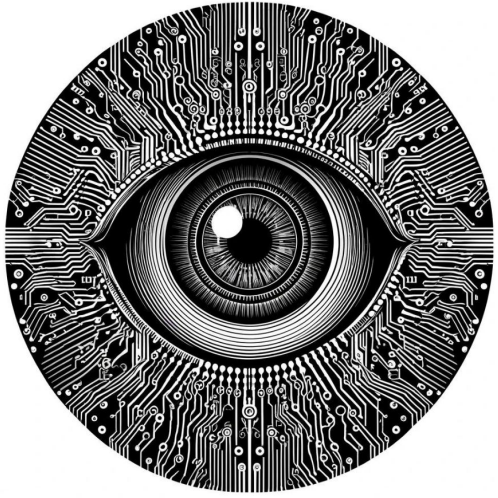
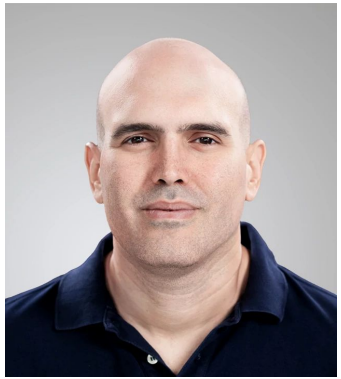
Workshop 6 - Multi-label Classification and Binary Cross Entropy Loss



Antonio Rueda-Toicen

About me

- AI Researcher at Hasso Plattner Institute, AI Engineer & DevRel for Voxel51
- Organizer of the Berlin Computer Vision Group
- Instructor at Nvidia's Deep Learning Institute and Berlin's Data Science Retreat
- Preparing a MOOC for OpenHPI (to be published in May)



LinkedIn

Step 1 - Discord Invite

https://discord.com/invite/fiftyone-community

Step 2 - Access Channel

https://discord.com/channels/1266527359511564372/1345119286041116763

#practical-computer-vision-workshops

Agenda

- Building a Feed Forward Network for Classification (review)
- Usage of Binary Cross Entropy Loss for multilabel classification

Notebooks

- Single label classification on pet images (review)
- Multilabel classification with binary cross entropy on satellite images

Dataset

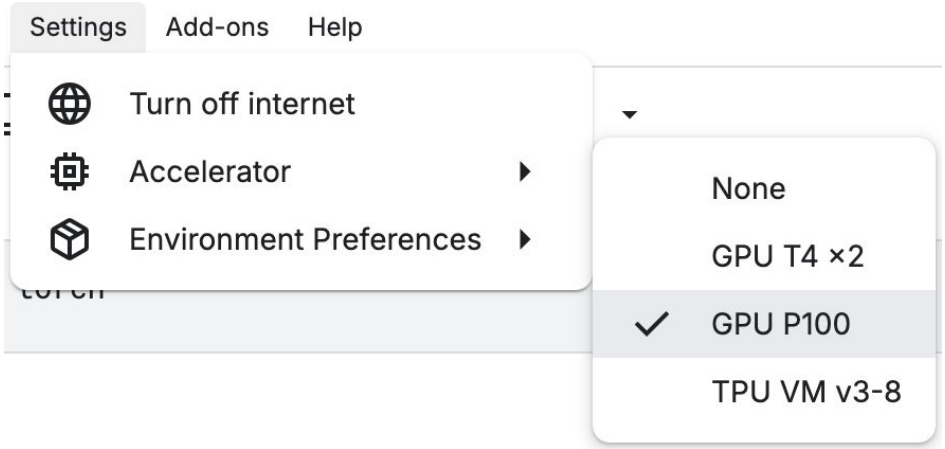
- Planet's dataset | Kaggle

Setup for today

- Setting up a Weights and Biases API token
- Setting up free GPU and TPU access in Kaggle Notebooks

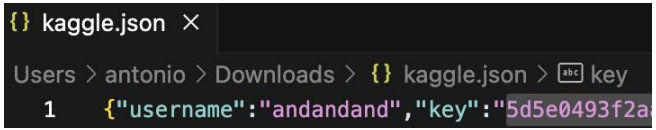
Kaggle Runtime Setup for Training

- Follow the Kaggle GPU Access Guide on our repository
- Settings -> Accelerator -> GPU P100



Google Colab Setup for Kaggle API keys

- Go to https://www.kaggle.com/settings and “Create New Token” on your API key
- Download and open the kaggle.json file



- In Google Colab, go to Secrets -> “Add New Secret”
- Create and enable KAGGLE_USERNAME and KAGGLE_KEY variables with the content of the JSON file

Residual block in Resnet18

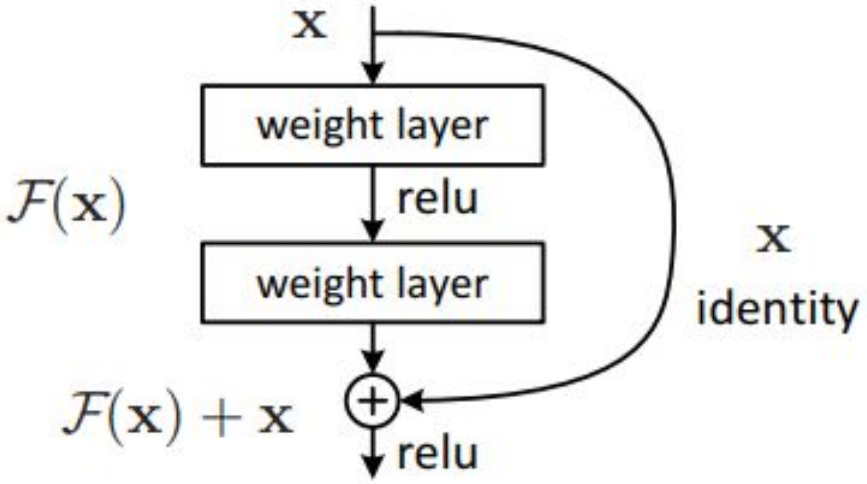


Diagram from [Deep Residual Learning for Image Recognition]

