

Classification

CISC 7026: Introduction to Deep Learning

University of Macau

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

Some requests from students:

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1. More coding, less theory

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2. More math/theory

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2. More math/theory
3. Too easy, go faster

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There are conflicting student needs

https://github.com/smorad/um_cisc_7026

1. Review
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

$$\nabla_{\mathbf{x}} f \left([x_1 \ x_2 \ \dots \ x_n]^\top \right) = \left[\frac{\partial f}{\partial x_1} \ \frac{\partial f}{\partial x_2} \ \dots \ \frac{\partial f}{\partial x_n} \right]^\top$$

Review

Gradients are important in deep learning for two reasons:

Review

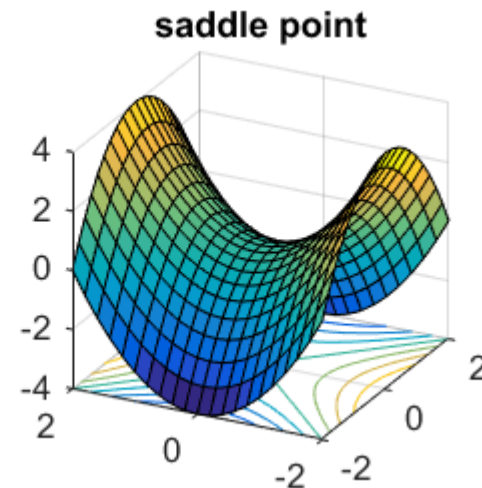
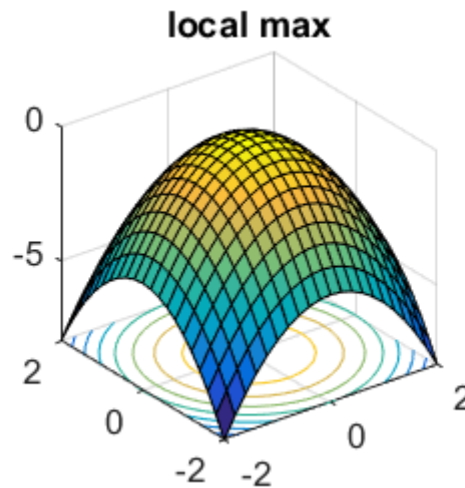
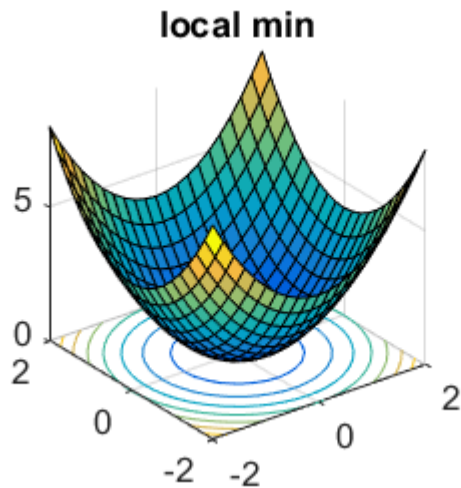
Gradients are important in deep learning for two reasons:

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

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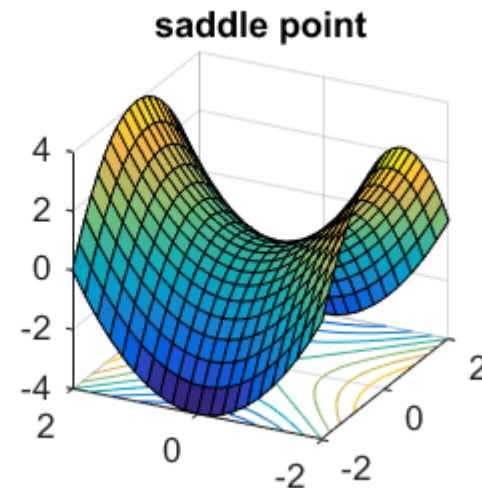
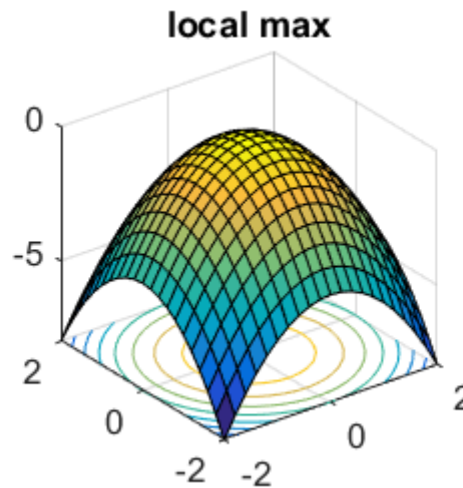
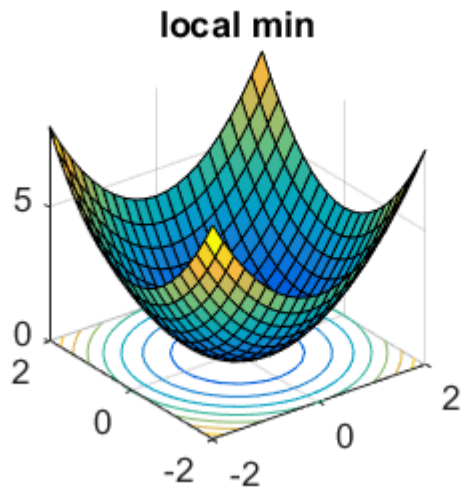
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With optimization, we attempt to find minima of loss functions

