Classification

CISC 7026: Introduction to Deep Learning

University of Macau

Admin

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Assignment 1 grades were released on moodle

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The scores were very good, with a mean of approximately 90/100

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

Admin

Some requests from students:

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1. More coding, less theory

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3. Too easy, go faster

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There are conflicting student needs

Admin

https://github.com/smorad/um_cisc_7026

Agenda

1. Review
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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Review

Last time, we reviewed derivatives

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

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and gradients

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

Review

Gradients are important in deep learning for two reasons:

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

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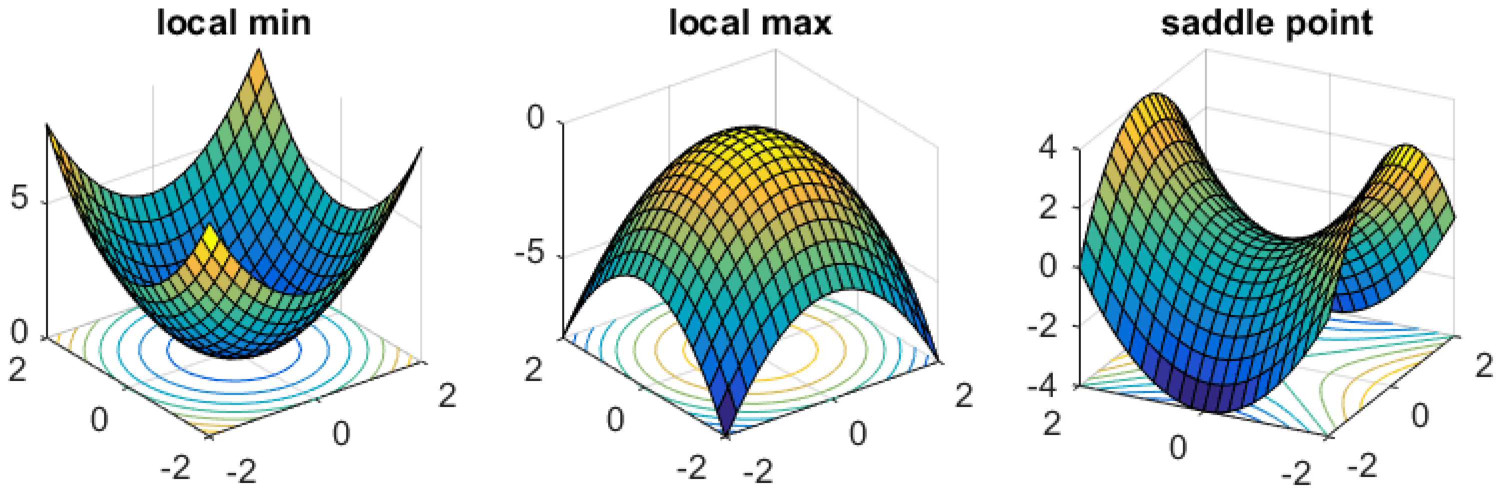

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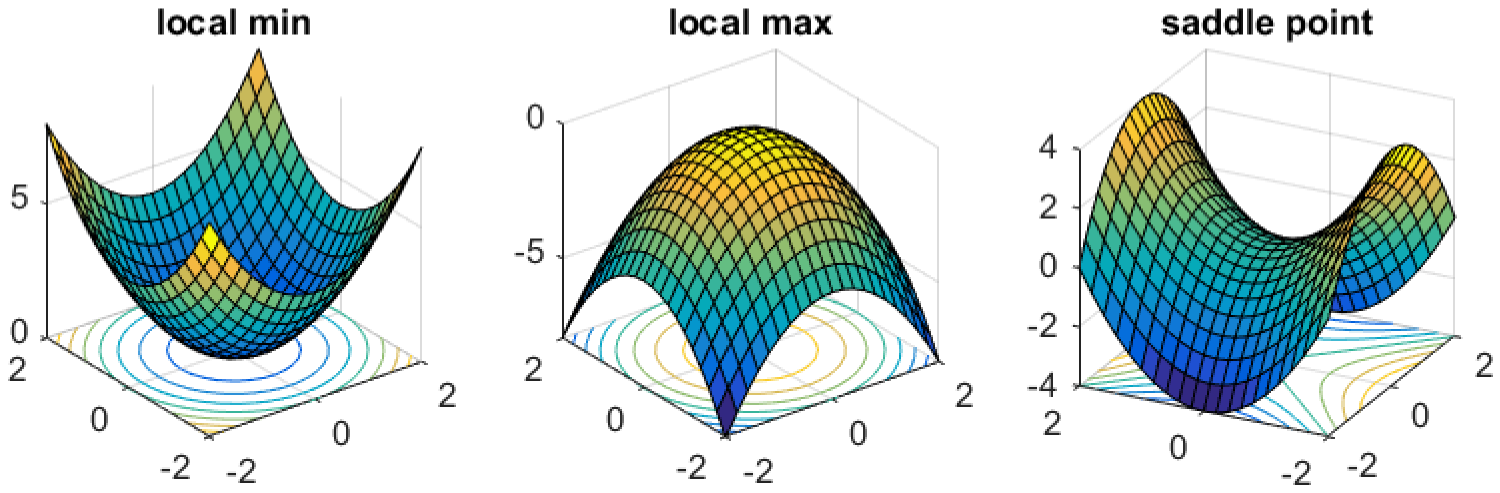
Reason 1: $f(\boldsymbol{x})$ has critical points at $\nabla_{\boldsymbol{x}} f(\boldsymbol{x}) = 0$



