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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There are conflicting student needs

Admin

https://github.com/smorad/um_cisc_7026

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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Last time, we reviewed derivatives

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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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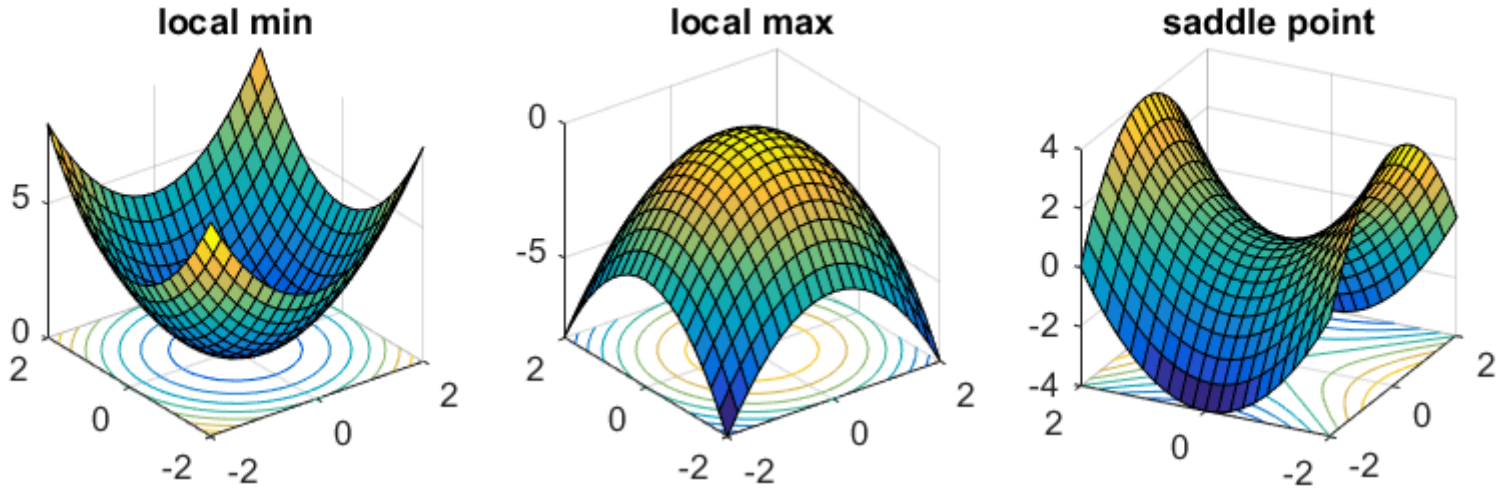

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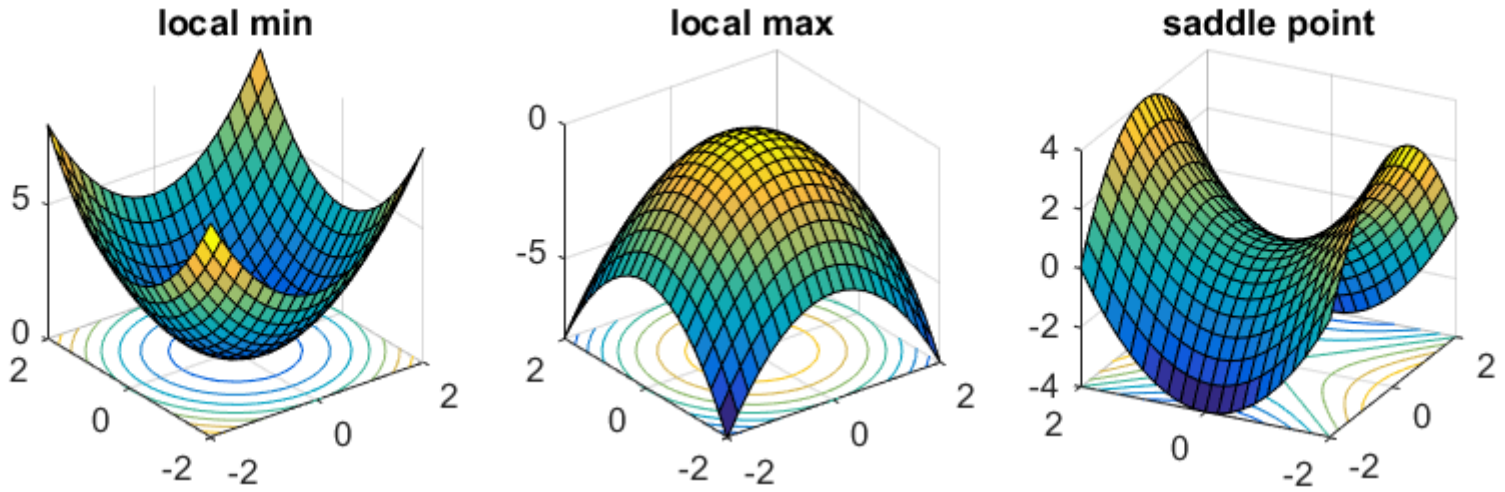

