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:

1. More coding, less theory

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- 2. More math/theory

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- 3. Too easy, go faster

- 1. More coding, less theory
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There are conflicting student needs

https://github.com/smorad/um_cisc_7026

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

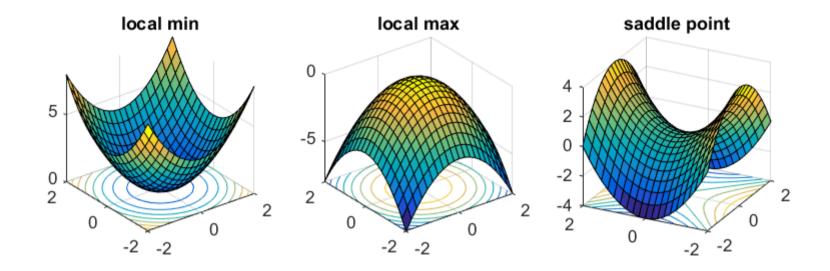
Gradients are important in deep learning for two reasons:

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Reason 1: f(x) has critical points at $\nabla_x f(x) = 0$

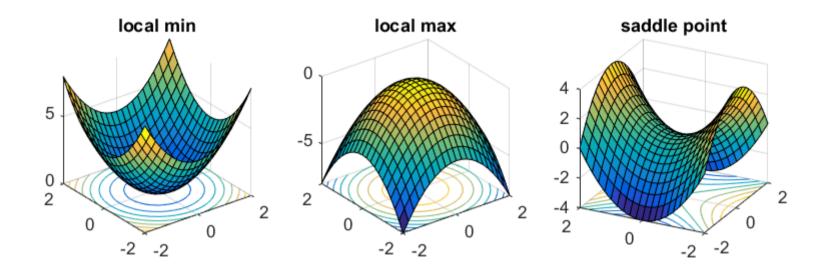
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With optimization, we attempt to find minima of loss functions

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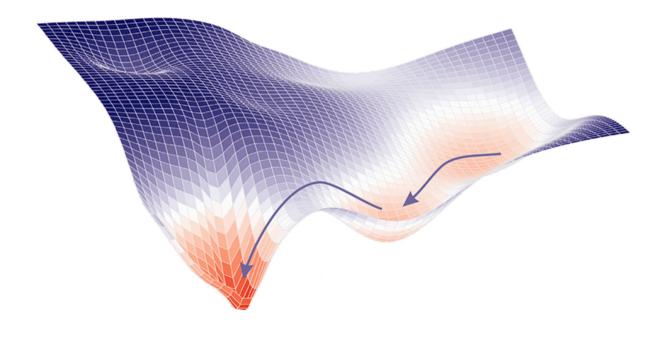
Gradients are important in deep learning for two reasons:

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

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



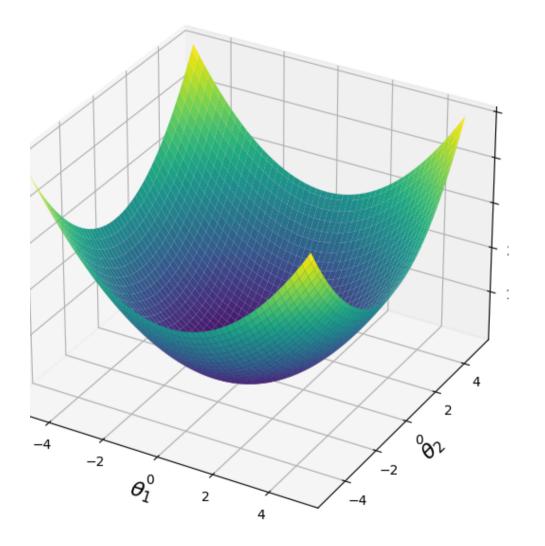
$$\mathcal{L}(oldsymbol{X},oldsymbol{Y},oldsymbol{ heta}) = \sum_{i=1}^n \left(fig(oldsymbol{x}_{[i]},oldsymbol{ heta}ig) - oldsymbol{y}_{[i]}
ight)^2$$