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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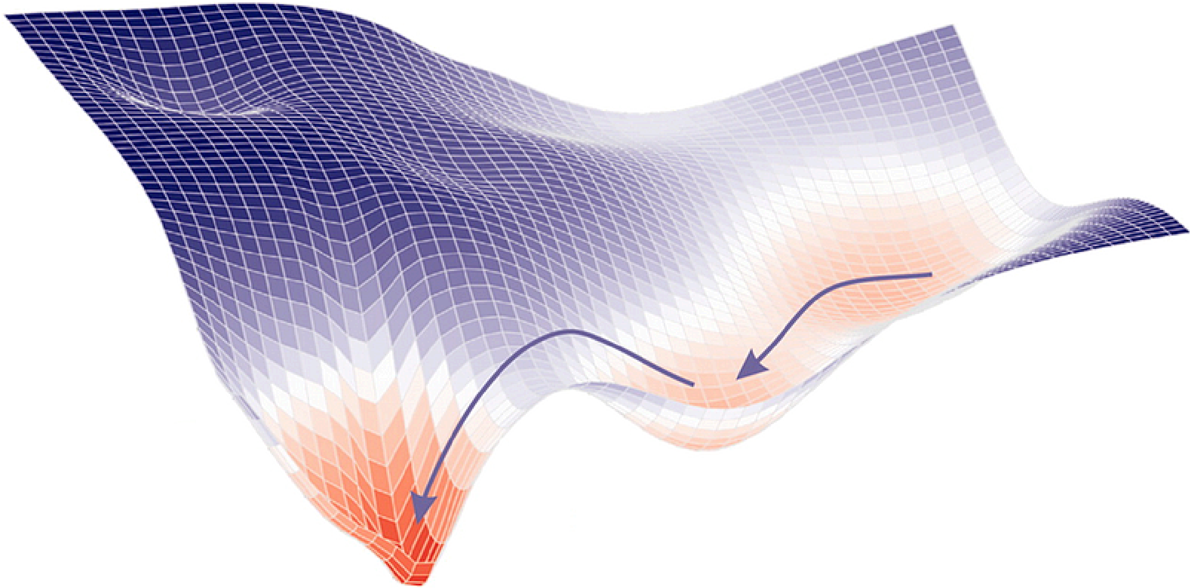

Review

First, we derived the solution to linear regression

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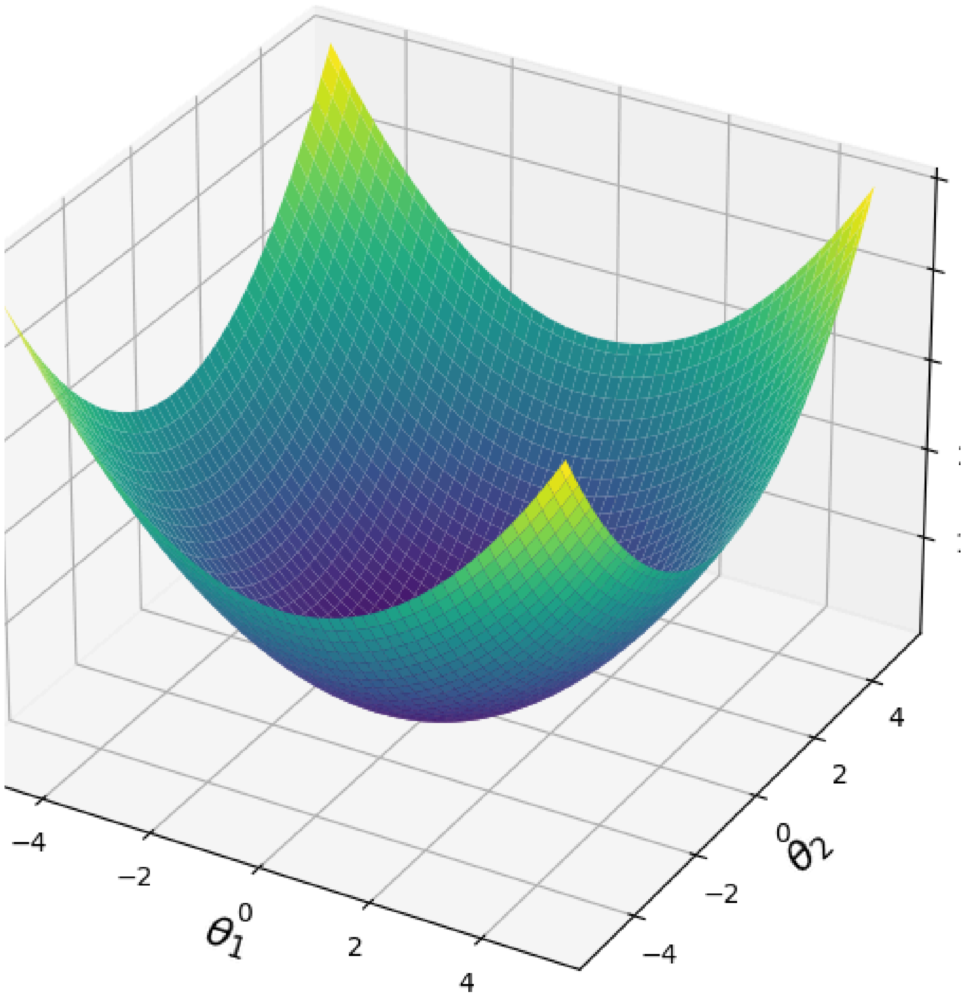
$$\mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta}) = \underbrace{\underbrace{(\boldsymbol{Y} - \boldsymbol{X}_D \boldsymbol{\theta})^\top}_{\text{Linear function of } \theta} \quad \underbrace{(\boldsymbol{Y} - \boldsymbol{X}_D \boldsymbol{\theta})}_{\text{Linear function of } \theta}}_{\text{Quadratic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

Review

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



Review

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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Now, we plug the model f into the loss function