With optimization, we attempt to find minima of loss functions

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

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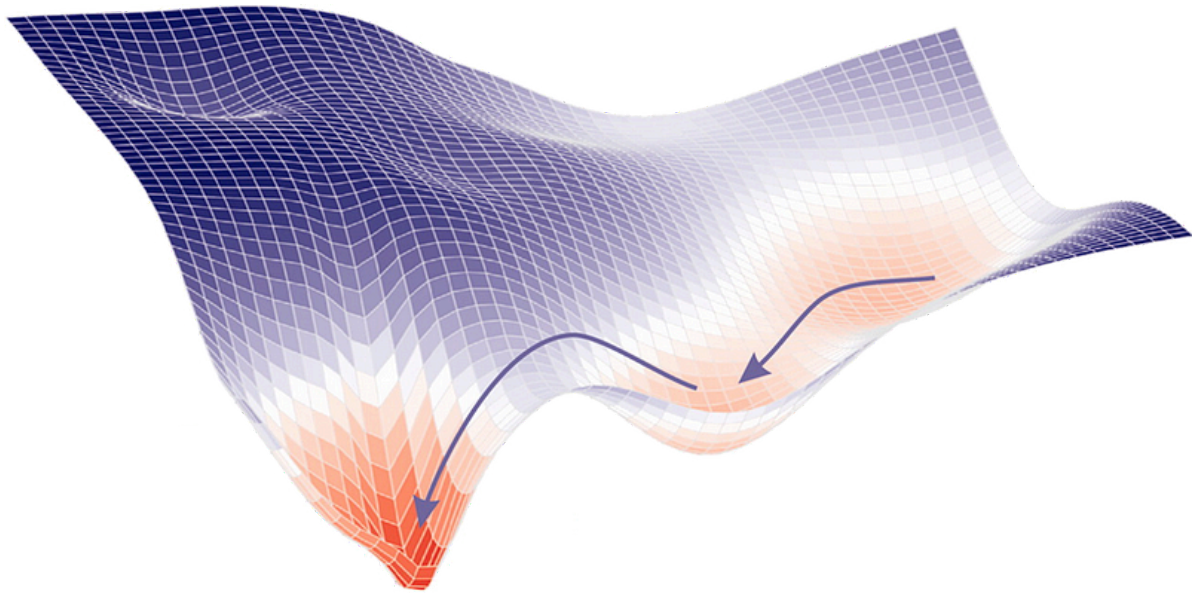

Review

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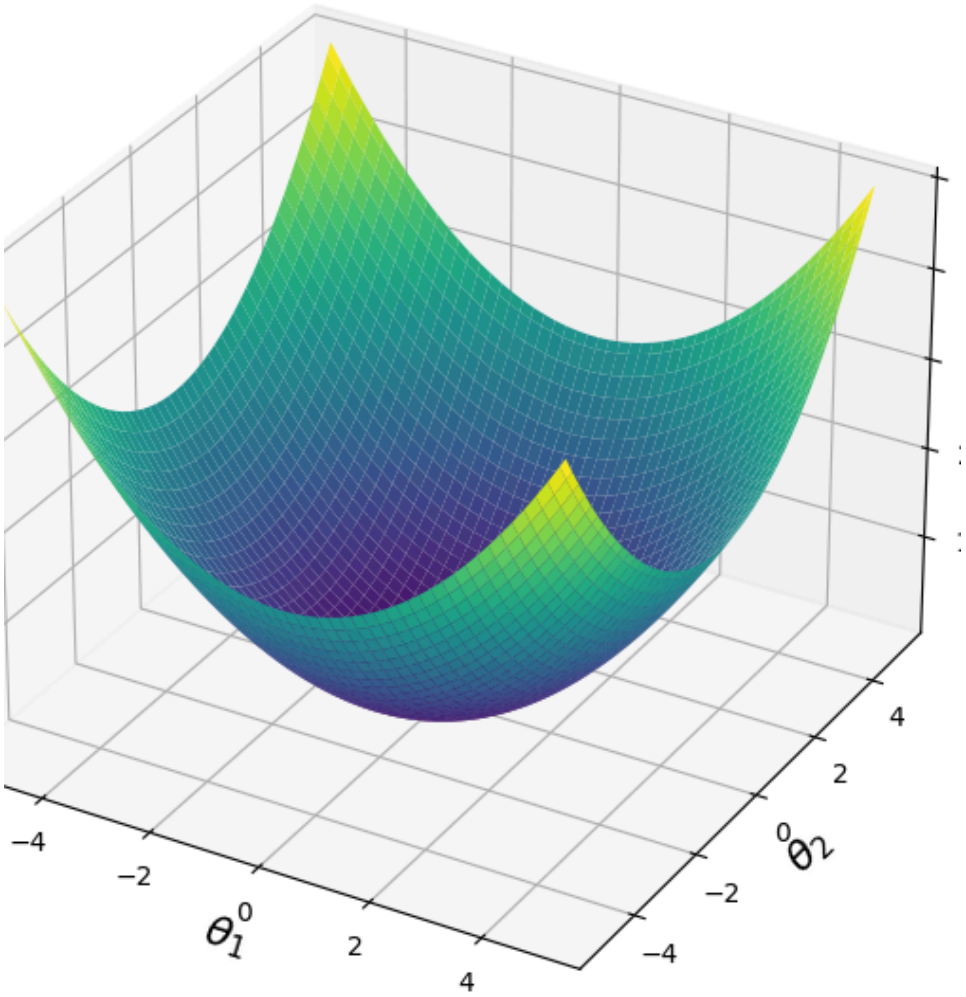
$$\mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta}) = \underbrace{\underbrace{(\boldsymbol{Y} - \boldsymbol{X}_D\boldsymbol{\theta})^\top}_{\text{Linear function of } \theta} \underbrace{(\boldsymbol{Y} - \boldsymbol{X}_D\boldsymbol{\theta})}_{\text{Linear function of } \theta}}_{\text{Quadratic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