Review

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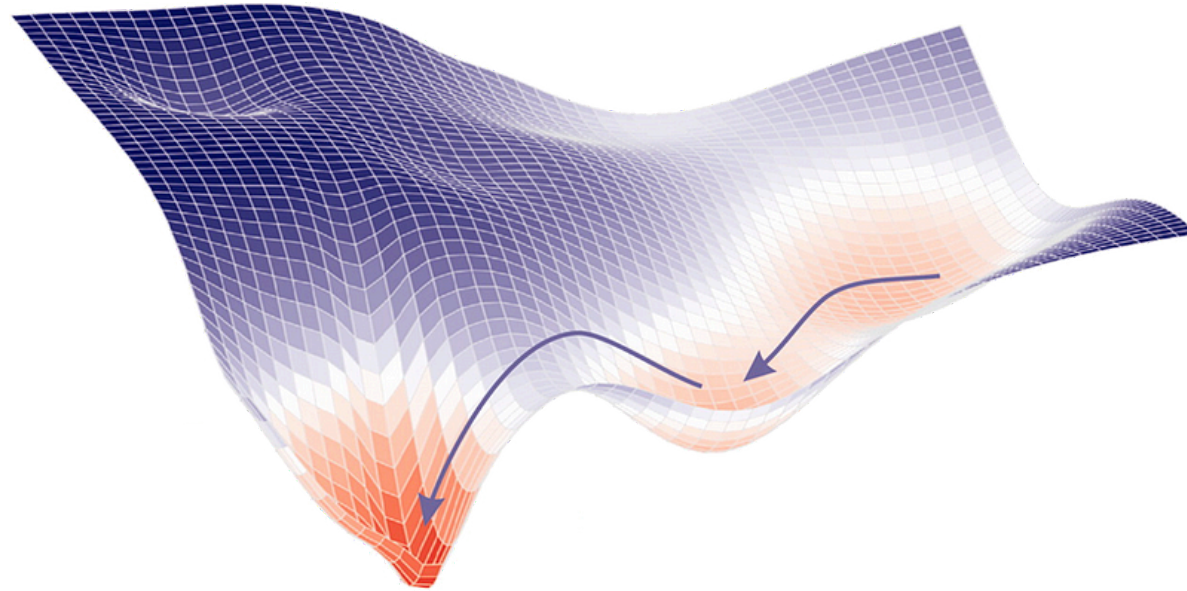
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Reason 2: For problems without analytical solutions, the gradient (slope) is necessary for gradient descent

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Review

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

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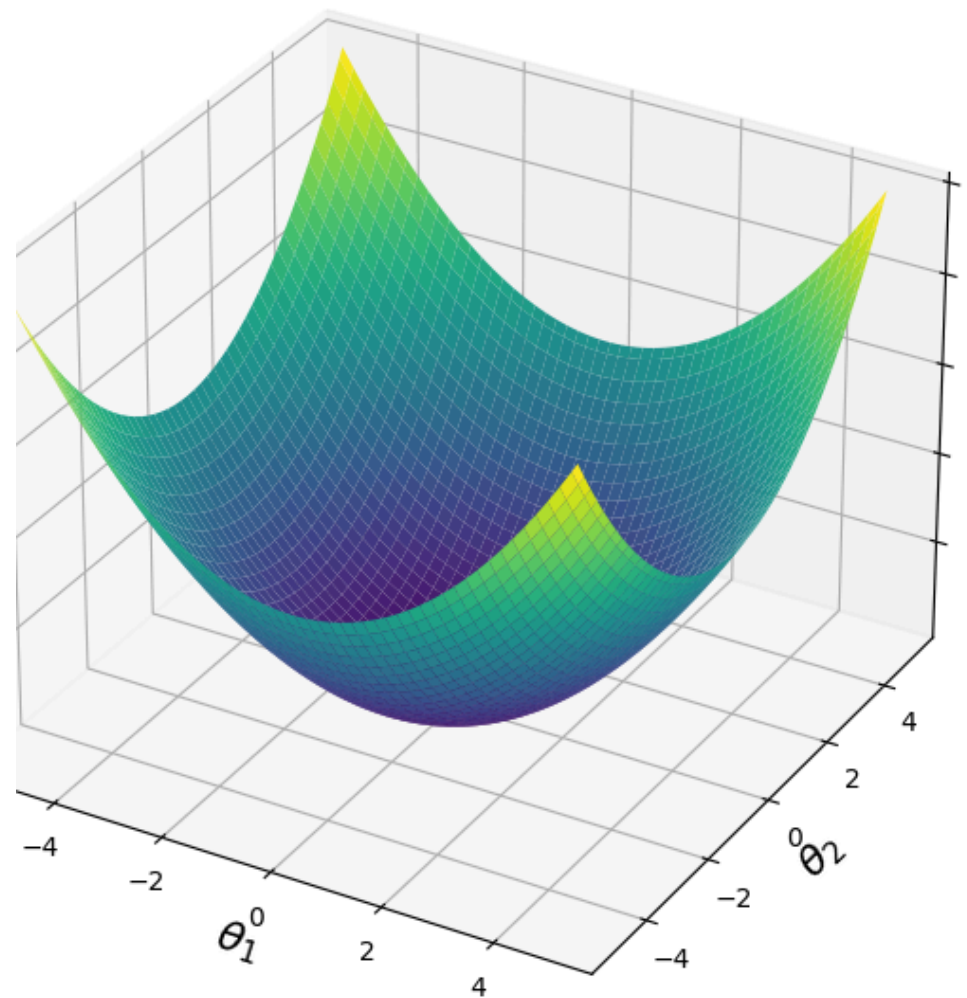
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$$\mathcal{L}(\mathbf{X}, \mathbf{Y}, \boldsymbol{\theta}) = \underbrace{(\mathbf{Y} - \mathbf{X}_D \boldsymbol{\theta})^\top}_{\text{Linear function of } \boldsymbol{\theta}} \underbrace{(\mathbf{Y} - \mathbf{X}_D \boldsymbol{\theta})}_{\text{Linear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