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

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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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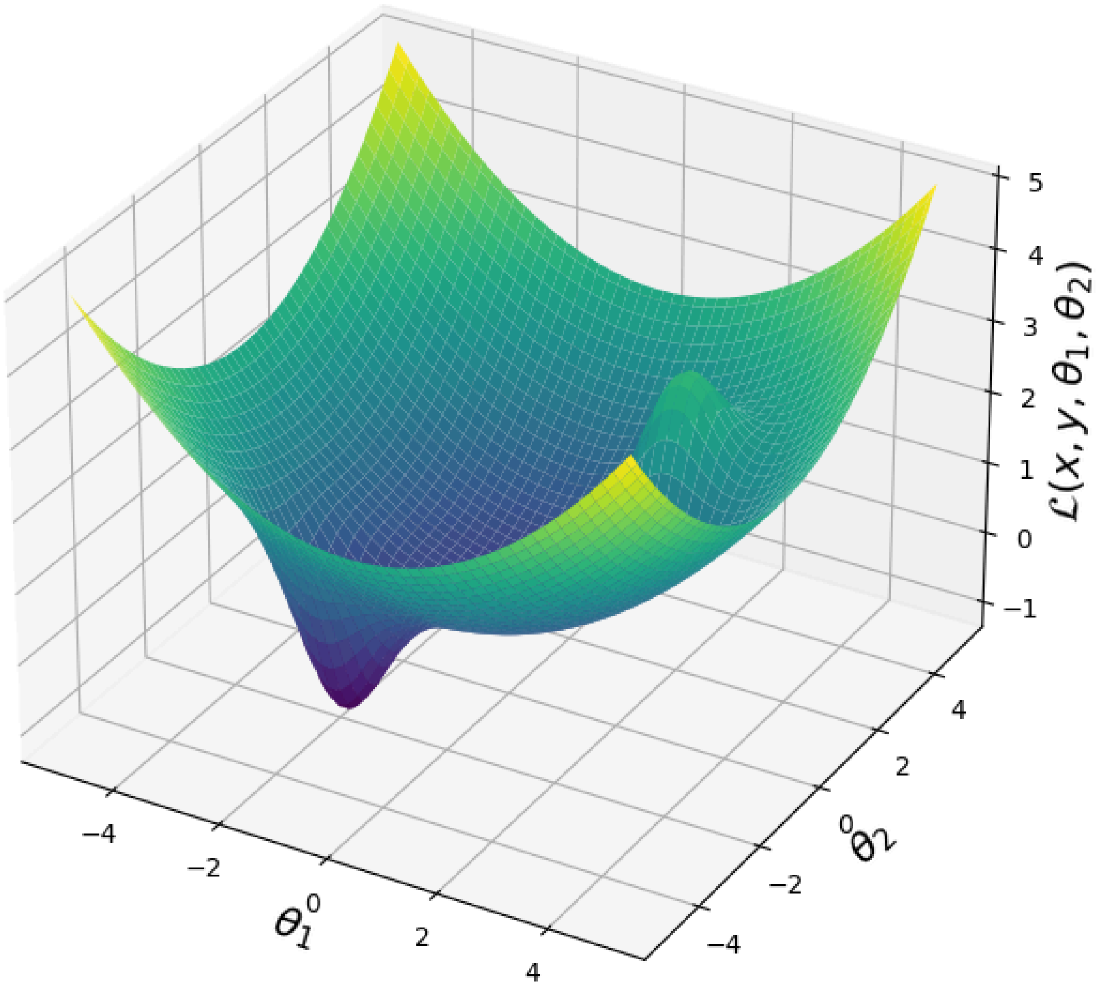
Gradient descent is an optimization method for differentiable functions

We went over both the intuition and mathematical definitions

Review

Review

Review



$\mathcal{L}(x, y, \theta_1, \theta_2)$
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($\boldsymbol{X}, \boldsymbol{Y}, \mathcal{L}, t, \alpha$)

  ▷ Randomly initialize parameters

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

  for $i \in 1...t$ **do**

    ▷ Compute the gradient of the loss

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

    ▷ Update the parameters using the negative gradient

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

  return $\boldsymbol{\theta}$

Review

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

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

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

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

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

Review

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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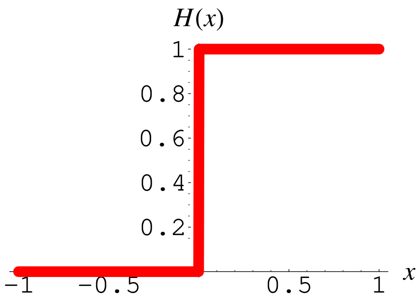

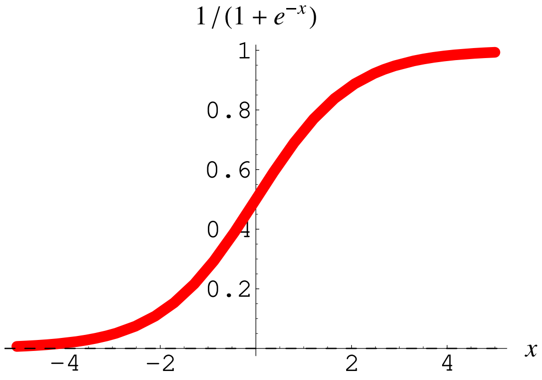

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

Review

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

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```python
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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Classification task

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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Classification task

Many problems in ML can be reduced to **regression** or **classification**

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Regression asks how many

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

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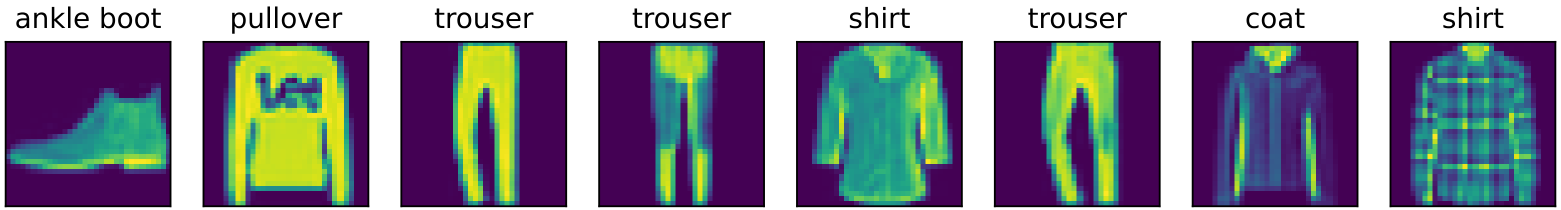
$X : \mathbb{Z}_{0,255}^{32 \times 32}$