Review

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



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Which solves

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

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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

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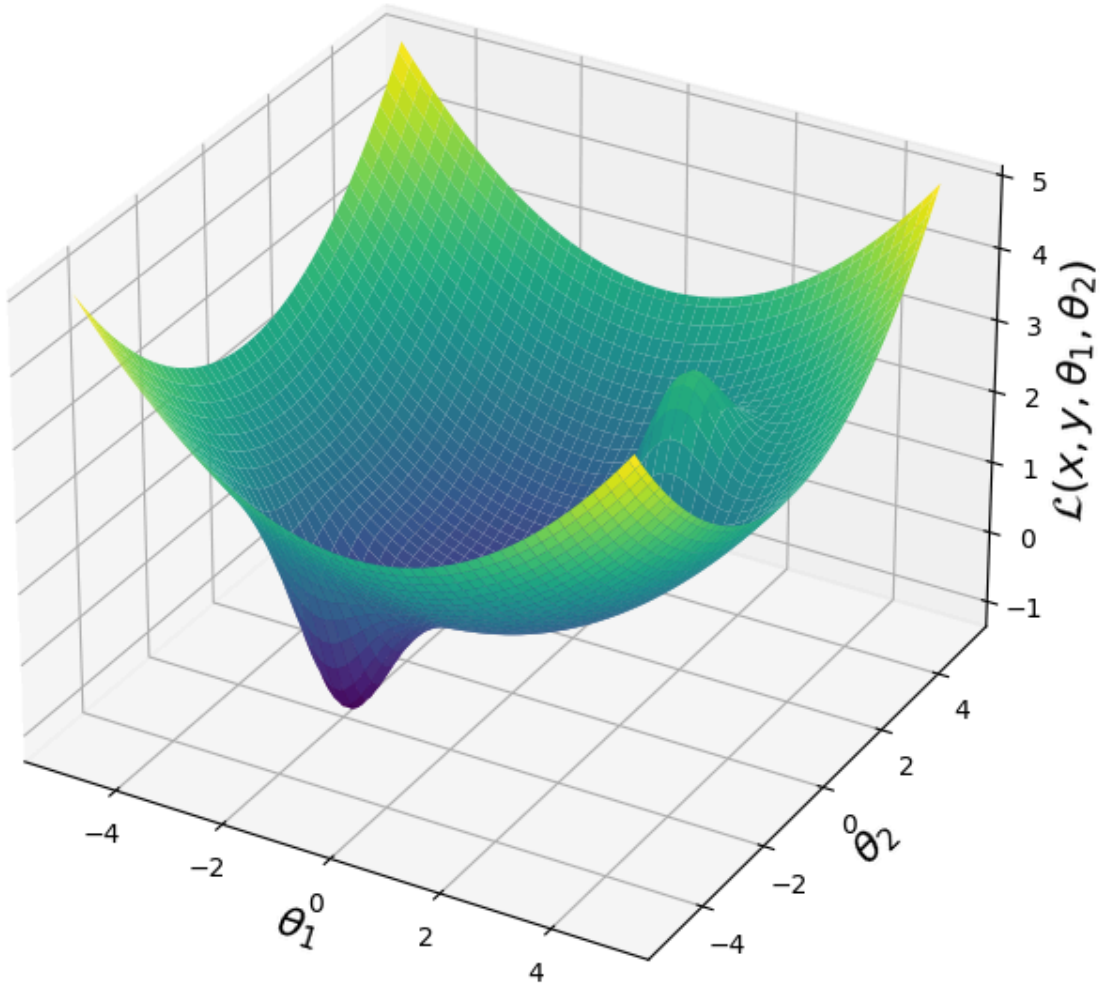
5
4
3
2
1
0
−1
$\mathcal{L}(x, y, \theta_1, \theta_2)$
−4
−2
θ_1^0
2
4
4
2
θ_2^0
−2
−4

Review

The gradient descent algorithm:

1: **function** GRADIENT DESCENT($\boldsymbol{X}$, $\boldsymbol{Y}$, $\mathcal{L}$, t, α)
2: ▷ Randomly initialize parameters
3: $\boldsymbol{\theta} \leftarrow \mathcal{N}(0, 1)$
4: **for** $i \in 1...t$ **do**
5: ▷ Compute the gradient of the loss
6: $\boldsymbol{J} \leftarrow \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$
7: ▷ Update the parameters using the negative gradient
8: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \boldsymbol{J}$
9: **return** $\boldsymbol{\theta}$

Review

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

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

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

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

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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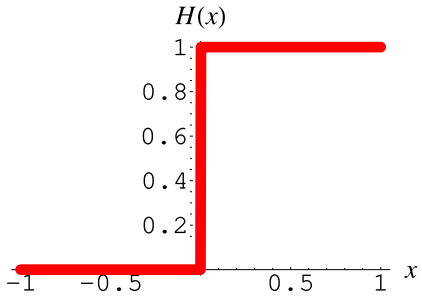