Understanding the Amazon from space

Planet: understanding the Amazon

The Planet satellite constellation

Tiny satellites show us the Earth as it changes in near-real-time | TED Talk

Planet’s Amazon Dataset on Kaggle

PLANET · FEATURED PREDICTION COMPETITION · 8 YEARS AGO

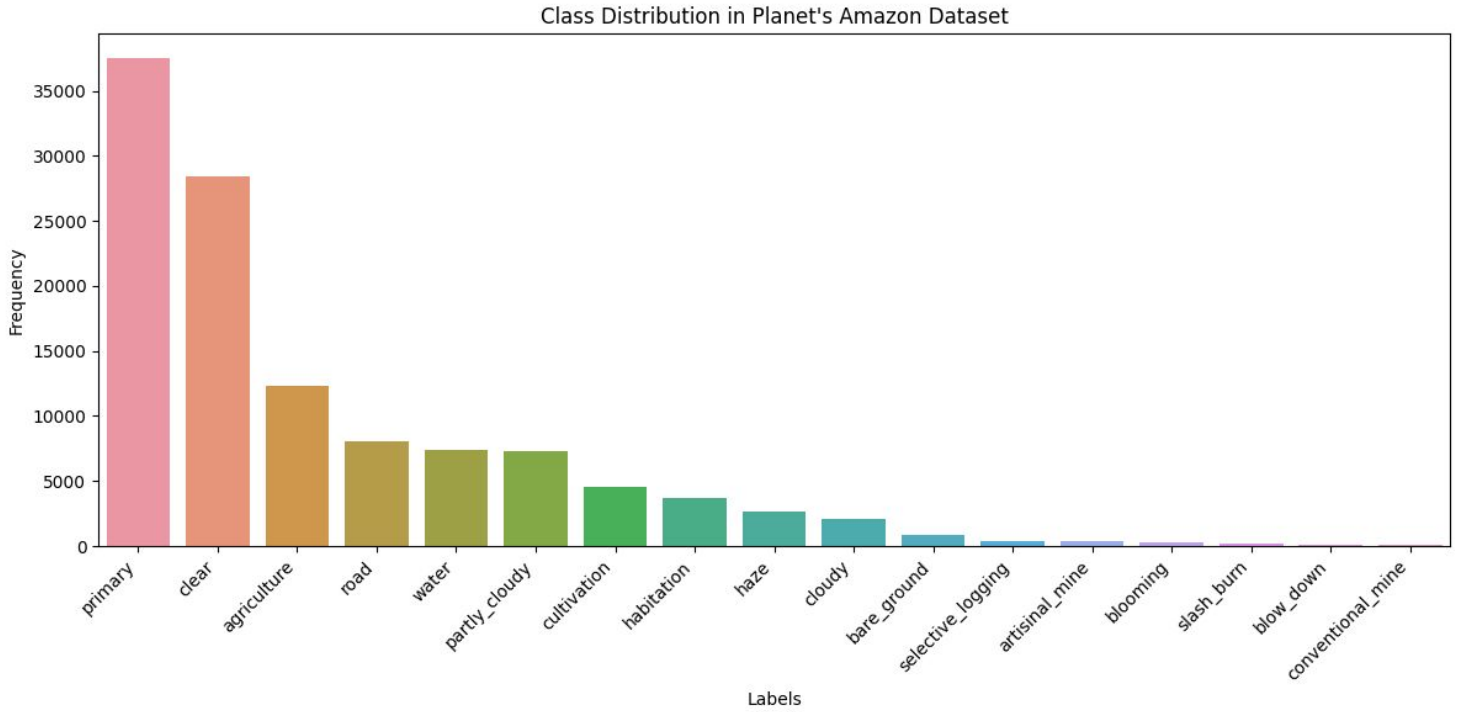
Late Submission

Planet: Understanding the Amazon from Space

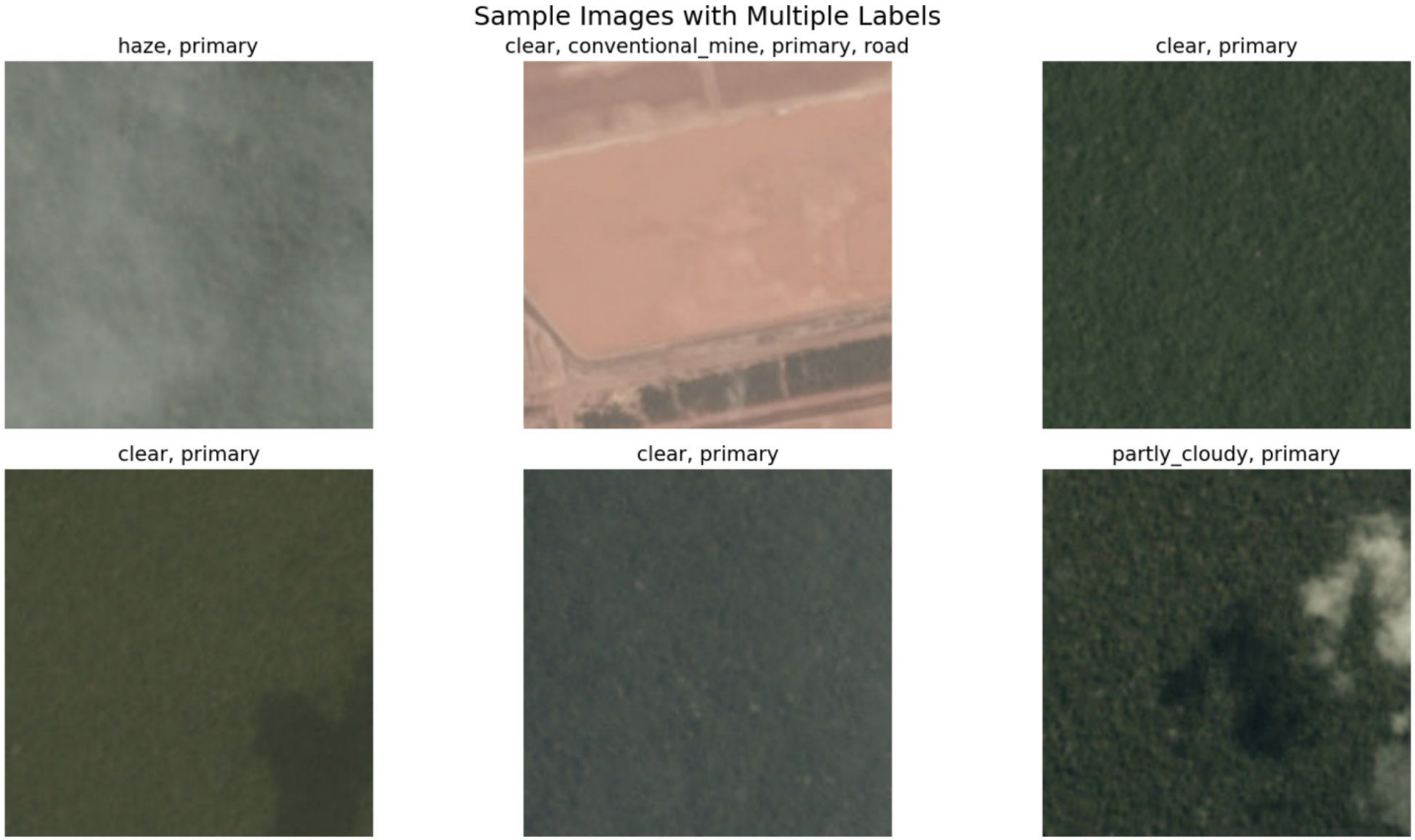
Use satellite data to track the human footprint in the Amazon rainforest

[Competition page on Kaggle]

Our class distribution is unbalanced



Our images have multiple labels



How we create a FiftyOne dataset

DATASET

Tags | Names | Classes | Description | ...