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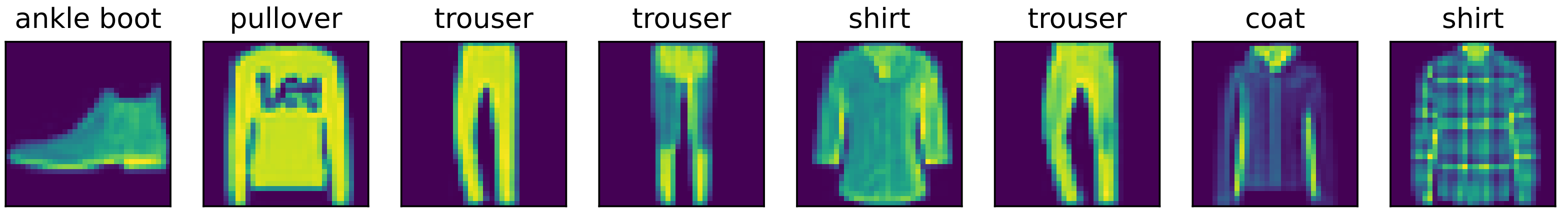

Y : {T-shirt, Trouser, Pullover, Dress, Coat, Sandal, Shirt, Sneaker, Bag, Ankle boot}

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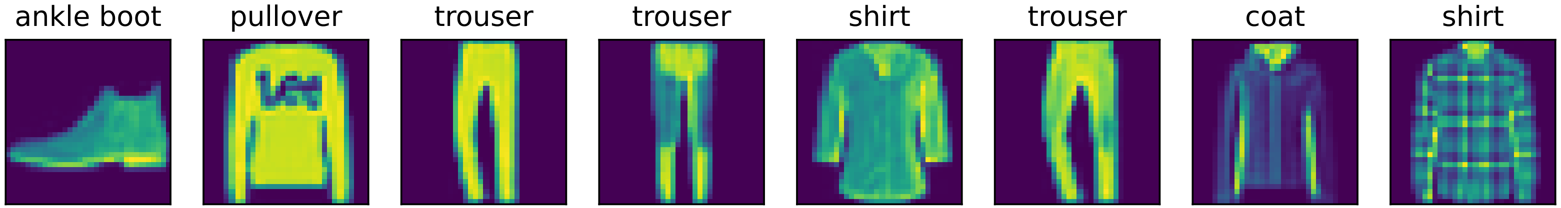

$Y : \{\text{T-shirt, Trouser, Pullover, Dress, Coat,}$
$\text{Sandal, Shirt, Sneaker, Bag, Ankle boot}\}$

Approach: Learn θ that produce **conditional probabilities**

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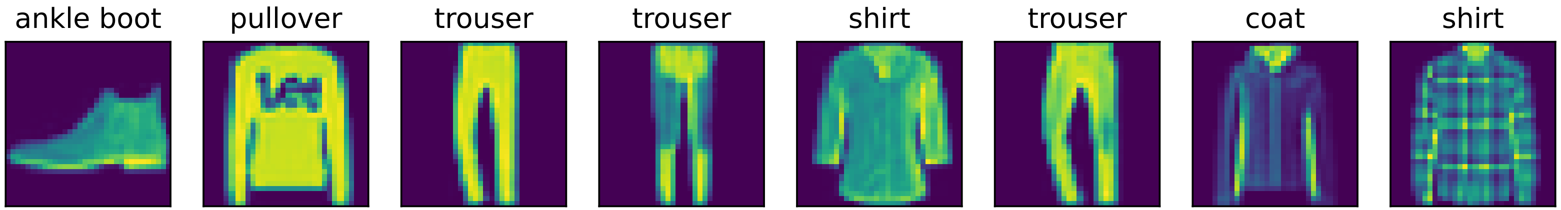
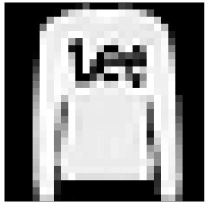


$Y : \{\text{T-shirt}, \text{Trouser}, \text{Pullover}, \text{Dress}, \text{Coat},$
$\text{Sandal}, \text{Shirt}, \text{Sneaker}, \text{Bag}, \text{Ankle boot}\}$

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

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



$$\left. \vphantom{\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}} \right) = \begin{bmatrix} 0.2 \\ 0.01 \\ \vdots \end{bmatrix}$$

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Experiment	Outcome

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An experiment yields one of many possible outcomes

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

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

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Experiment	Sample Space S

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Experiment	Sample Space S
Flip a coin	$S = \{\text{heads}, \text{tails}\}$

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Experiment	Sample Space S
Flip a coin	$S = \{\text{heads}, \text{tails}\}$
Walk outside	$S = \{\text{rain}, \text{sun}, \text{wind}, \text{cloud}\}$

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

Experiment	Sample Space S
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
Flip a coin	$P(\text{heads}) = 0.5$
Walk outside	$P(\text{rain}) = 0.15$

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The probability must be between 0 (never occurs) and 1 (always occurs)