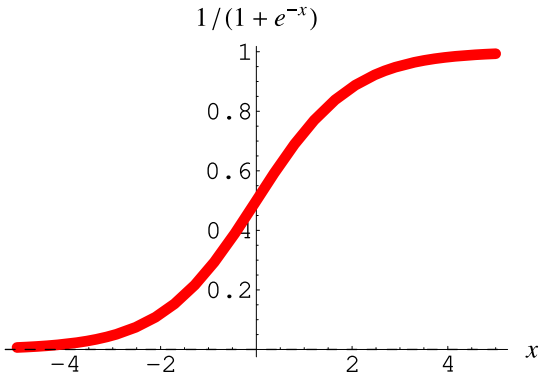

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

Review

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

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```
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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4. Probability review
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Torch Optimization Coding

First, a video of one application of gradient descent

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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

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

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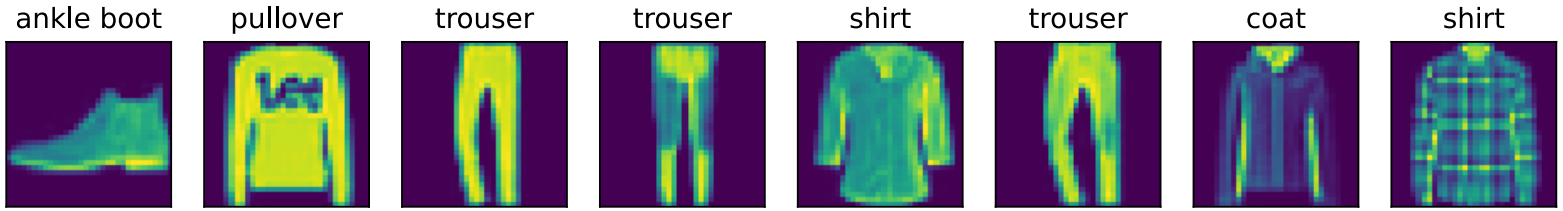
$$X : \mathbb{Z}_{0,255}^{32\times 32}$$



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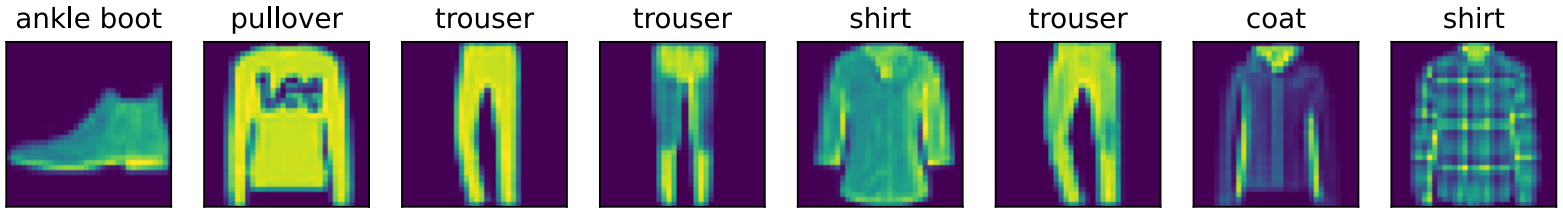

$Y : \{\text{T-shirt, Trouser, Pullover, Dress, Coat,}$

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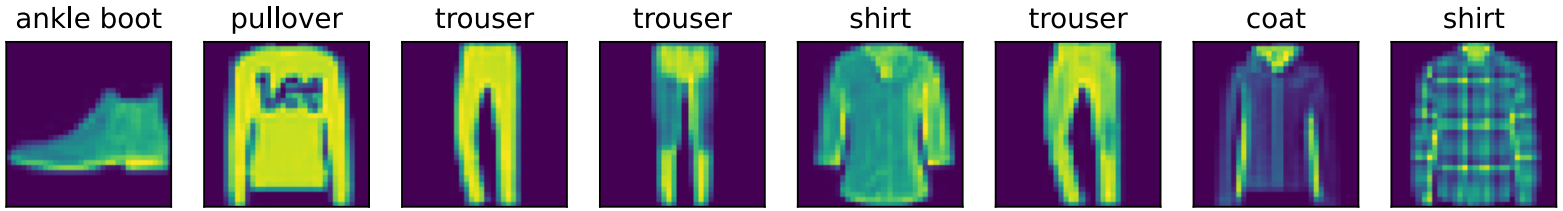

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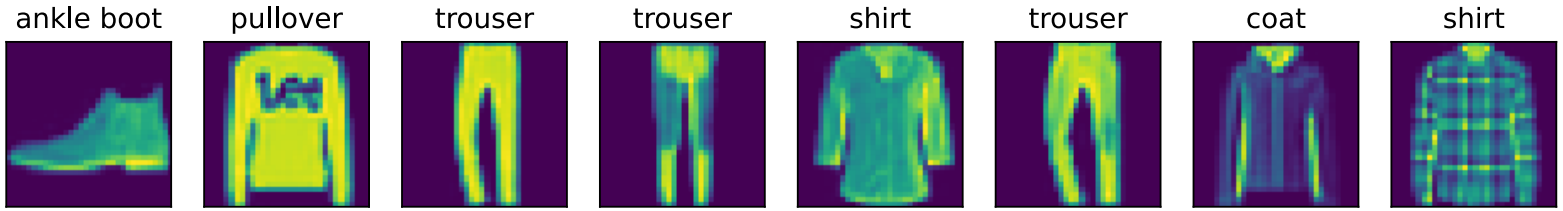