Quadratic function of $\boldsymbol{\theta}$

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 θ

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$$\nabla_{\theta} \mathcal{L}(\mathbf{X}, \mathbf{Y}, \theta) = 0$$

$$\theta = (\mathbf{X}_D^{\top} \mathbf{X}_D)^{-1} \mathbf{X}_D^{\top} \mathbf{Y}$$

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Which solves

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

Review

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

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

Loss function

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

Neural network model

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Now, we plug the model f into the loss function

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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

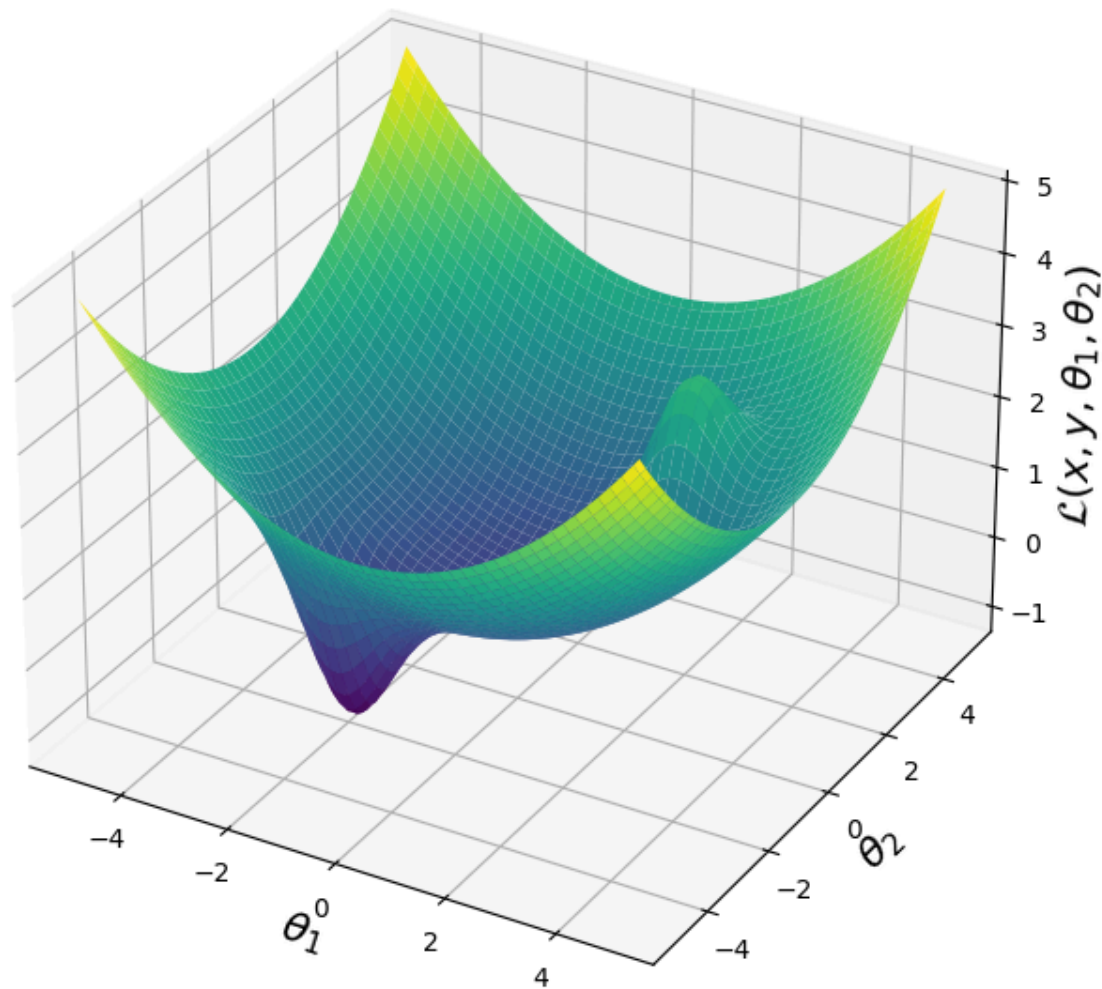
Review



Review



Review



Review

The gradient descent algorithm:

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

Review

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

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

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$$\nabla_{\theta} f(x, \theta) = \nabla_{\varphi, \psi, \dots, \xi} f(x, [\varphi \ \psi \ \dots \ \xi]^{\top}) = \begin{bmatrix} \nabla_{\varphi} f_1(x, \varphi) \\ \nabla_{\psi} f_2(z_1, \psi) \\ \vdots \\ \nabla_{\xi} f_{\ell}(z_{\ell-1}, \xi) \end{bmatrix}$$

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

Review

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

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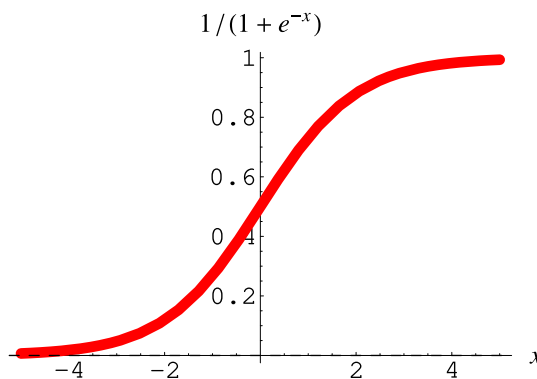
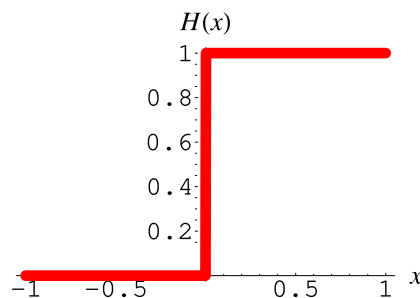
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We replaced it with a differentiable (soft) approximation called the sigmoid function