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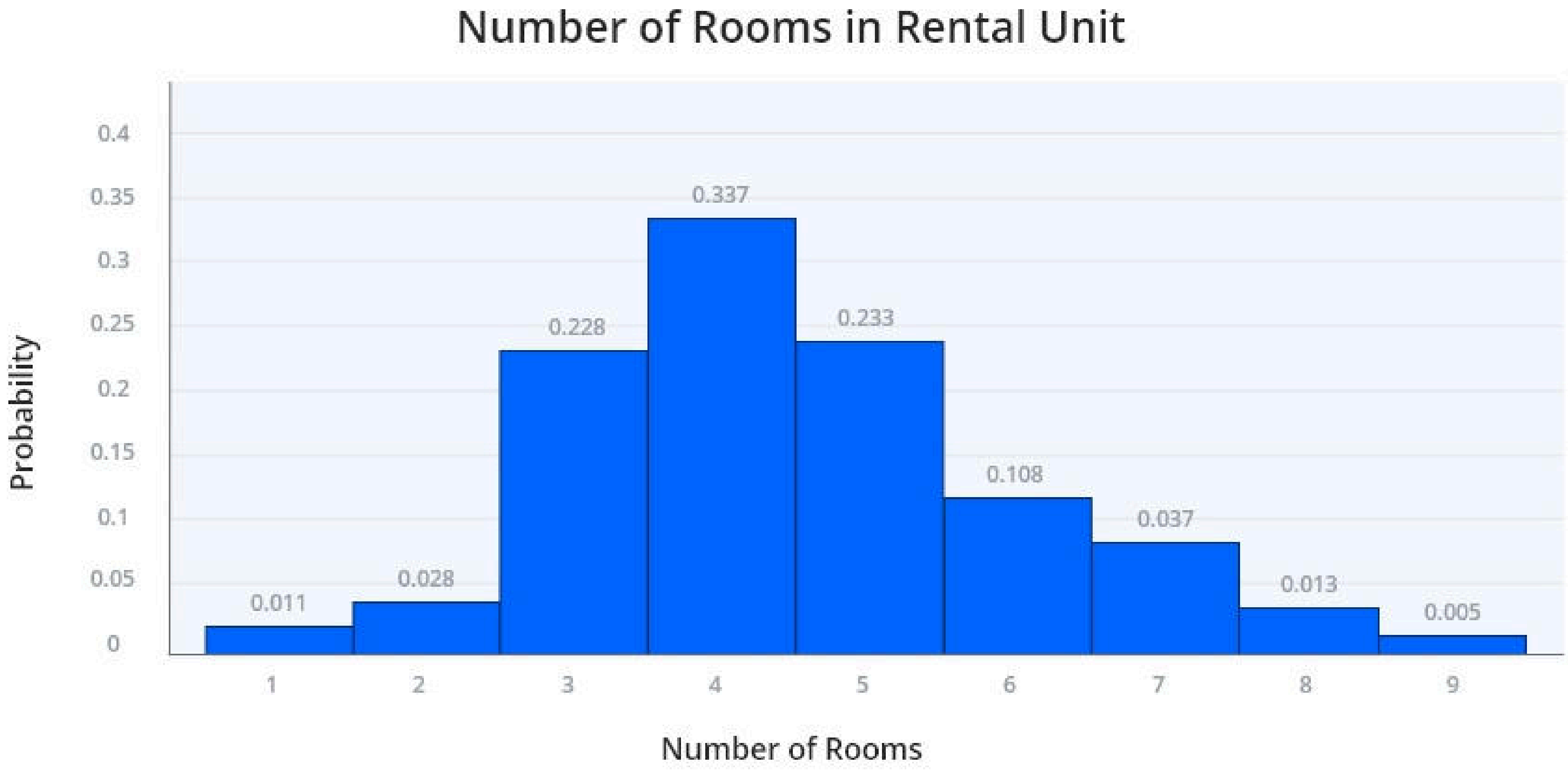
Flip a coin $\{P(\text{heads}) = 0.5, P(\text{tails}) = 0.5\}$

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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- Disjoint events
- Conditionally dependent events

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Flip a coin

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

Walk outside

$$P(\text{Rain}) = 0.1, P(\text{Cloud}) = 0.2$$
$$P(\text{Rain} \cap \text{Cloud}) \neq 0$$

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$$P(\text{Rain} \cap \text{Cloud}) = 0.1$$

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

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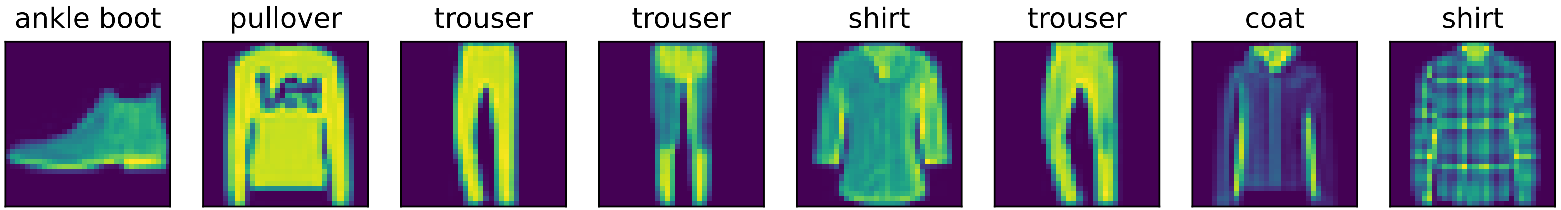
$X : \mathbb{Z}_{0,255}^{32 \times 32}$



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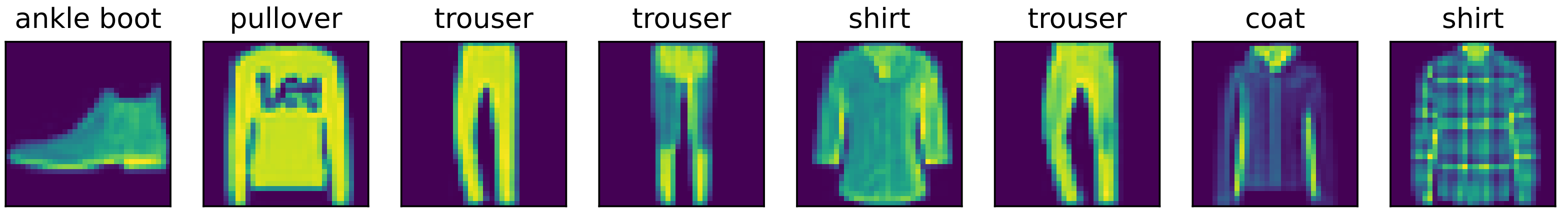