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$$f(\boldsymbol{x}, \boldsymbol{\theta}) = P(\boldsymbol{y} \mid \boldsymbol{x}) = P\left(\begin{bmatrix} \text{T-Shirt} \\ \text{Trouser} \\ \vdots \end{bmatrix} \middle| \quad \right) = \begin{bmatrix} 0.2 \\ 0.01 \\ \vdots \end{bmatrix}$$

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An experiment yields one of many possible outcomes

Classification tasks require **probability theory**, so let us review

In probability, we have **experiments** and **outcomes**

An experiment yields one of many possible outcomes

Experiment	Outcome

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

An **event** E is a specific subset of the sample space

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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

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Experiment	Probabilities
Flip a coin	$P(\text{heads}) = 0.5$
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$$0 \leq P(E) \leq 1$$

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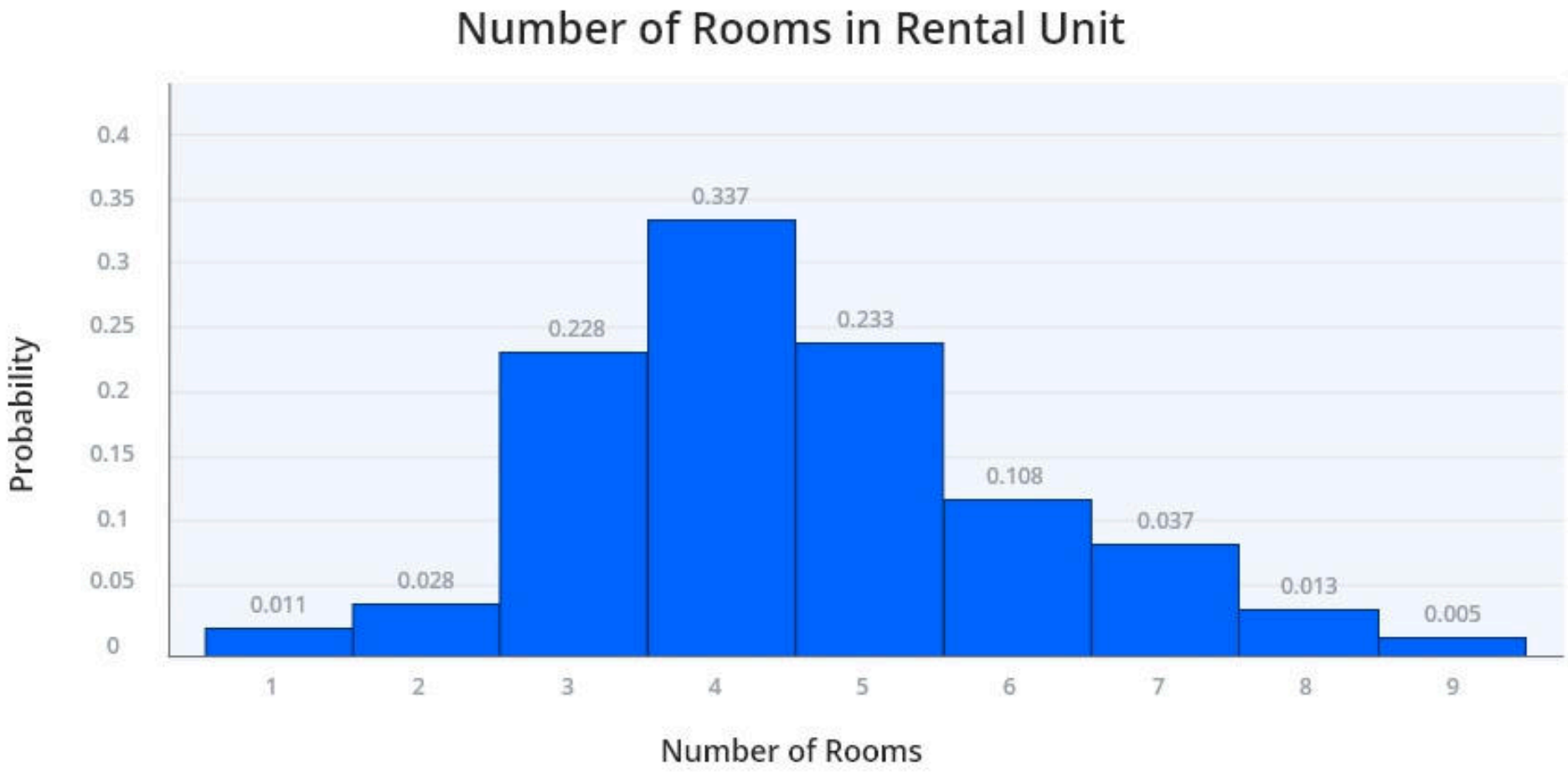
Flip a coin $\{P(\text{heads}) = 0.5, P(\text{tails}) = 0.5\}$

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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Flip a coin

$$P(\text{Heads}) = 0.5, P(\text{Tails}) = 0.5$$
$$P(\text{Heads} \cap \text{Tails}) = 0$$