SAMPLE 0

ID | Filepath | Tags | Label | Field

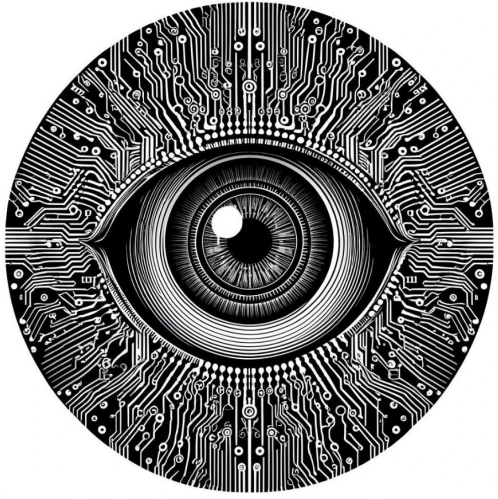
SAMPLE 1

ID | Filepath | Tags | Label | Field

SAMPLE 2

ID | Filepath | Tags | Label | Field

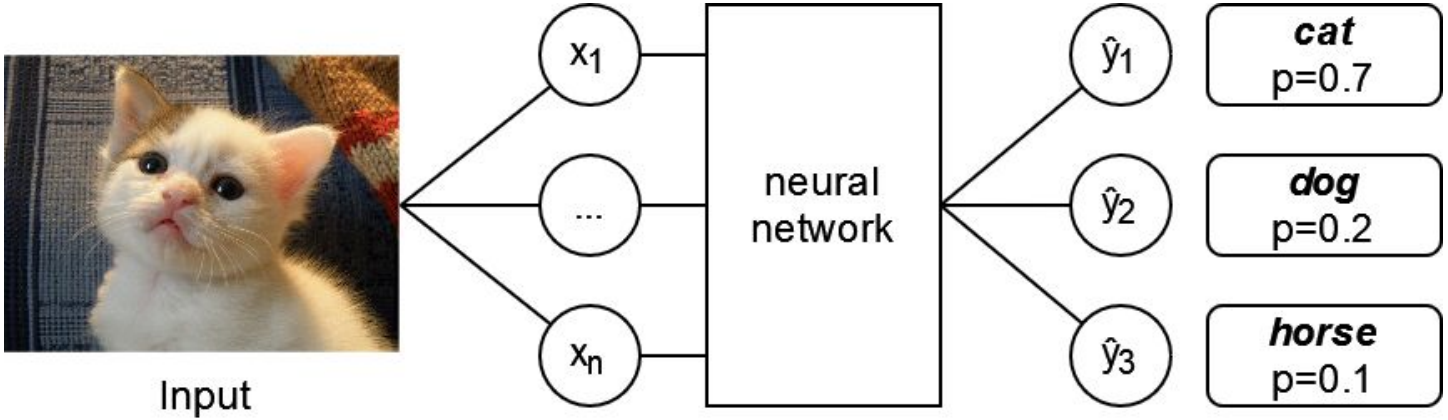
Building a Feedforward Network for Classification in PyTorch



Learning goals

- Create a multilayer neural network for classification in PyTorch
- Gain familiarity with the nn.Module syntax for network creation
- Understand usage of the softmax activation function
- Develop intuitions on Categorical Cross Entropy
- Use the Adam variant of stochastic gradient descent

Multiclass classification: n probabilities for n classes



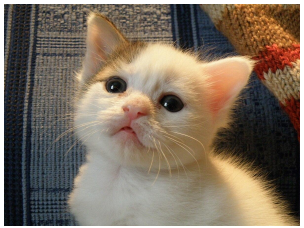
Classification $P(\hat{y}_{\text{cat}}) + P(\hat{y}_{\text{dog}}) + P(\hat{y}_{\text{horse}}) = 1$

Cross entropy loss

$y = 1.0$ $\hat{y} = 0.75$

$$H(p,q) = -\frac{1}{n}\sum_{i=1}^{n} p(x_i)\log q(x_i)$$

Labels y_i map to $p(x_i)$, predictions $\hat{y}_i$ map to $q(x_i)$. Suppose that we show the network, only the following image (n=1).



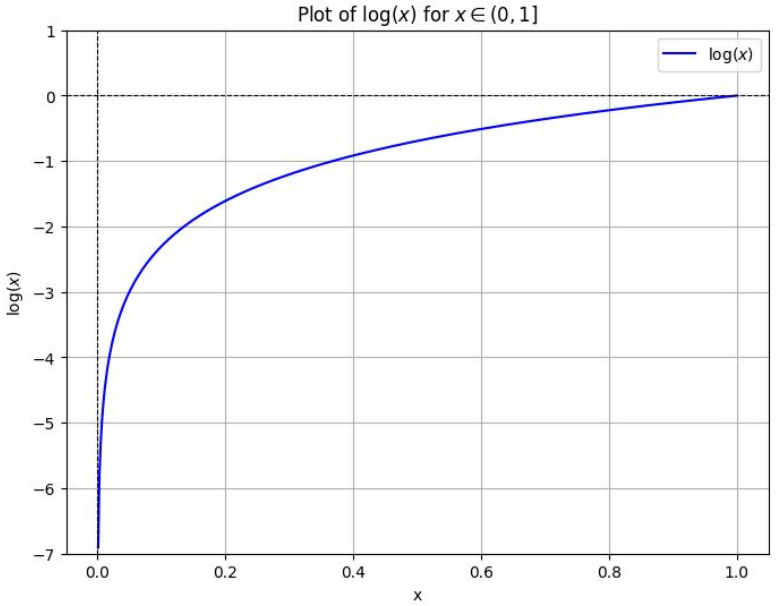
"one hot encoding" 🔥 = only one true label

The label for the image is encoded as y = [1, 0, 0] (i = 0 = cat, i = 1 = dog, i = 2 = horse)

- First the network outputs **$\hat{y}$ = [0.75, 0.25, 0.0]**
- Then the network outputs **$\hat{y}$ = [0.99, 0.01, 0.0]** **(if trained correctly)**