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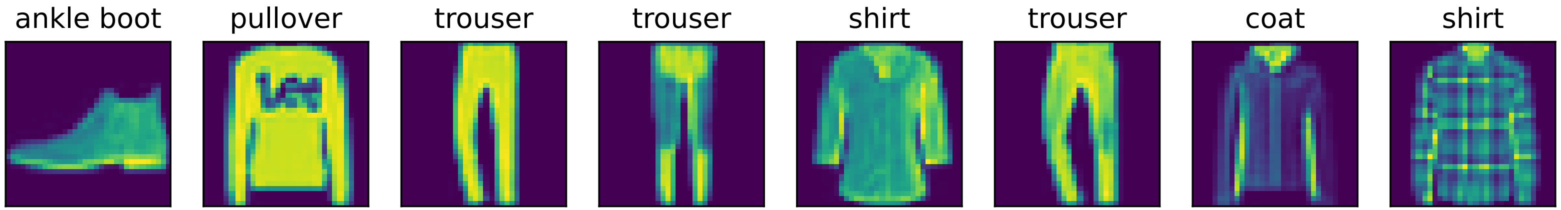

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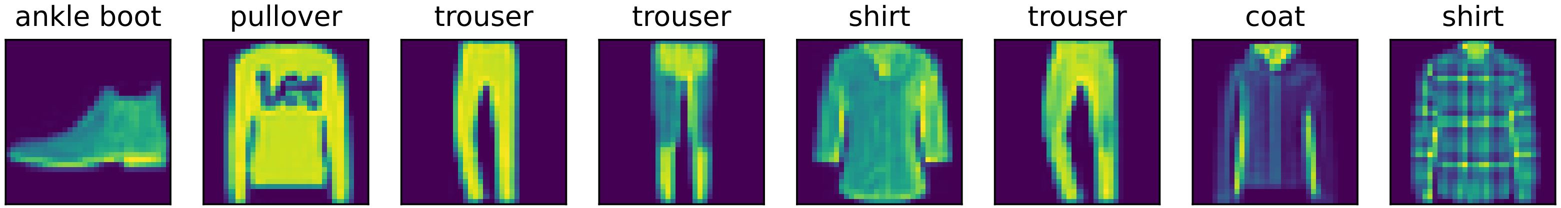

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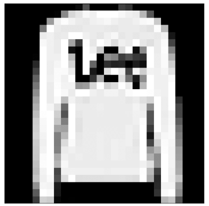
$$f(\boldsymbol{x}, \boldsymbol{\theta}) = P(\boldsymbol{y} \mid \boldsymbol{x}) = P\left(\begin{bmatrix} \text{T-Shirt} \\ \text{Trouser} \\ \vdots \end{bmatrix} \middle| \right.$$



$$\left. \vphantom{\begin{bmatrix} a \\ b \\ c \end{bmatrix}} \right) = \begin{bmatrix} 0.2 \\ 0.01 \\ \vdots \end{bmatrix}$$

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Answer: $f : \mathbb{R}^{d_x} \times \Theta \mapsto \mathbb{R}^{d_y}$

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Answer: No! Because probabilities must be $\in (0, 1)$ and sum to one

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$$\boldsymbol{v} = \left\{ \begin{bmatrix} v_1 \\ \vdots \\ v_{d_y} \end{bmatrix} \middle| \quad \sum_{i=1}^{d_y} v_i = 1; \quad v_i \in (0, 1) \right\}$$

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

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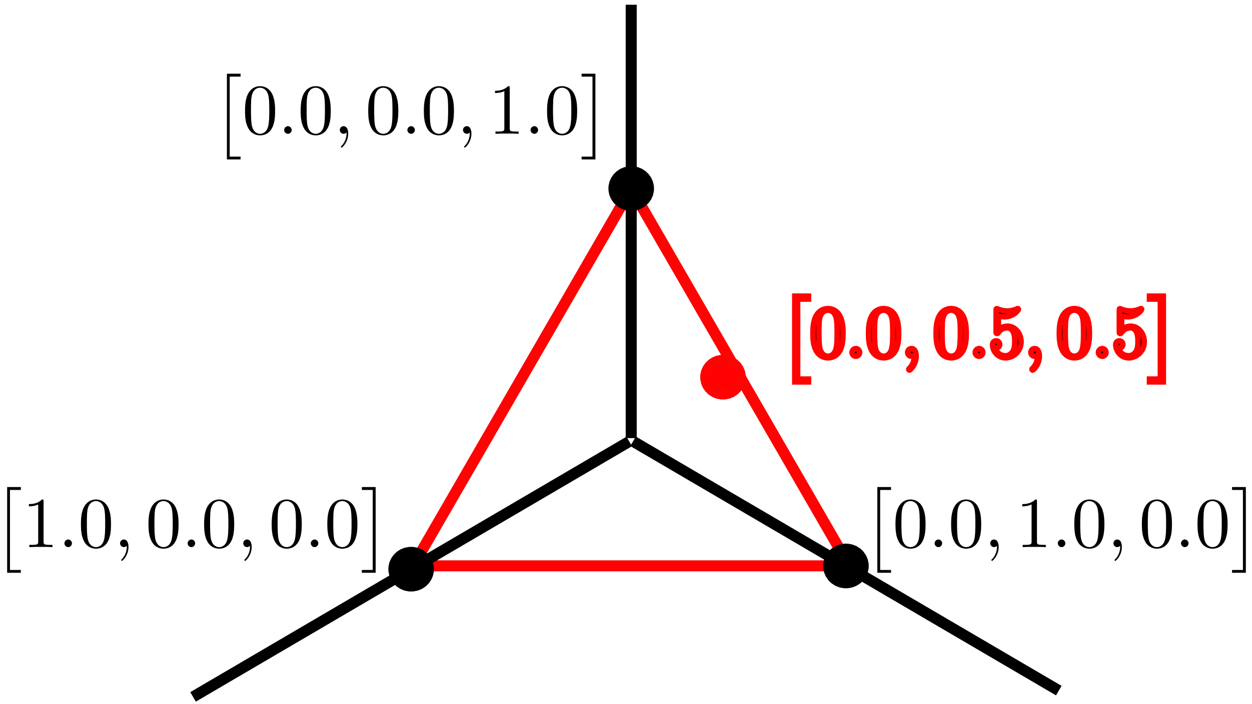

