \mid \quad \right) \\ P\left(\text{Bag} \mid \quad \right) \end{bmatrix} = \begin{bmatrix} 0.6 \\ 0.4 \end{bmatrix}$$





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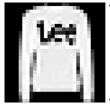
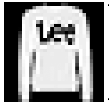
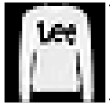
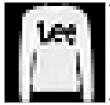



$$\boldsymbol{y}_{[i]} = \begin{bmatrix} P\left(\text{Shirt} \mid \quad \right) \\ P\left(\text{Bag} \mid \quad \right) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

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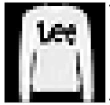
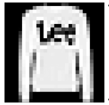
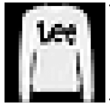
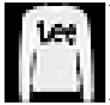
$f(\boldsymbol{x}_{[i]}, \boldsymbol{\theta}) = \Big[$ $P(\text{Shirt} \mid$  $)$; $P(\text{Bag} \mid$  $)$ $\Big] = \begin{bmatrix} 0.6 \\ 0.4 \end{bmatrix}$

$\boldsymbol{y}_{[i]} = \Big[$ $P(\text{Shirt} \mid$  $)$; $P(\text{Bag} \mid$  $)$ $\Big] = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

What loss function should we use for classification?

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Instead, we use the **cross-entropy loss**

$$f(\boldsymbol{x}_i, \boldsymbol{\theta}) = \begin{bmatrix} 0.6 \\ 0.4 \end{bmatrix}, \boldsymbol{y}_i = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

We could use the square error like linear regression

$$(0.6 - 1)^2 + (0.4 - 0)^2$$

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Let us derive it

We can model $f(\boldsymbol{x}, \boldsymbol{\theta})$ and $\boldsymbol{y}$ as probability distributions

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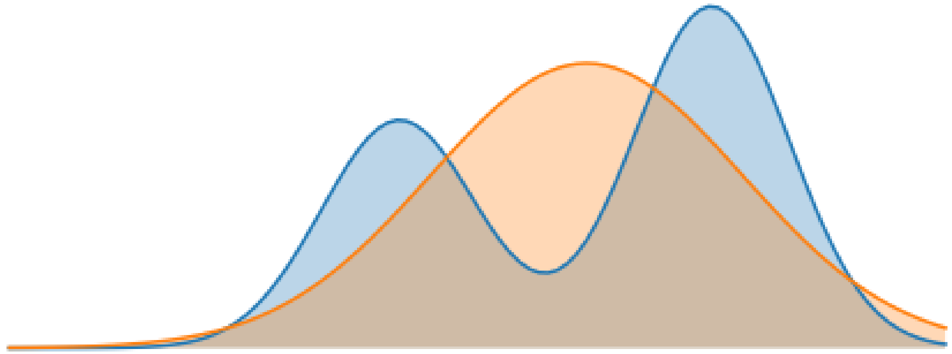

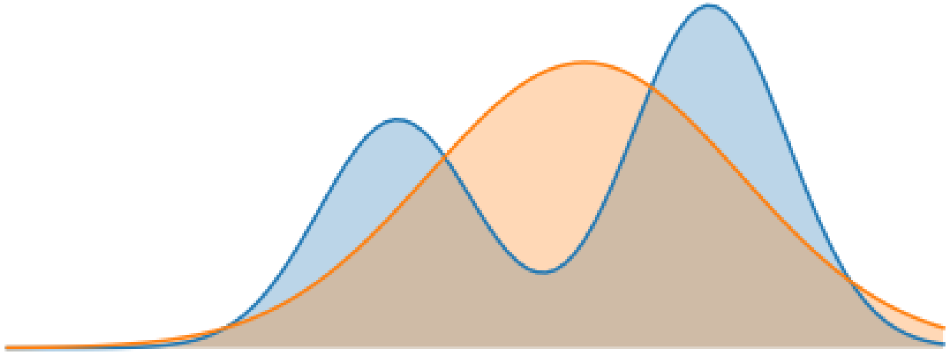

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Plug in our two distributions $P = f$ and $Q = \boldsymbol{y}$

$$\mathrm{KL}(P(\boldsymbol{y} \mid \boldsymbol{x}), f(\boldsymbol{x}, \boldsymbol{\theta})) = \sum_{i=1}^{d_y} P(y_i \mid \boldsymbol{x}) \log \frac{P(y_i \mid \boldsymbol{x})}{f(\boldsymbol{x}, \boldsymbol{\theta})_i}$$

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Rewrite the logarithm using the sum rule of logarithms

$$\mathrm{KL}(P(\boldsymbol{y} \mid \boldsymbol{x}), f(\boldsymbol{x}, \boldsymbol{\theta})) = \sum_{i=1}^{d_y} P(y_i \mid \boldsymbol{x}) \left(\log P(y_i \mid \boldsymbol{x}) - \log f(\boldsymbol{x}, \boldsymbol{\theta})_i\right)$$

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Split the sum into two parts

$$= \sum_{i=1}^{d_y} P(y_i \mid \boldsymbol{x}) \log P(y_i \mid \boldsymbol{x}) - \sum_{i=1}^{d_y} P(y_i \mid \boldsymbol{x}) \log f(\boldsymbol{x}, \boldsymbol{\theta})_i$$

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The first term is constant, and we will minimize the loss. So $\arg\min_{\boldsymbol{\theta}} \mathcal{L} + k = \arg\min_{\boldsymbol{\theta}} \mathcal{L}$. Therefore, we can ignore the first term.

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This is the loss for a classification task! We call this the **cross-entropy** loss function

$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\theta}) = -\sum_{i=1}^{d_y} P(y_i \mid \boldsymbol{x}) \log f(\boldsymbol{x}, \boldsymbol{\theta})_i$$

By minimizing the loss, we make $f(\boldsymbol{x}, \boldsymbol{\theta}) = \boldsymbol{y}$

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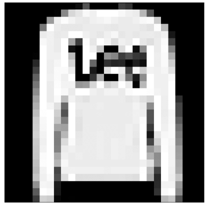
$$f(\boldsymbol{x}, \boldsymbol{\theta}) = P(\boldsymbol{y} \mid \boldsymbol{x}) = P\left(\begin{bmatrix} \text{boot} \\ \text{dress} \\ \vdots \end{bmatrix} \middle| \right.$$  $$\left. \right)$$

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2. Torch optimization coding
3. Classification task
4. Probability review
5. Define model f
6. **Define loss function $\mathcal{L}$**
7. Find $\boldsymbol{\theta}$ that minimize $\mathcal{L}$
8. Coding

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$$\nabla_{\boldsymbol{\theta}} \operatorname{softmax}(\boldsymbol{z}) = \operatorname{softmax}(\boldsymbol{z}) \odot (1 - \operatorname{softmax}(\boldsymbol{z}))$$

This is because softmax is a multi-class generalization of the sigmoid function

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The rest of this course will examine neural network architectures

Classification