Intuition for the log function in cross entropy loss

$$y = [1, 0, 0] \quad \text{where} \quad i = 0\ (\text{cat}),\ i = 1\ (\text{dog}),\ i = 2\ (\text{horse})$$



$$\ln(1) = \log(1) = 0$$

$$y_0 = 1 \quad \text{and} \quad \hat{y}_0 = 1$$

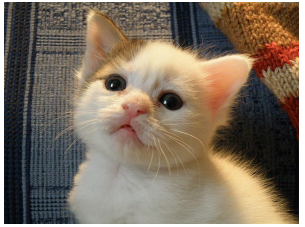
$$\text{Cross Entropy Loss} = -1 \cdot \log(1) = 0 \quad \text{(perfect prediction, no loss)}$$

$$y_0 = 1 \quad \text{and} \quad \hat{y}_0 = 0.01$$

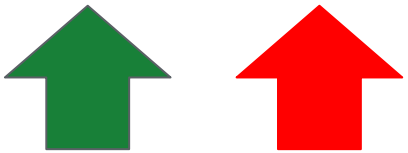
$$\text{Cross Entropy Loss} = -(1 \cdot \log(0.01)) = 4.65 \quad \text{(bad prediction, high los}$$

Implementing cross entropy loss from probabilities for a single sample

```python
import torch

# Example predicted probabilities from model
y_hat = torch.tensor([0.75, 0.25, 0.0])

# True label: y = [1, 0, 0]
y = torch.tensor([1, 0, 0], dtype=torch.float32)

def cross_entropy(y, y_hat):
    epsilon = 1e-15 # equal to 1 times 10^-15 (very small number)
    # Adding epsilon prevents log(0) which is undefined
    log_probs = torch.log(y_hat + epsilon)
    # Notice that the sum would only give a value different
    # than zero on the index of true_label
    # we are computing a single sample
    # so n = 1 (batch dimension)
    return -torch.sum(y * log_probs)

loss = cross_entropy(y, y_hat)
# Gives us tensor(0.287), not perfect, but not the worst possible
```



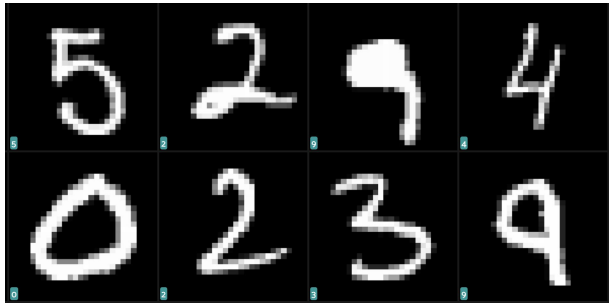
`y = [1, 0, 0]` `y_hat = [0.75, 0.25, 0.0]`



$$H(y, \hat{y}) = -\frac{1}{n} \sum_{i=1}^{n} y_i \log \hat{y}_i$$

A minimal network for classification

```python
import torch.nn as nn

# Model
model = nn.Sequential(

    # Flatten the input image
    nn.Flatten(),

    # The number of input features is the number of pixels in the image
    nn.Linear(in_features=28 * 28, out_features = 128),

    # We add a non-linearity
    nn.ReLU(),

    # We create 10 scores, aka 'logits', one for each class that we have
    # Notice that there is no ReLU after nn.Linear
    nn.Linear(in_features=128, out_features = 10)
)
```



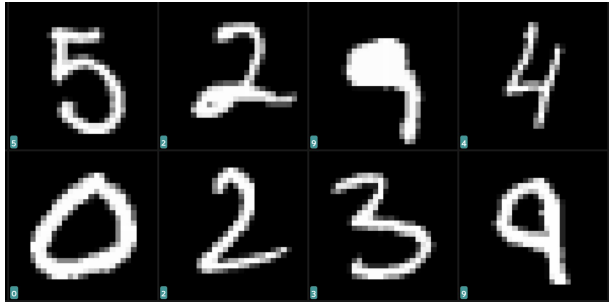
Tip: do not confuse these "logits" with the function described on https://en.wikipedia.org/wiki/Logit

$$f(x) = \ln\left(\frac{x}{1-x}\right)$$

❌ these "logits" are **not** this ^

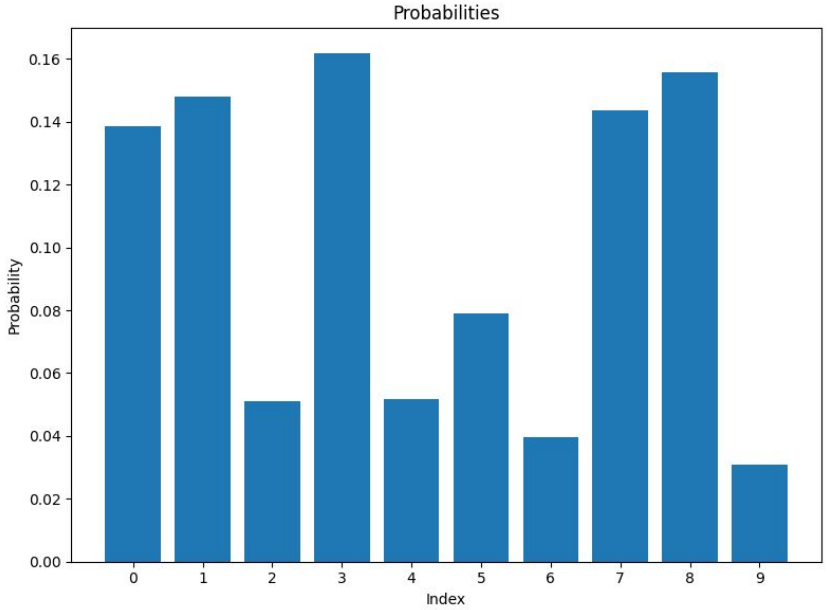
Using the nn.Module syntax

```
import torch.nn as nn

class MNISTClassifier(nn.Module):
    def __init__(self):
        super().__init__()
        # Instead of Sequential, we define each module as a class attribute
        self.flatten = nn.Flatten()
        self.fc1 = nn.Linear(in_features=28 * 28, out_features=128)
        self.relu = nn.ReLU()
        self.fc2 = nn.Linear(in_features=128, out_features=10)

    def forward(self, x):
        # Define the forward pass and set a breakpoint
        import pdb; pdb.set_trace()
        x = self.flatten(x)
        x = self.fc1(x)
        x = self.relu(x)
        x = self.fc2(x) # notice no relu here
        return x

# Create an instance of the model
model = MNISTClassifier()
```