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

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

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

```
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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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

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

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Classification asks which one

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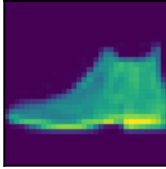
So far, we only looked at regression. Now, let us look at classification

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

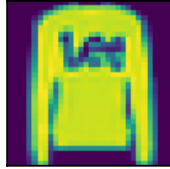
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$$X : \mathbb{Z}_{0,255}^{32 \times 32}$$

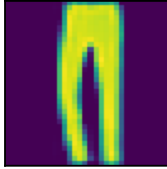
ankle boot



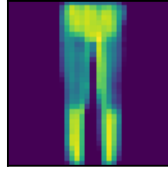
pullover



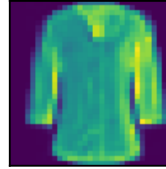
trouser



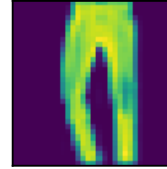
trouser



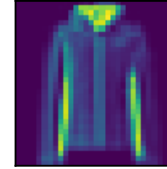
shirt



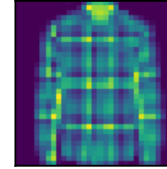
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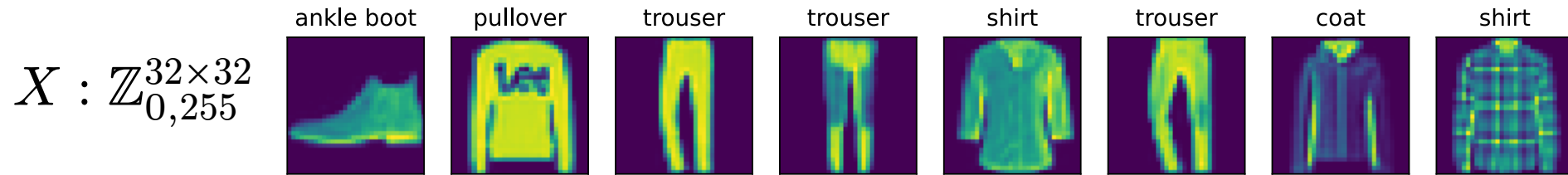
coat



shirt

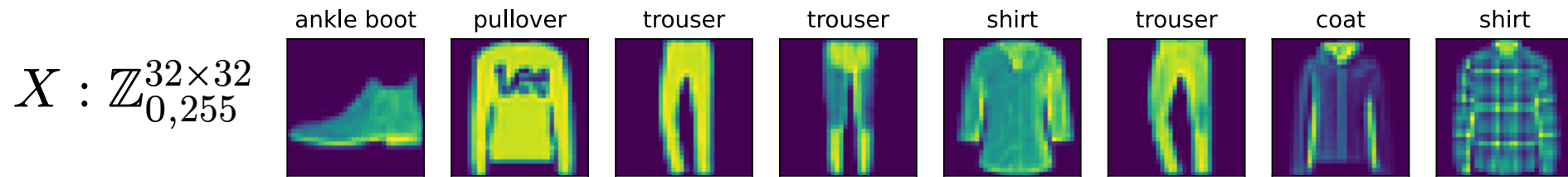


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$Y : \{\text{T-shirt, Trouser, Pullover, Dress, Coat, Sandal, Shirt, Sneaker, Bag, Ankle boot}\}$

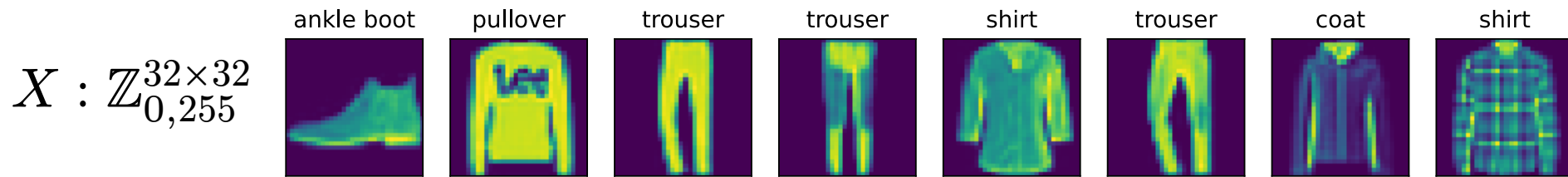
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Approach: Learn θ that produce **conditional probabilities**

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

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

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Outcome

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Experiment

Outcome

Flip a coin

Heads

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An experiment yields one of many possible outcomes

Experiment

Outcome

Flip a coin

Heads

Walk outside

Rain

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Walk outside

$S = \{\text{rain, sun, wind, cloud}\}$

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Experiment

Sample Space

Event

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Event

Flip a coin

$S = \{\text{heads, tails}\}$

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$E = \{\text{rain, wind}\}$