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

Walk outside

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

$$P(\text{Rain} \mid \text{Cloud}) = \frac{0.1}{0.2} = 0.5$$

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

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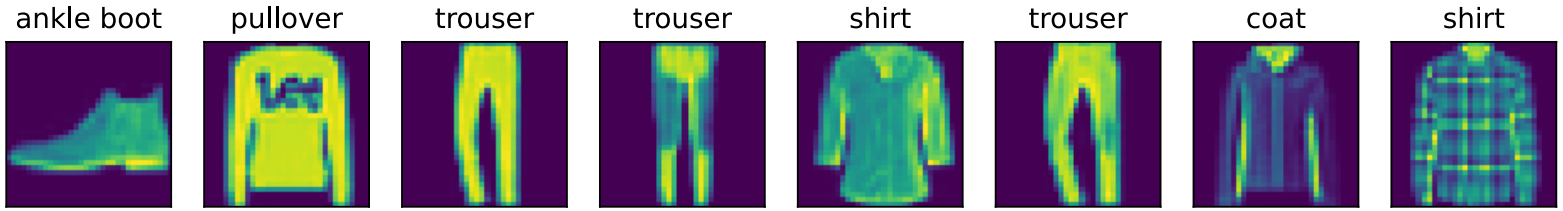
$$X : \mathbb{Z}_{0,255}^{32\times32}$$



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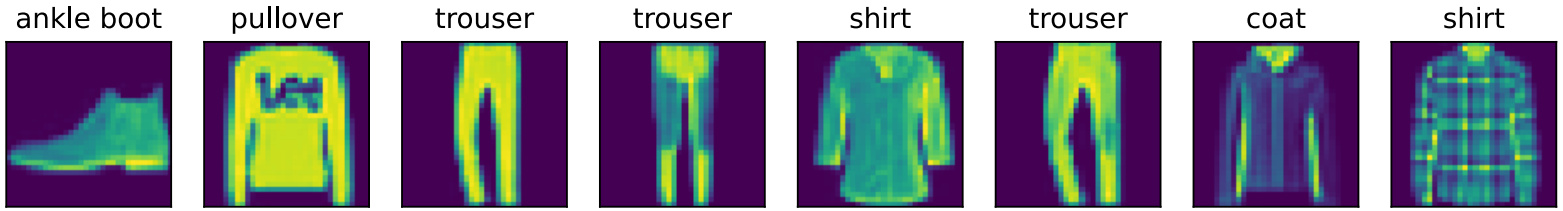

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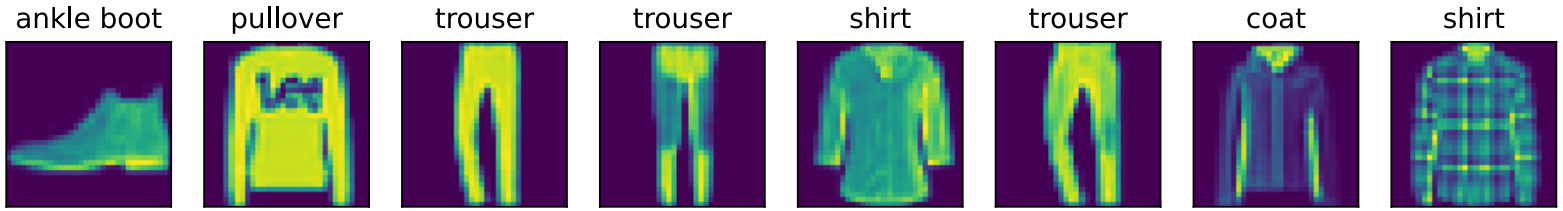

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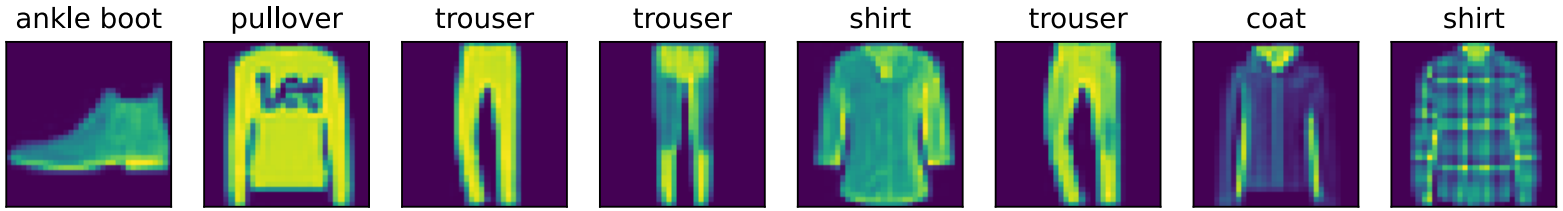

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$$f(\boldsymbol{x}, \boldsymbol{\theta}) = P(\boldsymbol{y} \mid \boldsymbol{x}) = P\left(\begin{bmatrix} \text{T-Shirt} \\ \text{Trouser} \\ \vdots \end{bmatrix} \middle| \quad \right) = \begin{bmatrix} 0.2 \\ 0.01 \\ \vdots \end{bmatrix}$$

Agenda

1. Review
2. Torch optimization coding
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4. **Probability review**
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Answer: No! Because probabilities must be $\in (0, 1)$ and sum to one