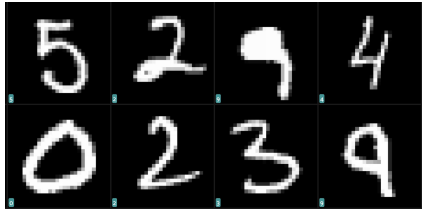


The softmax function

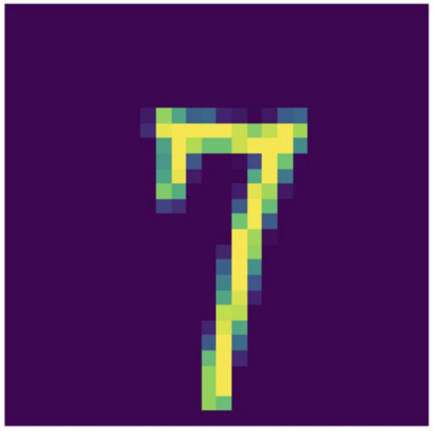
$$\text{Softmax}(x_i) = \frac{\exp(x_i)}{\sum_j \exp(x_j)}$$

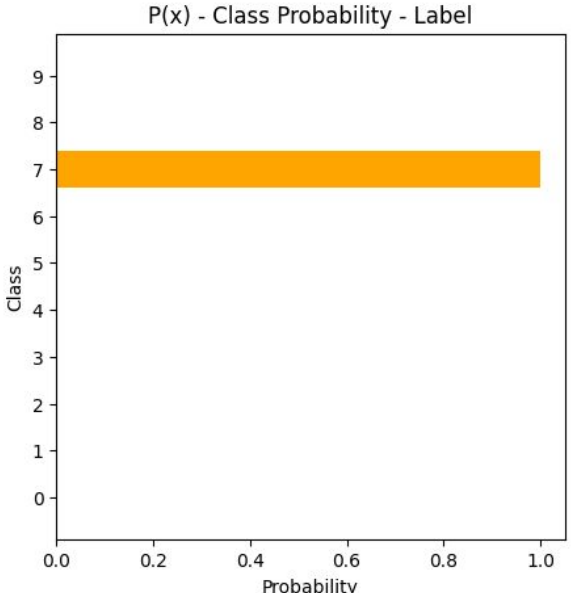


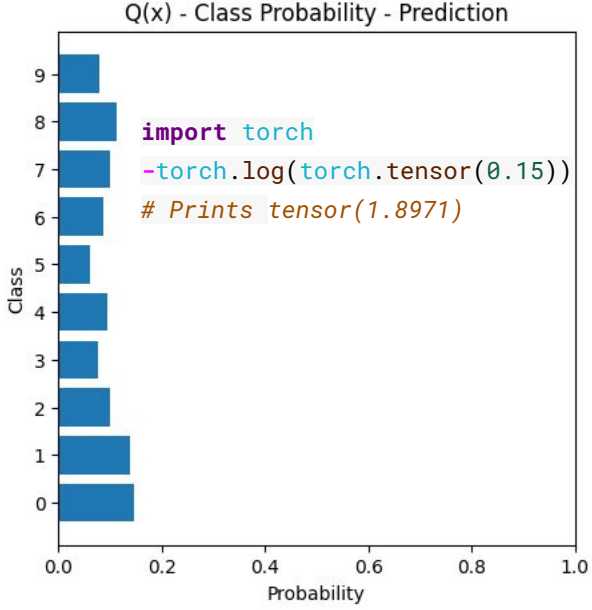

```
import torch.nn.functional as F
logits = torch.tensor([ 0.7645,  0.8300, -0.2343,  0.9186, -0.2191,  0.2018, -0.4869,  0.8000, 0.8815, -0.7336])
probabilities = F.softmax(logits, dim=0)
print(probabilities.sum()) # prints tensor(1.00)
```



High cross entropy loss - high disagreement between P(x) = y and Q(x) = ŷ

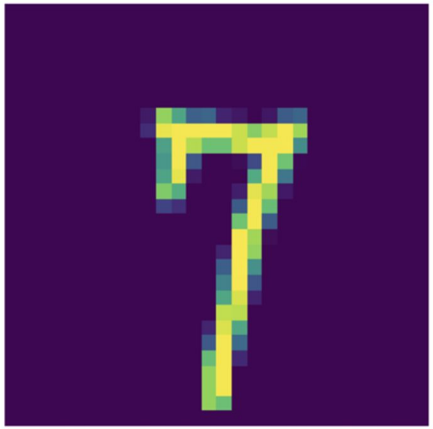


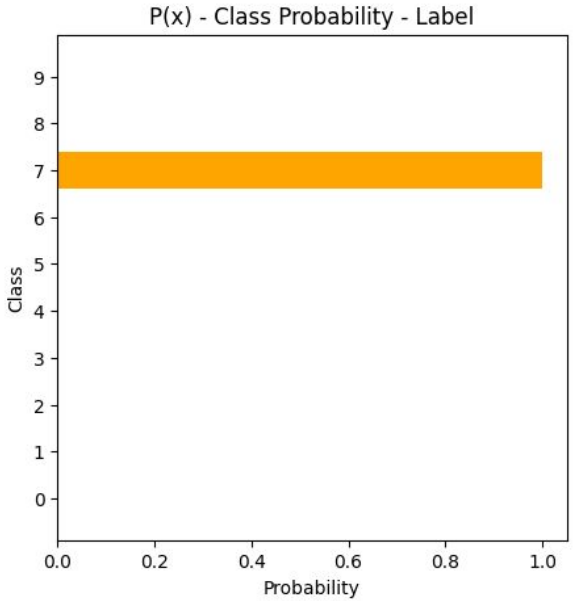


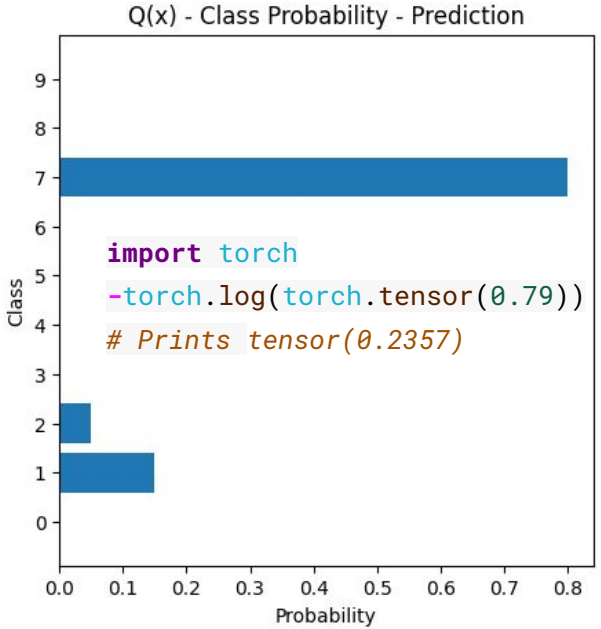


$$H(p,q) = -\frac{1}{n}\sum_{i=1}^{n} p(x_i)\log q(x_i) = H(y,\hat{y}) = -\frac{1}{n}\sum_{i=1}^{n} y_i \log \hat{y}_i$$