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

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

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Experiment

Probabilities

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Experiment

Probabilities

Flip a coin

$$P(\text{heads}) = 0.5$$

Walk outside

$$P(\text{rain}) = 0.15$$

The **probability** measures how likely an event is to occur

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

$$0 \leq P(A) \leq 1; \quad \forall A \in S$$

Experiment

Probabilities

Flip a coin

$$P(\text{heads}) = 0.5$$

Walk outside

$$P(\text{rain}) = 0.15$$

Take from closet

$$P(\text{Shirt}) = 0.1$$

When we define P as a function, we call it a **distribution**

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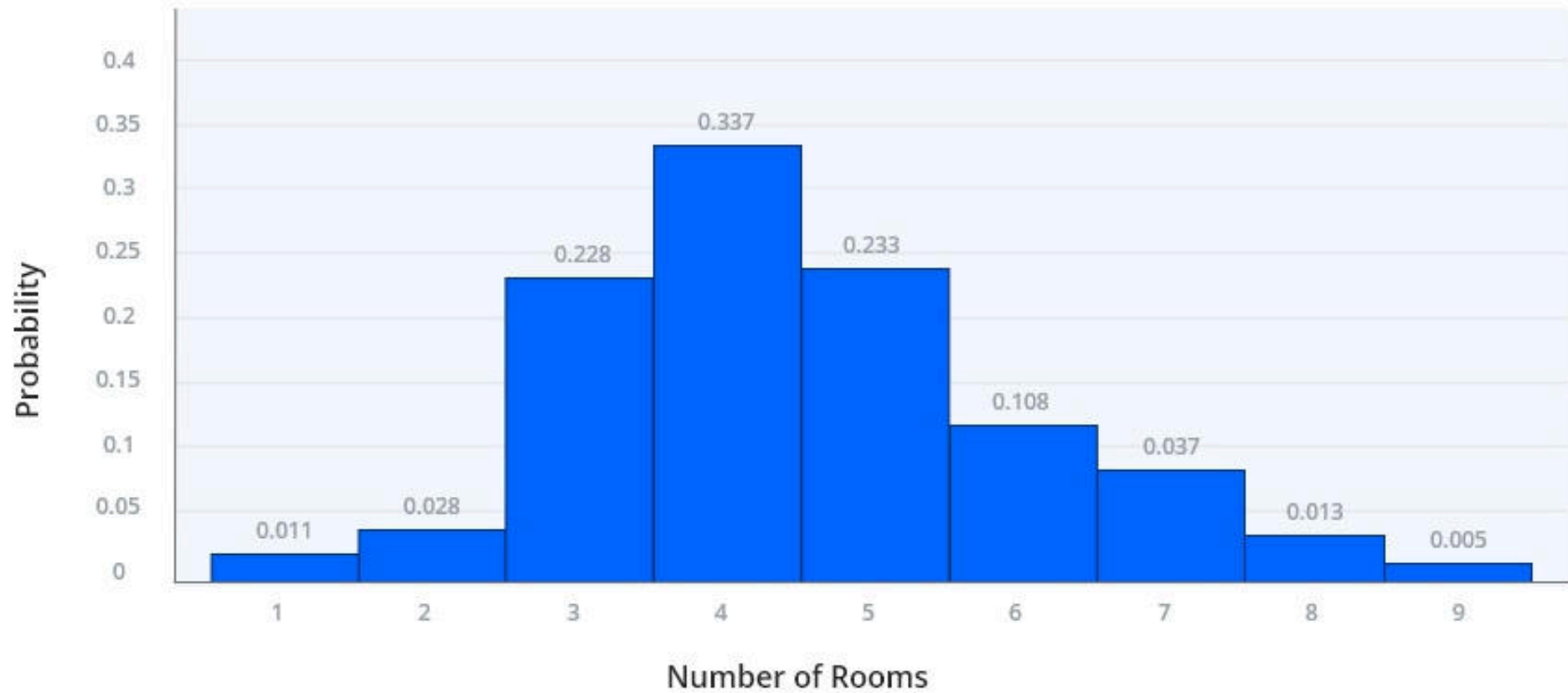
$$\sum_{x \in E} P(x) = 1$$

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

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

The distribution is a function, so we can plot it

Number of Rooms in Rental Unit



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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With disjoint events, $P(A \cap B) = 0$

Flip a coin

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

Be careful!

Walk outside

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

Events A is **conditionally dependent** on B if B occurring tells us about the probability of A

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$$P(A \mid B) = \frac{P(A \cap B)}{P(B)}$$

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

Walk outside

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

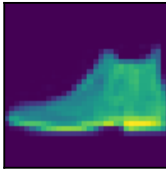
$$P(\text{Rain} \mid \text{Cloud}) = \frac{0.2}{0.4} = 0.5$$

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

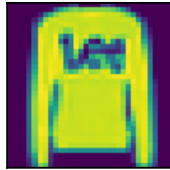
Task: Given a picture of clothes, predict the text description

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

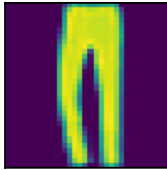
ankle boot



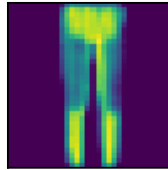
pullover



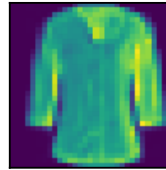
trouser



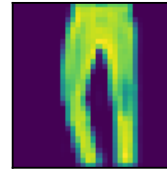
trouser



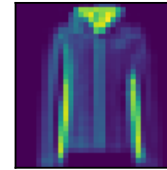
shirt



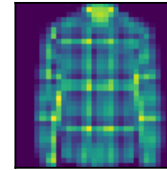
trouser



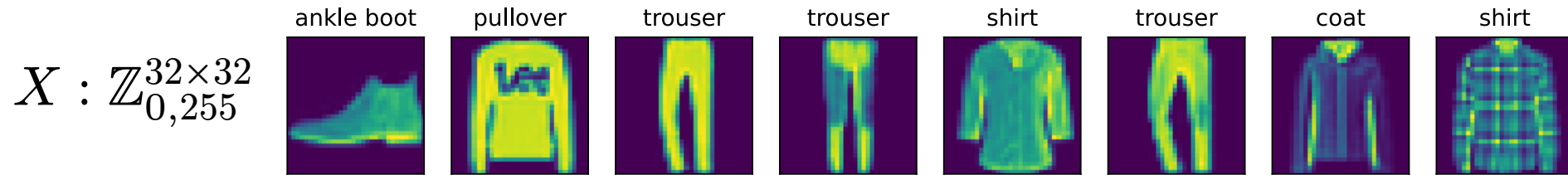
coat



shirt

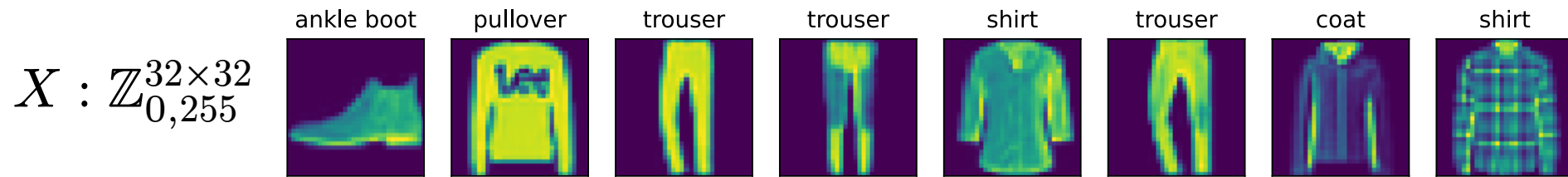