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

$$egin{aligned} \mathcal{L}(m{X}, m{Y}, m{ heta}) &= \sum_{i=1}^n \left(fig(m{x}_{[i]}, m{ heta}ig) - m{y}_{[i]} ig)^2 \\ \mathcal{L}(m{X}, m{Y}, m{ heta}) &= (m{Y} - m{X}_D m{ heta})^{ op} (m{Y} - m{X}_D m{ heta}) \\ \mathcal{L}(m{X}, m{Y}, m{ heta}) &= \underbrace{(m{Y} - m{X}_D m{ heta})^{ op}}_{ ext{Linear function of } m{ heta}} \underbrace{(m{Y} - m{X}_D m{ heta})}_{ ext{Linear function of } m{ heta}} \\ &= \underbrace{(m{Y} - m{X}_D m{ heta})^{ op}}_{ ext{Quadratic function of } m{ heta}} \underbrace{(m{Y} - m{X}_D m{ heta})}_{ ext{Constrainty}} \underbrace{(m{Y} - m{X}_D m{ heta})}_{ ext{Quadratic function of } m{ heta}} \end{aligned}$$

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



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Which solves

$$rg\min_{oldsymbol{ heta}} \mathcal{L}(oldsymbol{X}, oldsymbol{Y}, oldsymbol{ heta})$$

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

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

Loss function

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 heta

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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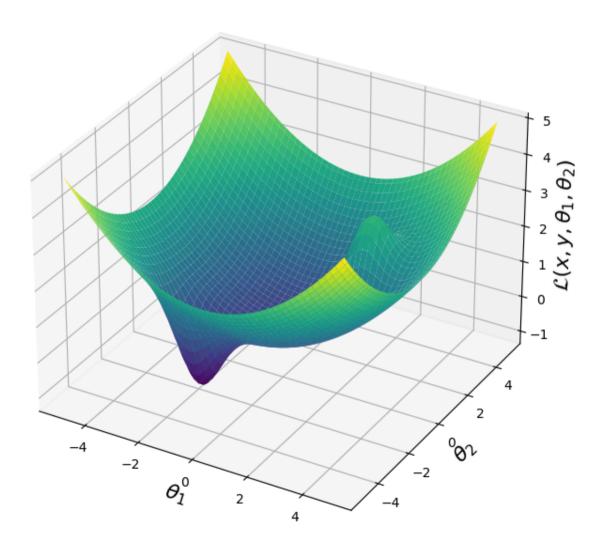
Gradient descent is an optimization method for differentiable functions

We went over both the intuition and mathematical definitions









The gradient descent algorithm:

```
1:function Gradient Descent(\boldsymbol{X}, \boldsymbol{Y}, \mathcal{L}, t, \alpha)
```

- 2: > Randomly initialize parameters
- 3: $\theta \leftarrow \mathcal{N}(0,1)$
- 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: b Update the parameters using the negative gradient
- 8: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} \alpha \boldsymbol{J}$
- 9: return θ

$$abla_{m{ heta}} \mathcal{L}(m{X}, m{Y}, m{ heta}) = \sum_{i=1}^n 2ig(fig(m{x}_{[i]}, m{ heta}ig) - m{y}_{[i]}ig)
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$$\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)$$

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

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

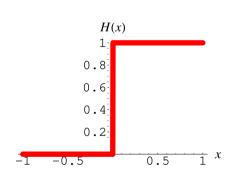
We ran into issues computing the gradient of a layer because of the Heaviside step function

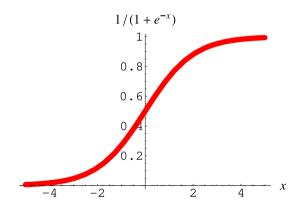
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We replaced it with a differentiable (soft) approximation called the sigmoid function

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

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

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 = 0.0001theta = theta - alpha * J

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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Torch Optimization Coding

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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Lecture 5: Classification

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

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Regression asks how many

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Regression asks how many

• How long will I live?