Low cross entropy loss - low disagreement between y and ŷ







$$H(y, \hat{y}) = -\frac{1}{n}\sum_{i=1}^{n} y_i \log \hat{y}_i$$

$$\text{Cross Entropy} = -\log(\hat{y}_i)$$

with index i being the one true class

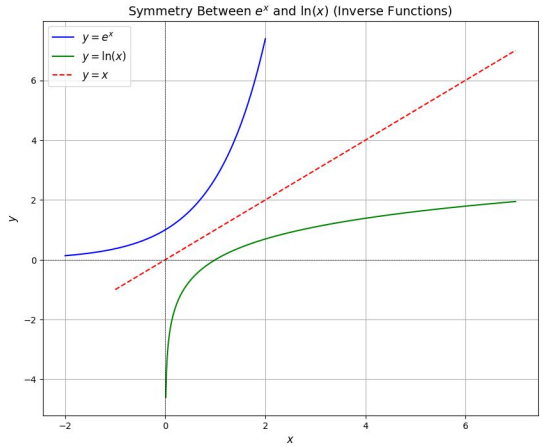
Quirks of nn.CrossEntropyLoss

```
# Compute output
logits = model(input_image)

# Turn output into probabilities, useful for interpretation
probabilities = F.softmax(logits)

# CrossEntropyLoss will compute log-softmax on the raw logits
# because it is more numerically stable
ce_loss = nn.CrossEntropyLoss()
ce_loss(logits, labels)
```

$$\text{Softmax}(x_i) = \frac{\exp(x_i)}{\sum_j \exp(x_j)} \qquad \text{LogSoftmax}(\mathbf{x})_i = x_i - \log\left(\sum_{j=1}^{n} \exp(x_j)\right)$$

Turning LogSoftmax into interpretable probabilities

$$p_i = \exp(\log p_i) = e^{\ln p_i}$$




```
import torch.nn.functional as F
logits = torch.tensor([ 0.7645,  0.8300, -0.2343,
                        0.9186, -0.2191,  0.2018,
                        -0.4869,  0.8000, 0.8815,
                        -0.7336])
log_probabilities = F.log_softmax(logits, dim=0)
print(log_probabilities.sum()) # prints tensor (-24.6857)
probabilities = torch.exp(log_probabilities)
print(probabilities.sum()) # prints tensor(1.00)
```

$$\text{Softmax}(x_i) = \frac{\exp(x_i)}{\sum_j \exp(x_j)}$$

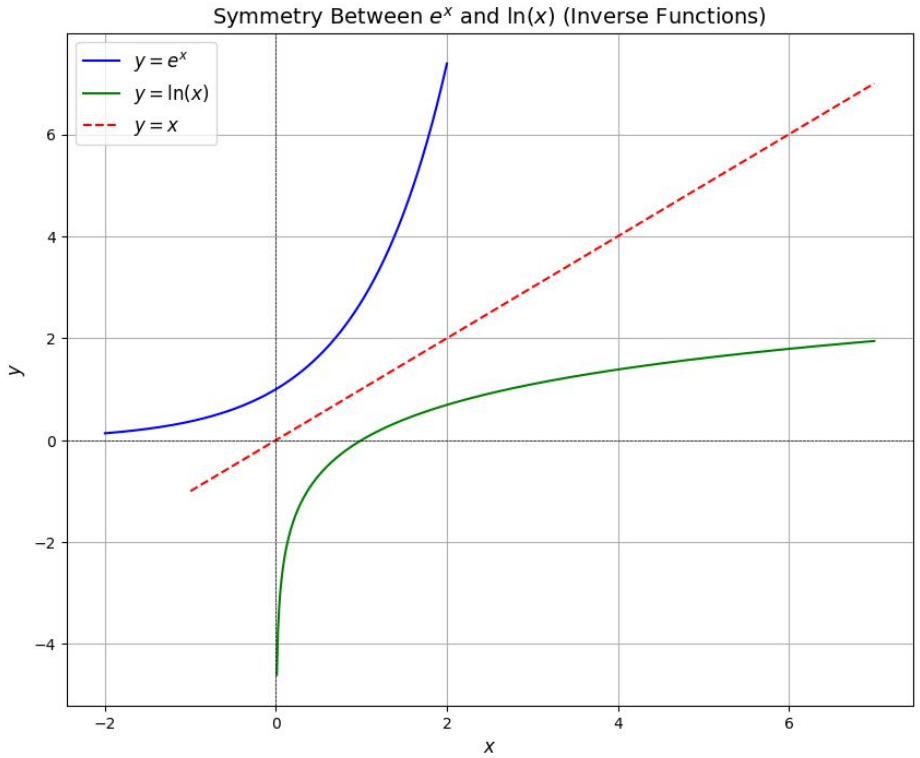
$$\text{LogSoftmax}(\mathbf{x})_i = x_i - \log\left(\sum_{\cdot}^{n} \exp(x_j)\right)$$

Why do we use log(x) = ln(x)?