Task: Given a picture of clothes, predict the text description



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

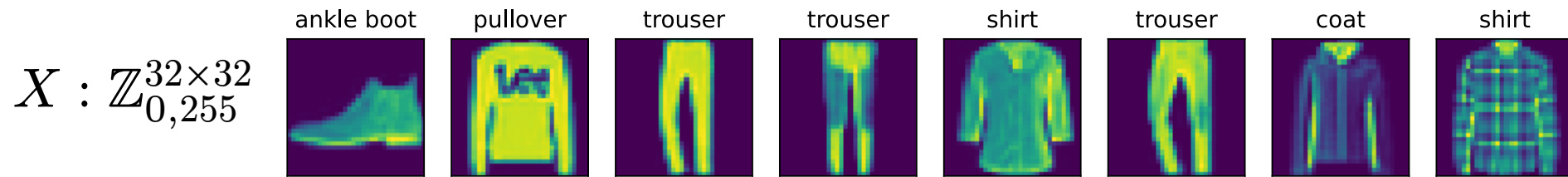
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Approach: Learn θ that produce **conditional probabilities**

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

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

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 θ that minimize \mathcal{L}
8. Coding

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Answer: No! Because probabilities must sum to one

How can we represent a distribution as a vector?

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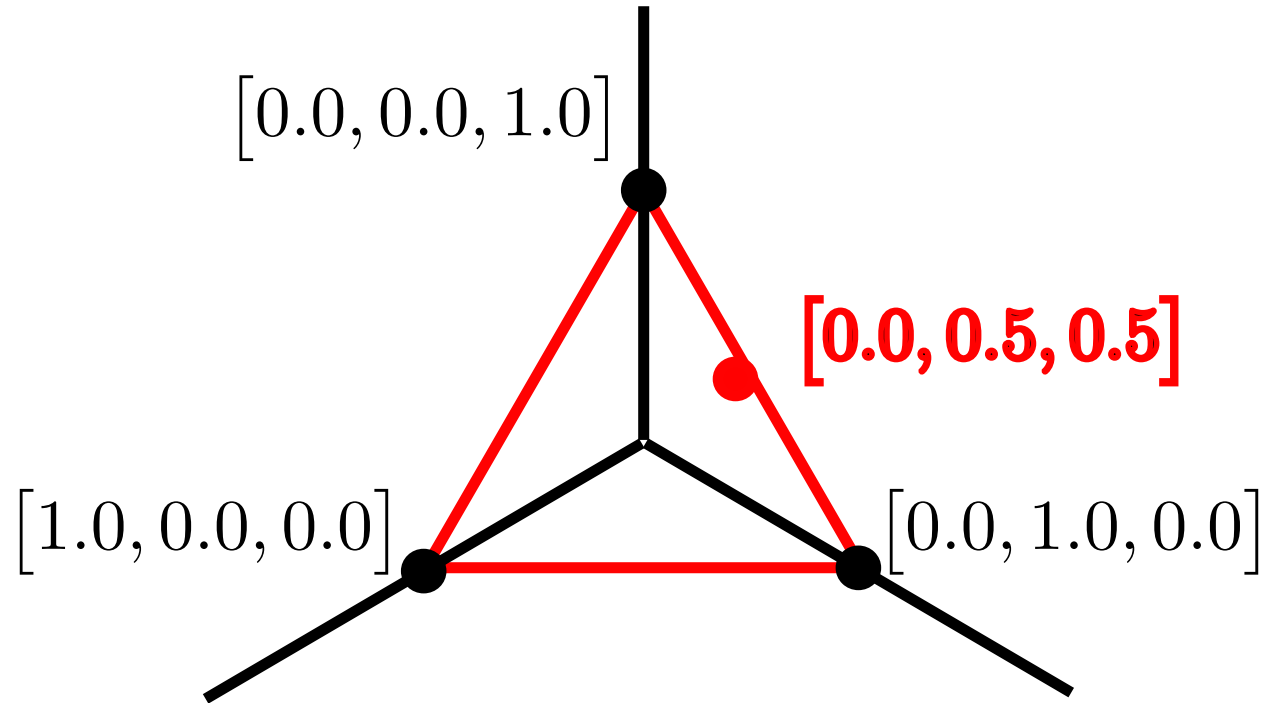
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$$\Delta^{d_y-1}$$

The simplex Δ^k is an $k - 1$ -dimensional triangle in k -dimensional space

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

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

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

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

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

$$\begin{aligned} f_1(\mathbf{x}, \boldsymbol{\varphi}) &= \sigma(\boldsymbol{\varphi}^\top \mathbf{x}) \\ &\vdots \\ f_\ell(\mathbf{x}, \boldsymbol{\xi}) &= \text{softmax}(\boldsymbol{\xi}^\top \mathbf{x}) \end{aligned}$$

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Now, our neural network can output probabilities

$$f(\mathbf{x}, \boldsymbol{\theta}) = \begin{bmatrix} P(\text{Ankle boot} \mid \text{img}) \\ P(\text{Bag} \mid \text{img}) \\ \vdots \end{bmatrix}$$

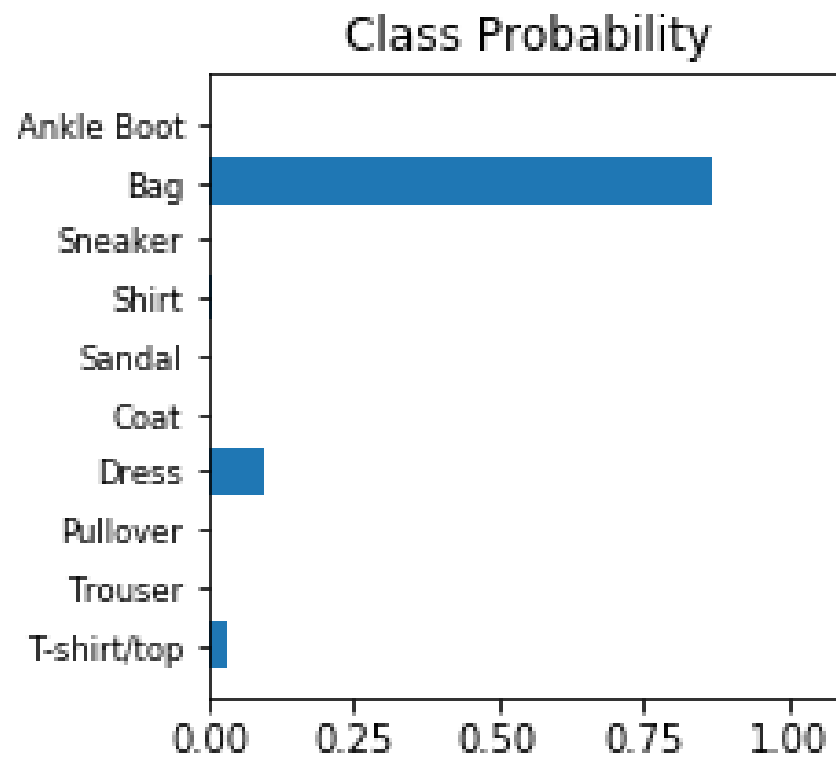
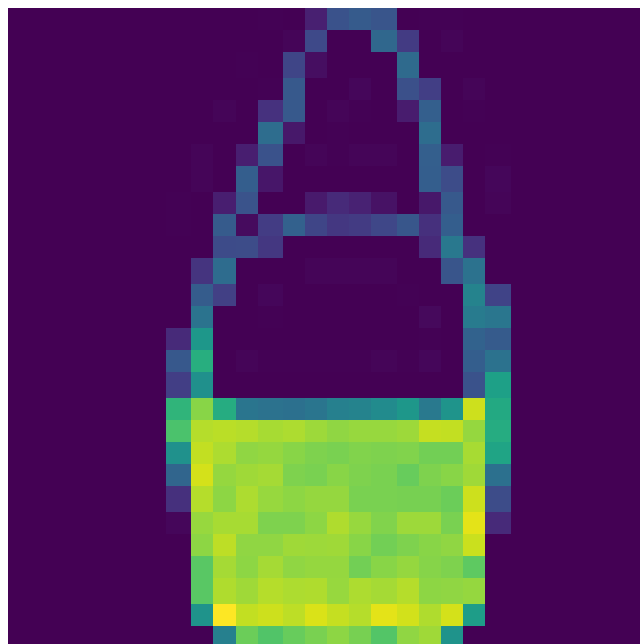
Question: Why do we output probabilities instead of a binary values

$$f(\mathbf{x}, \boldsymbol{\theta}) = \begin{bmatrix} P(\text{Shirt} \mid \text{Image}) \\ P(\text{Bag} \mid \text{Image}) \end{bmatrix}$$

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

Answer 1: Outputting probabilities results in differentiable functions

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



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Consider the following prediction and truth

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

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What loss function should we use for classification?