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- How long will I live?
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• Is this a dog or muffin?

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- How long will I live?
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- Is this a dog or muffin?
- Will it rain tomorrow? Yes or no?

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- How long will I live?
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Classification asks which one

- Is this a dog or muffin?
- Will it rain tomorrow? Yes or no?
- What color is this object?

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Regression asks how many

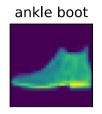
- How long will I live?
- How much rain will there be tomorrow?
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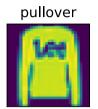
Classification asks which one

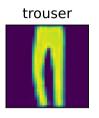
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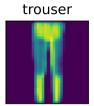
So far, we only looked at regression. Now, let us look at classification

 $X:\mathbb{Z}_{0,255}^{32 imes32}$

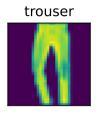


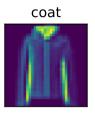


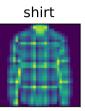






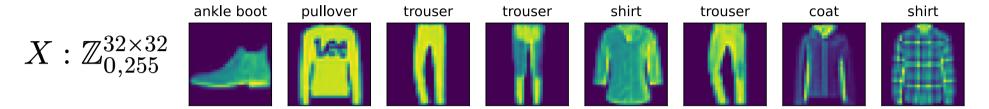






 $X: \mathbb{Z}_{0,255}^{32 imes 32}$ ankle boot pullover trouser trouser shirt trouser coat shirt $X: \mathbb{Z}_{0,255}^{32 imes 32}$

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



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

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

 $X: \mathbb{Z}_{0,255}^{32 imes32}$ ankle boot pullover trouser trouser shirt trouser coat shirt $X: \mathbb{Z}_{0,255}^{32 imes32}$

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

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

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

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An experiment yields one of many possible outcomes

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Experiment

Outcome

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

An experiment yields one of many possible outcomes

Experiment

Outcome

Flip a coin

Heads

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

An experiment yields one of many possible outcomes

Experiment Outcome

Flip a coin Heads

Walk outside Rain

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

An experiment yields one of many possible outcomes

Experiment Outcome

Flip a coin Heads

Walk outside Rain

Grab clothing from closest Coat

Experiment

Sample Space S

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

Experiment

Sample Space S

Flip a coin

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

Walk outside

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

Experiment

Sample Space S

Flip a coin

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

Walk outside

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

Take clothing from closet

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

Experiment

Sample Space

Event

Experiment

Sample Space

Event

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

$$E = \{\text{heads}\}$$

Experiment

Sample Space

Event

Flip a coin

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

$$E = \{\text{heads}\}$$

Walk outside

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

Experiment

Sample Space

Event

Flip a coin

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

$$E = \{\text{heads}\}$$

Walk outside

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

{T-shirt, Trouser,

Take from closet

$$\frac{\text{Pullover, Dress,}}{\text{Coat, Sandal, Shirt,}} E = \{\text{Shirt, T-Shirt, Coat}\}$$

Sneaker, Bag, Ankle boot}

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

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$$0 \le P(E) \le 1$$

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Experiment

Probabilities

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

$$0 \le P(E) \le 1$$

Experiment

Flip a coin

Probabilities

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

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

$$0 \le P(E) \le 1$$

Experiment

Flip a coin

Walk outside

Probabilities

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

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

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

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

$$0 \le P(E) \le 1$$

Experiment

Flip a coin

Walk outside

Take from closet

Probabilities

P(heads) = 0.5

P(rain) = 0.15

P(Shirt) = 0.1

$$P: E \mapsto (0,1)$$

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The probabilities (distribution) over the sample space S must sum to one