$$p_i = \exp(\log p_i) = e^{\ln p_i}$$

$$\frac{d}{dx} e^x = e^x$$

$$\frac{d}{dx} \ln(x) = \frac{1}{x}$$



Cross entropy loss from logits

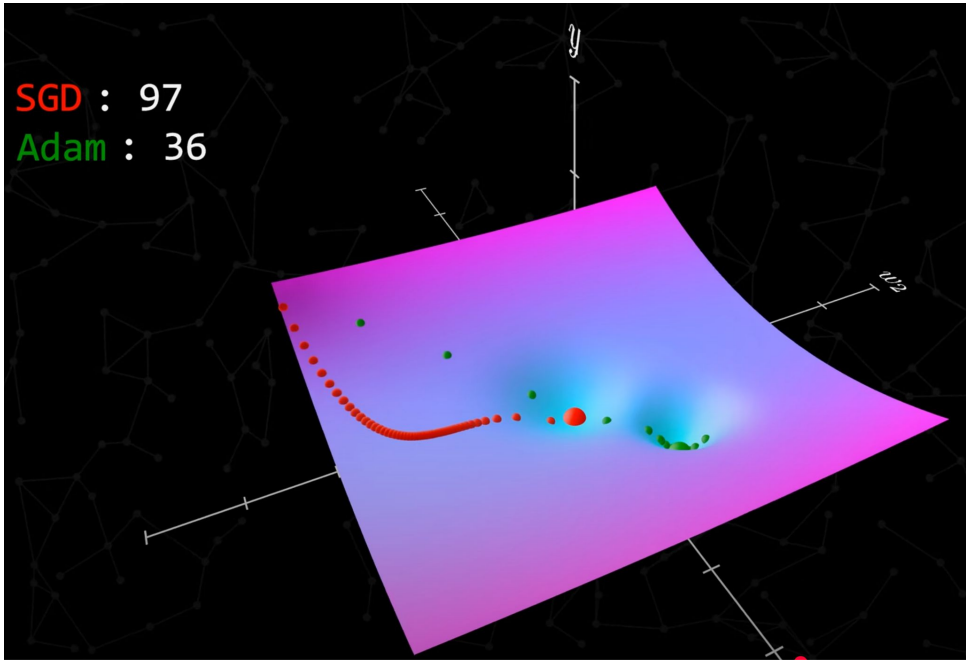
```python
import torch
import torch.nn.functional as F

def cross_entropy_loss(logits, labels):
    """
    Calculate cross entropy loss from logits using log softmax

    Args:
        logits: Tensor of shape (batch_size, num_classes) containing raw model outputs
        labels: Tensor of shape (batch_size,) containing class indices (0-9 for MNIST)

    Returns:
        loss: Scalar tensor with the mean loss
    """
    # Apply log softmax to get log probabilities
    log_probs = F.log_softmax(logits, dim=1)

    # Calculate negative log likelihood loss
    # This efficiently computes cross entropy without explicitly creating one-hot vectors
    loss = F.nll_loss(log_probs, labels)
```

“negative of the log of the likelihood (of the correct class” = F.nll_loss

$$\text{Cross Entropy} = -\log(\hat{y}_i)$$

with index i being the one true class

Extra: Adam vs Stochastic Gradient Descent



Adaptive Gradients with Momentum (ADAM) is
variant of stochastic gradient descent that per
well in many problems.

```
from torch.optim import Adam
optimizer = Adam(
            model.parameters(),
            lr=0.001)

# Compute gradients and update weights
ce_loss.backward()
optimizer.step()
```

Image from "Who is Adam and what is he optimizing?"

Summary

Feedforward neural networks for image classification

- Convert pixel inputs into class probabilities
- The number of output units determines the number of scores that we can produce
- The Adam optimizer is a variant of SGD that works well in practice

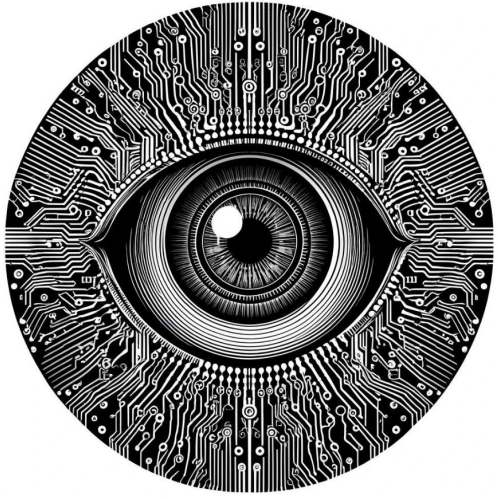
Classification pipeline

- We use one-hot encoding when we want to predict a single label per image
- We convert the raw output scores (logits) to probabilities using softmax

Cross entropy loss

- Measures classification prediction quality (agreement of probabilities in y hat and y)
- Used with log-softmax in PyTorch for numerical stability

Usage of Binary Cross Entropy Loss

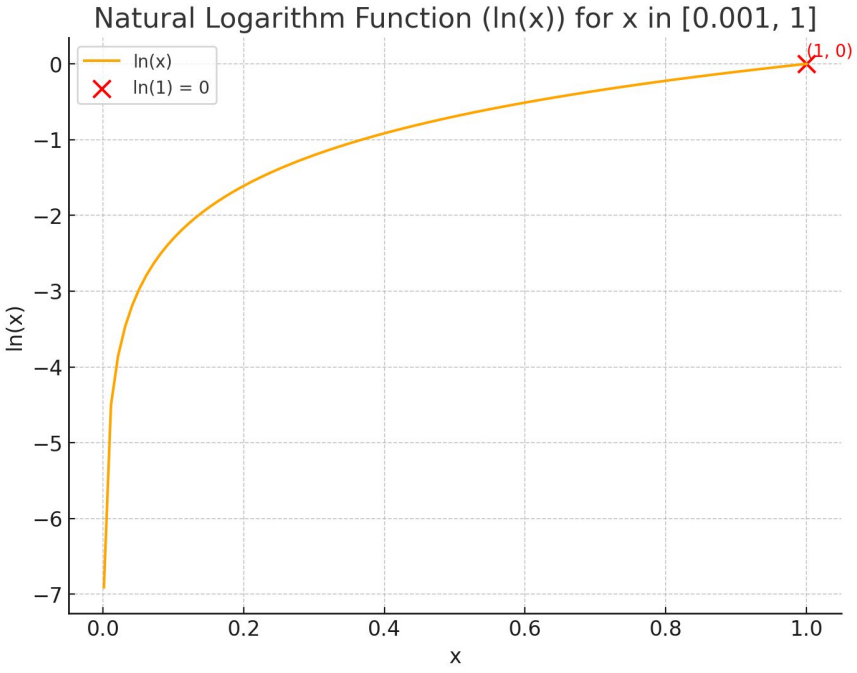


Antonio Rueda-Toicen

Learning goals

- Encode class labels as probability distributions
- Understand differences between categorical and binary cross entropy loss
- Describe differences between sigmoid and softmax activation functions
- Design network architectures with agreement between the classification task, output layer, activation function, and loss function