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

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

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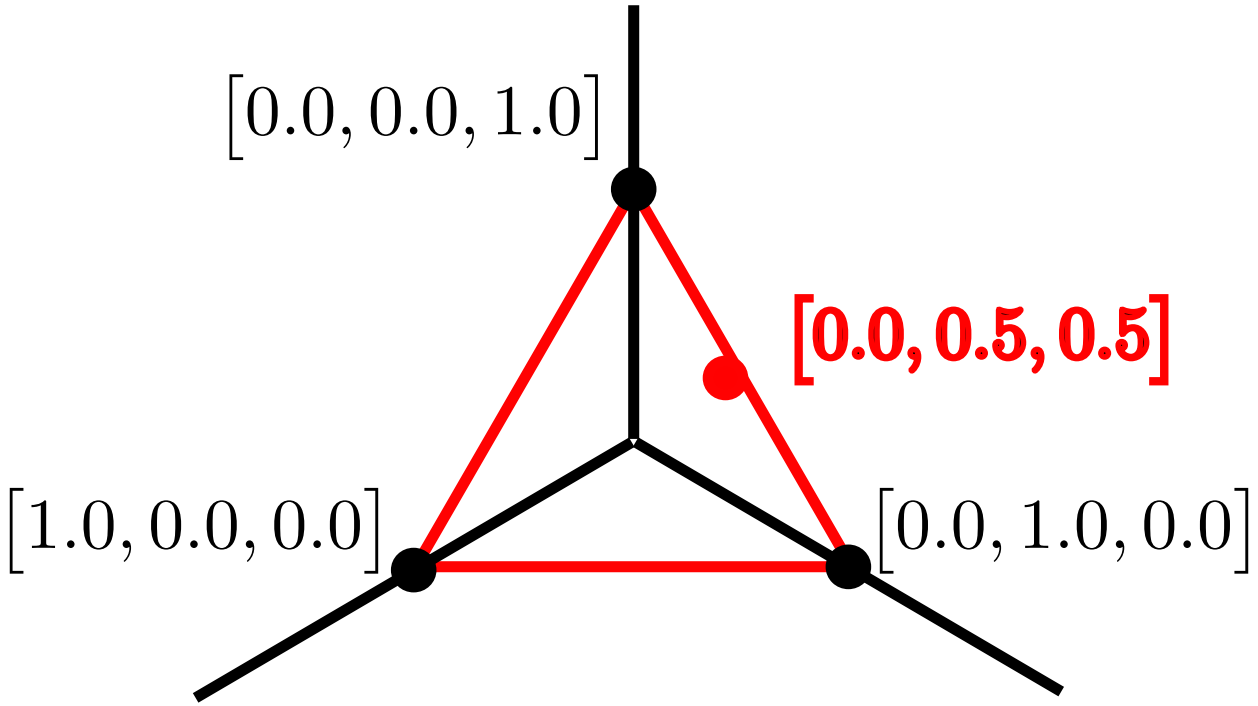

It has only $k-1$ free variables, because $x_k = 1 - \sum_{i=1}^{k-1} x_i$

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

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$$g : \mathbb{R}^{d_y} \mapsto \Delta^{d_y - 1}$$

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

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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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$$\vdots$$
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Now, our neural network can output probabilities

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

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

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

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Answer 1: Outputting probabilities results in differentiable functions

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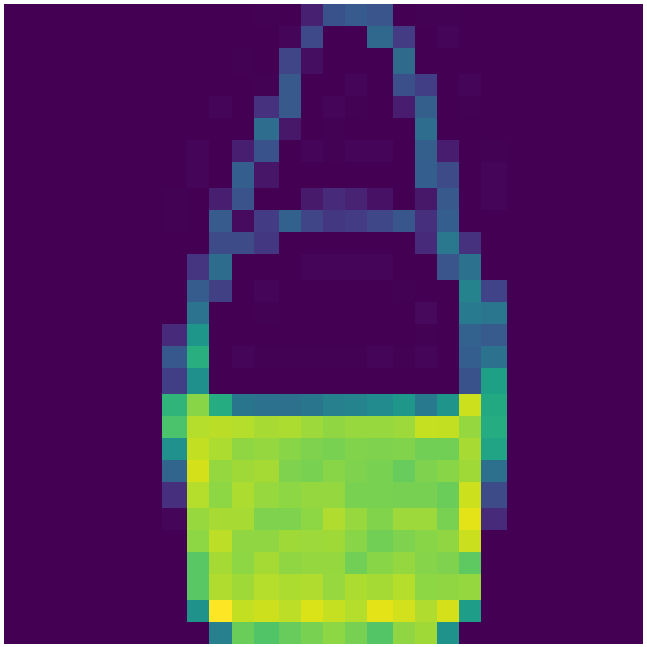
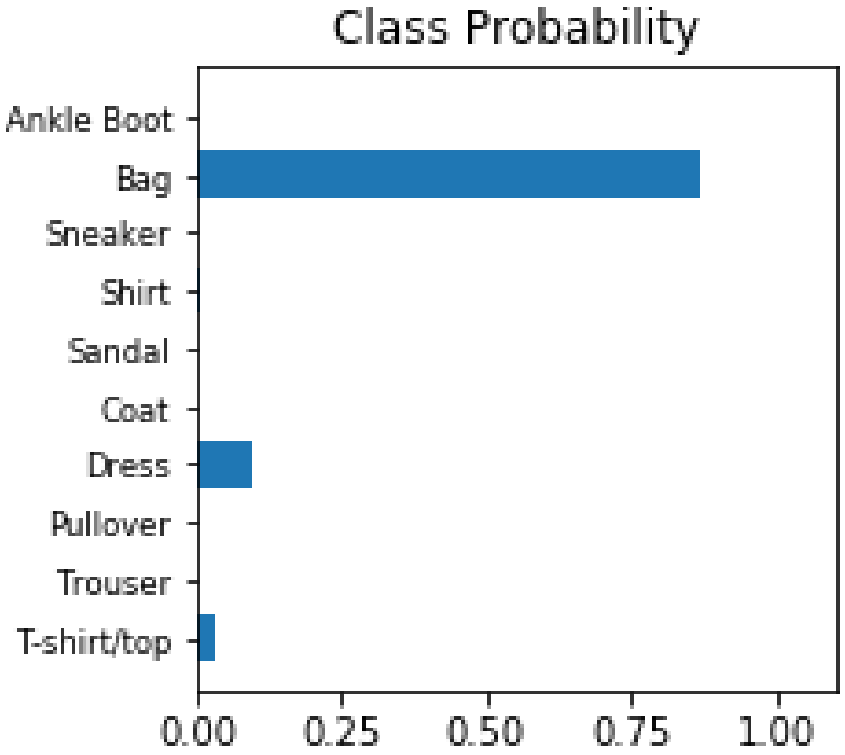
Answer 1: Outputting probabilities results in differentiable functions