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

$$P: E \mapsto (0,1)$$

The probabilities (distribution) over the sample space S must sum to one

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

Flip a coin

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

$$P: E \mapsto (0,1)$$

The probabilities (distribution) over the sample space S must sum to one

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

Flip a coin

Take clothing from closet

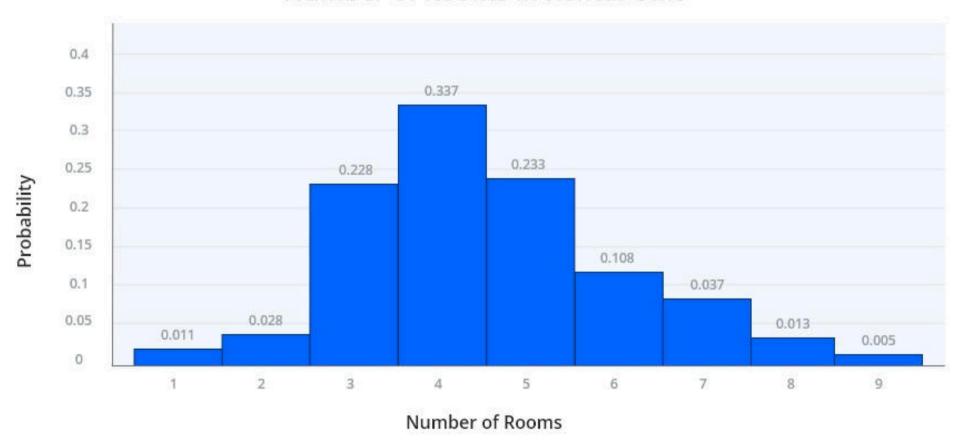
$$\{P(\text{heads}) = 0.5, P(\text{tails}) = 0.5\}$$

$$\{P(\text{T-shirt}) = 0.1, P(\text{Trouser}) = 0.08,$$

$$P(\text{Pullover}) = 0.12, ...\}$$

The distribution is a function, so we can plot it

Number of Rooms in Rental Unit



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

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

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

Be careful!

Walk outside

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

 $P(\text{Rain} \cap \text{Sun}) \neq 0$

$$P(\text{cloud}) = 0.2, P(\text{rain}) = 0.1$$

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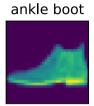
Walk outside

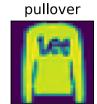
$$P(\text{Rain} \cap \text{Cloud}) = 0.1$$

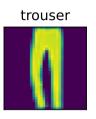
$$P(\text{Cloud}) = 0.2$$

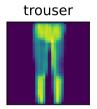
$$P(\text{Rain} \mid \text{Cloud}) = \frac{0.1}{0.2} = 0.5$$

 $X:\mathbb{Z}_{0,255}^{32 imes32}$

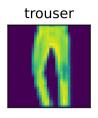


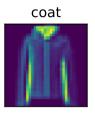


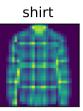






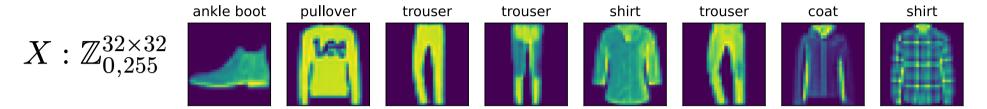






 $X: \mathbb{Z}_{0,255}^{32 imes 32}$ ankle boot pullover trouser trouser shirt trouser coat shirt $X: \mathbb{Z}_{0,255}^{32 imes 32}$

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



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

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

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- 1. Review
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We want our model to predict the probability of each outcome

Question: What is the function signature of f?

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

Question: Can we use this model to predict probabilities?

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

How can we represent a probability distribution for a neural network?