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

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We could use the square error like linear regression

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

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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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How do we measure the difference between probability distributions?

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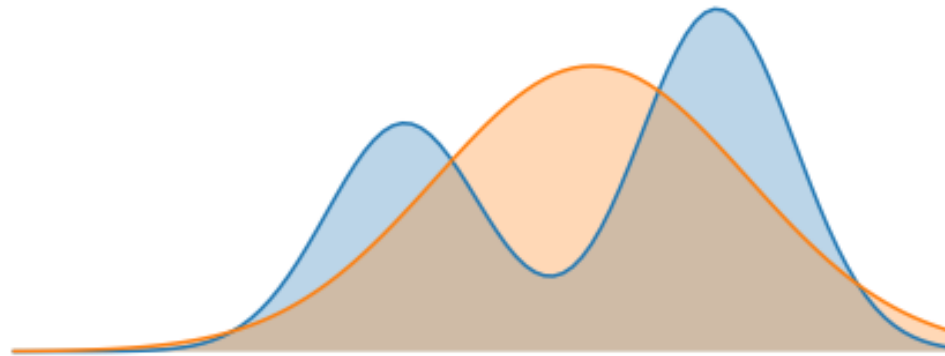
How do we measure the difference between probability distributions?

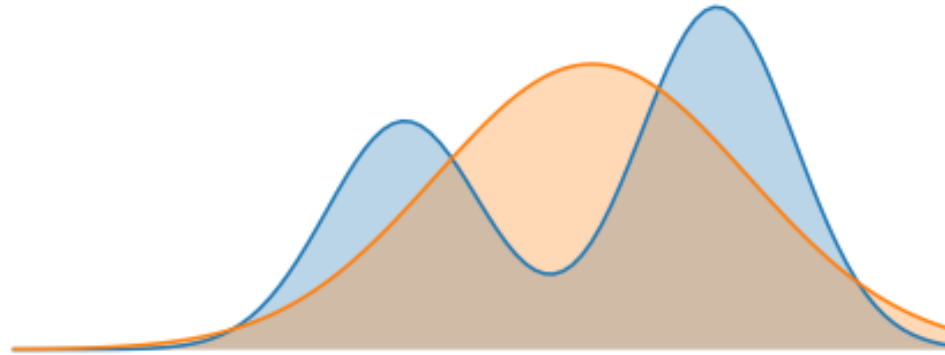
We use the **Kullback-Leibler Divergence (KL)**

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$$\text{KL}(P, Q) = \sum_i P(i) \log \frac{P(i)}{Q(i)}$$

First, write down KL-divergence

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Plug in our two distributions $P = f$ and $Q = y$

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

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Rewrite the logarithm using the sum rule of logarithms

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

Split the sum into two parts

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

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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

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

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

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$$f(\mathbf{x}, \boldsymbol{\theta}) = P(\mathbf{y} \mid \mathbf{x}) = P \left(\begin{bmatrix} \text{boot} \\ \text{dress} \\ \vdots \end{bmatrix} \mid \begin{img alt="A small, pixelated grayscale image of a boot, likely a Chelsea boot, used as an input example for the model." data-bbox="662 708 754 868"/> \right)$$

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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 θ that minimize \mathcal{L}
8. Coding

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Find θ just like before, using gradient descent

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$$\nabla_{\theta} \text{softmax}(\mathbf{z}) = \text{softmax}(\mathbf{z}) \odot (1 - \text{softmax}(\mathbf{z}))$$

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

Coding

<https://colab.research.google.com/drive/1BGMIE2CjlJOH-D2r9AariPDVgxjWlqG?usp=sharing>