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

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

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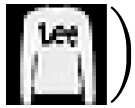
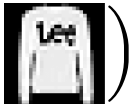
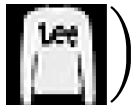
$$P\left(\boldsymbol{y}_{[i]} \mid \boldsymbol{x}_{[i]}\right) = \begin{bmatrix} P\left(\text{Shirt} \mid \text{  }\right) \\ P\left(\text{Bag} \mid \text{  }\right) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Our neural network also outputs some distribution

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

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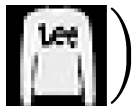
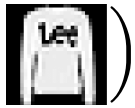
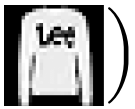
$$P\left(\boldsymbol{y}_{[i]} \mid \boldsymbol{x}_{[i]}\right) = \begin{bmatrix} P\left(\text{Shirt} \mid \text{  }\right) \\ P\left(\text{Bag} \mid \text{  }\right) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Our neural network also outputs some distribution

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

What loss function should we use for classification?

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Let us derive it

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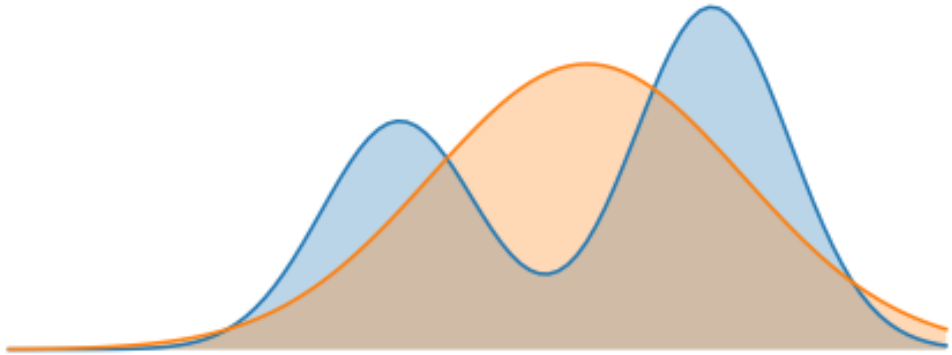

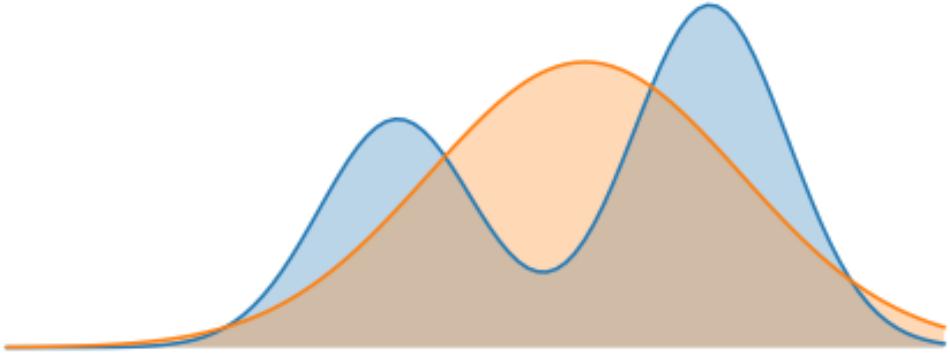

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Plug in our two distributions $P = f$ and $Q = \boldsymbol{y}$

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

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Rewrite the logarithm using the sum rule of logarithms

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

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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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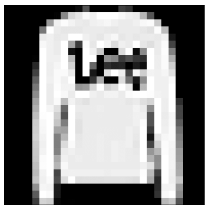

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Agenda

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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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

Coding

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

Admin

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