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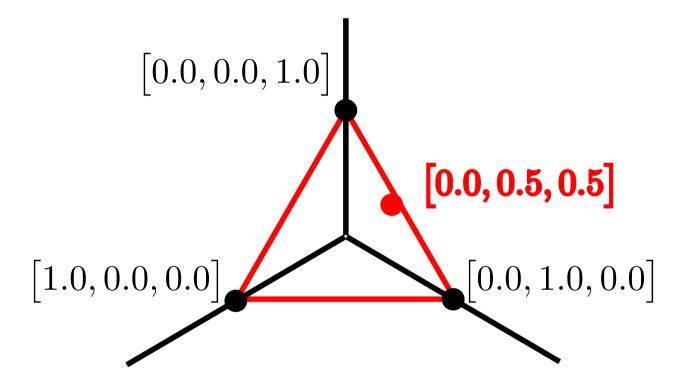
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$$\Delta^{d_y-1}$$

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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So we need a function that maps to the simplex

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

Then, we can combine f and g

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

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

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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

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

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

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

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

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Now, our neural network can output probabilities

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

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

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

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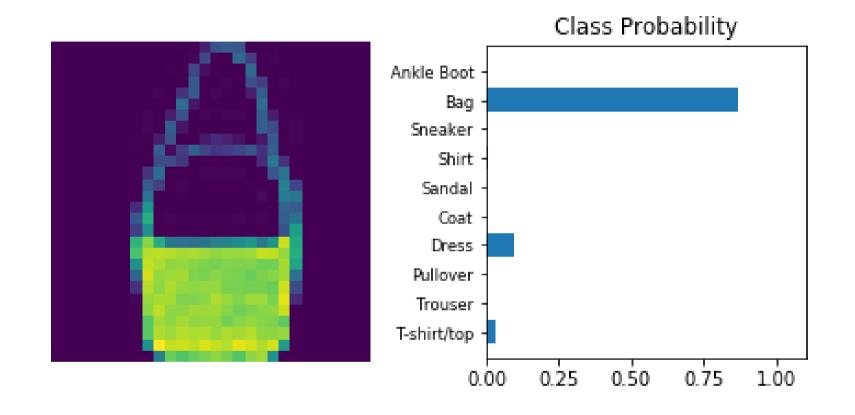
Answer 1: Outputting probabilities results in differentiable functions

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Answer 1: Outputting probabilities results in differentiable functions

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



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Consider the following prediction and truth

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What loss function should we use for classification?

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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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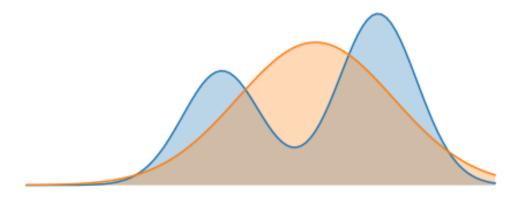
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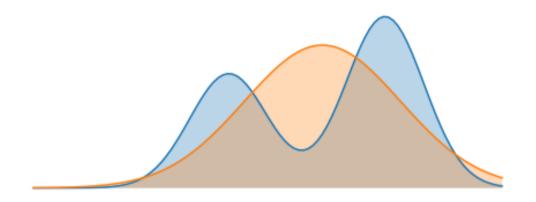
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First, write down KL-divergence

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Plug in our two distributions P = f and Q = 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 $\arg\min_{\theta} \mathcal{L} + k = \arg\min_{\theta} \mathcal{L}$. 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

$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\theta}) = -\sum_{i=1}^{d_y} P(y_i \mid \boldsymbol{x}) \log f(\boldsymbol{x}, \boldsymbol{\theta})_i; \quad f(\boldsymbol{x}, \boldsymbol{\theta}) = \begin{bmatrix} 0.6 \\ 0.4 \end{bmatrix}; \quad \boldsymbol{y} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

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Agenda

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- 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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Find θ just like before, using gradient descent

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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

https://colab.research.google.com/drive/1BGMIE2CjlLJOH-D2r9 AariPDVgxjWlqG?usp=sharing

Admin

Homework 3 is released, you have two weeks to complete it

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https://colab.research.google.com/drive/1LainS20p6c3YVRFM4

XgHRBODh6dvAaT2?usp=sharing#scrollTo=q8pJST5xFt-p