It has only $k - 1$ free variables, because $x_k = 1 - \sum_{i=1}^{k-1} x_i$

$$f: \mathbb{R}^{d_x} \times \Theta \mapsto \mathbb{R}^{d_y}$$

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Then, we can combine f and g

$$g(f) : \mathbb{R}^{d_x} \times \Theta \mapsto \Delta^{d_y - 1}$$

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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)

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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

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

$$\vdots$$

$$f_\ell(\boldsymbol{x}, \boldsymbol{\xi}) = \text{softmax}(\boldsymbol{\xi}^\top \overline{\boldsymbol{x}})$$

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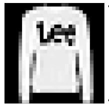
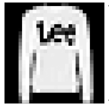
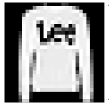
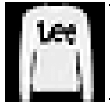
Now, our neural network can output probabilities

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \begin{bmatrix} P\left(\text{Ankle boot} \mid \quad \right) \\ P\left(\text{Bag} \mid \quad \right) \\ \vdots \end{bmatrix} = \begin{bmatrix} 0.25 \\ 0.08 \\ \vdots \end{bmatrix}$$





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

$f(\boldsymbol{x}, \boldsymbol{\theta}) =$ [$P\big(\text{Shirt} \mid$  $\big)$, $P\big(\text{Bag} \mid$  $\big)$, $\vdots$] $= \begin{bmatrix} 0.25 \\ 0.08 \\ \vdots \end{bmatrix}; \quad f(\boldsymbol{x}, \boldsymbol{\theta}) = \begin{bmatrix} 1 \\ 0 \\ \vdots \end{bmatrix}$

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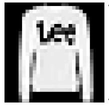

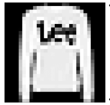

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Answer 1: Outputting probabilities results in differentiable functions

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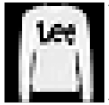

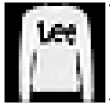

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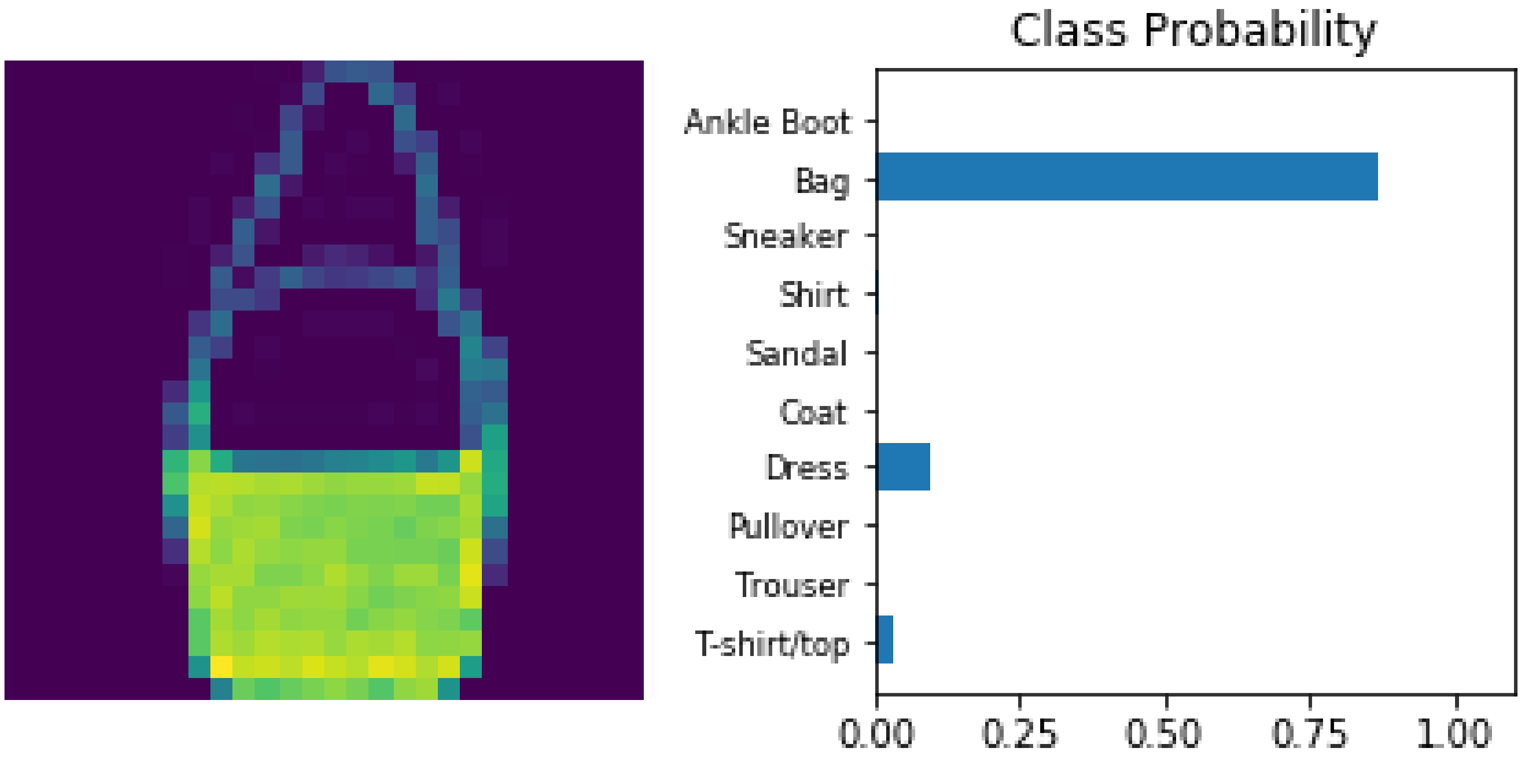
Answer 1: Outputting probabilities results in differentiable functions

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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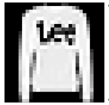
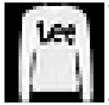
We consider the label $\boldsymbol{y}_{[i]}$ as a conditional distribution

$P\left(\boldsymbol{y}_{[i]} \mid \boldsymbol{x}_{[i]}\right) =$

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

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

$= \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

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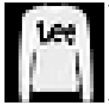
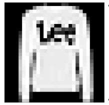
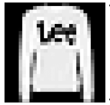
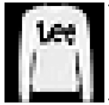
$P(\boldsymbol{y}_{[i]} \mid \boldsymbol{x}_{[i]}) = \Bigg[$ $P(\text{Shirt} \mid$  $)$

$P(\text{Bag} \mid$  $)$ $\Bigg] = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

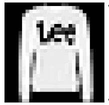
Our neural network also outputs some distribution

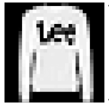
$f(\boldsymbol{x}_{[i]}, \boldsymbol{\theta}) = \Bigg[$ $P(\text{Shirt} \mid$  $)$

$P(\text{Bag} \mid$  $)$ $\Bigg] = \begin{bmatrix} 0.6 \\ 0.4 \end{bmatrix}$

We consider the label $\boldsymbol{y}_{[i]}$ as a conditional distribution

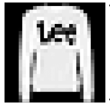
$$P\left(\boldsymbol{y}_{[i]} \mid \boldsymbol{x}_{[i]}\right) = \begin{bmatrix} P(\text{Shirt} \mid \square_1) \\ P(\text{Bag} \mid \square_2) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

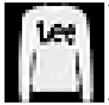
$\square_1$: 

$\square_2$: 

Our neural network also outputs some distribution

$$f\left(\boldsymbol{x}_{[i]}, \boldsymbol{\theta}\right) = \begin{bmatrix} P(\text{Shirt} \mid \square_3) \\ P(\text{Bag} \mid \square_4) \end{bmatrix} = \begin{bmatrix} 0.6 \\ 0.4 \end{bmatrix}$$

$\square_3$: 

$\square_4$: 

What loss function should we use for classification?

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Let us derive it

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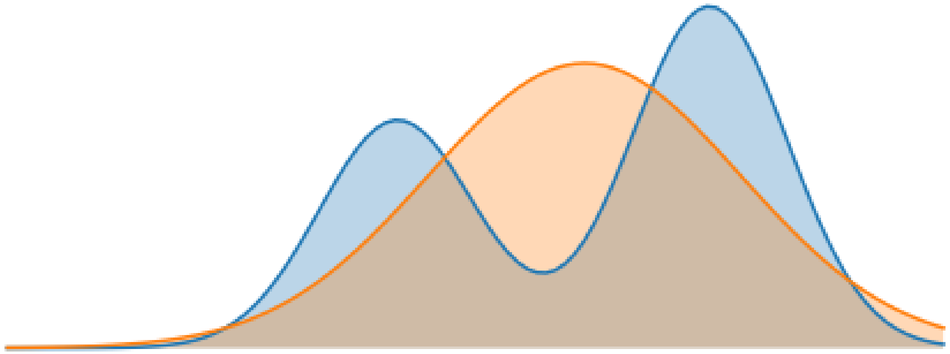

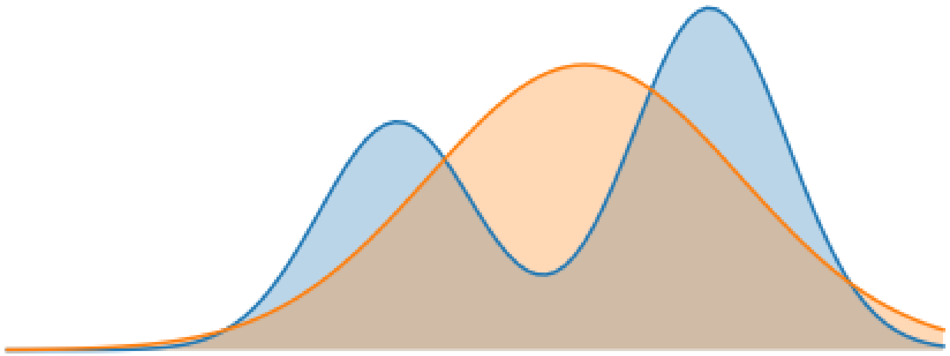

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Plug in our two distributions $P = f$ and $Q = \boldsymbol{y}$

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

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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

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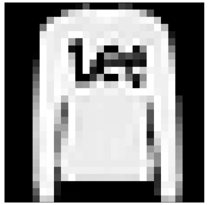

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$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\theta}) = \left[-\sum_{j=1}^{n} \sum_{i=1}^{d_y} P\left(y_{[j],i} \mid \boldsymbol{x}_{[j]}\right) \log f\left(\boldsymbol{x}_{[j]}, \boldsymbol{\theta}\right)_i\right]$$

Agenda

1. Review
2. Torch optimization coding
3. Classification task
4. Probability review
5. Define model f
6. **Define loss function $\mathcal{L}$**
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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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Relax

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The rest of this course will examine neural network architectures

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https://colab.research.google.com/drive/1BGMIE2CjlLJOH-D2r9AariPDVgxjWlqG?usp=sharing

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