The logarithm function and cross entropy



$$H(y, \hat{y}) = -\sum_{i=1}^{C} y_i \log(\hat{y}_i)$$

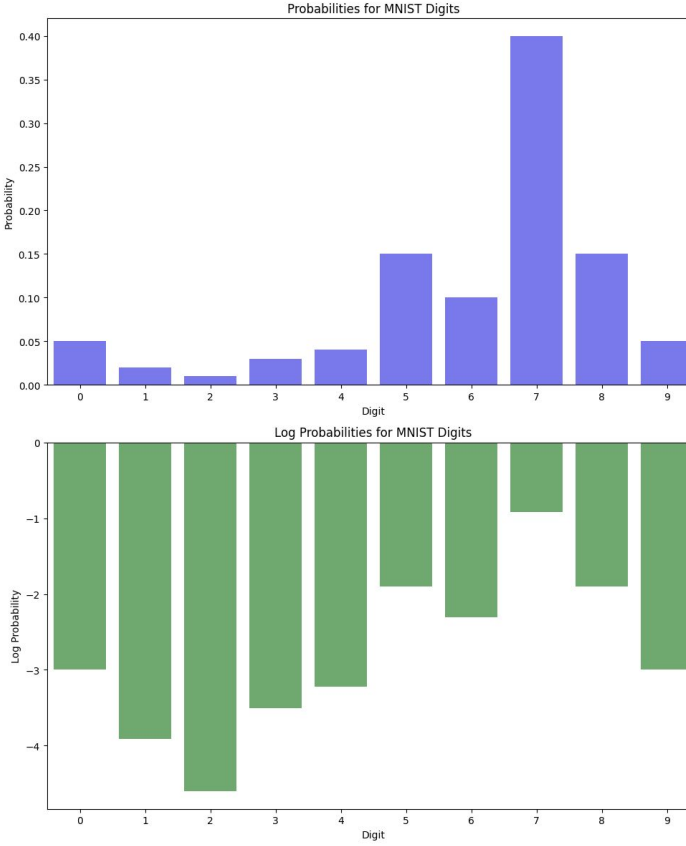
Predicting a single label from multiple classes with a neural network

$$\text{softmax}(x_i) = \frac{\exp(x_i)}{\sum_{j=1}^{n} \exp(x_j)}$$

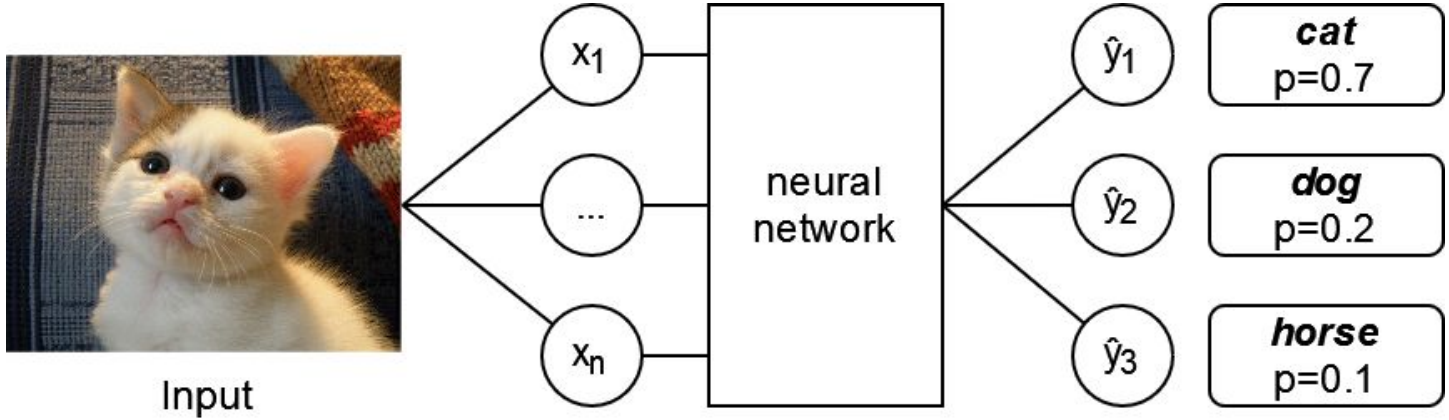
MNIST has a single label per image

$$\log \text{softmax}(x_i) = x_i - \log \sum_{j=1}^{n} \exp(x_j)$$

$$H(y, \hat{y}) = -\sum_{i=1}^{C} y_i \log(\hat{y}_i)$$



Single label classification: n probabilities for n classes




```
model = nn.Sequential(
    # We get raw logits as output
    nn.Linear(input_size, 3),
)

criterion = nn.CrossEntropyLoss()
loss = criterion(predictions, targets)
```

$$P(\hat{y}_{\text{cat}}) + P(\hat{y}_{\text{dog}}) + P(\hat{y}_{\text{horse}}) = 1$$

$$\text{softmax}(x_i) = \frac{\exp(x_i)}{\sum_{j=1}^{n} \exp(x_j)}$$

Binary Cross Entropy

Used to model events such as

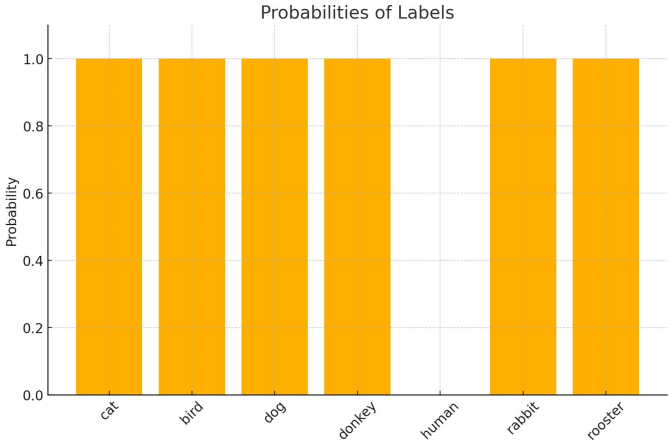
$$P(A) = 1 - P(B)$$

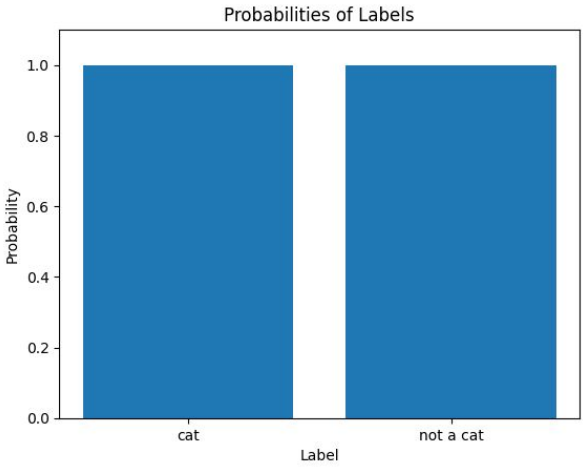
$$\text{BinaryCrossEntropy}(y, \hat{y}) = -\left[y \cdot \log(\hat{y}) + (1 - y) \cdot \log(1 - \hat{y})\right]$$

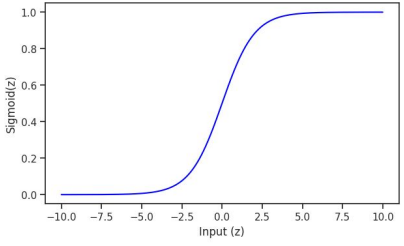
Compare with categorical cross entropy
when having a single class and a single data point

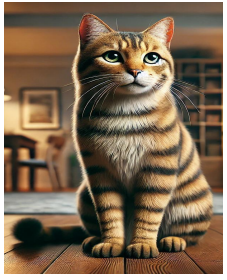
$$H(y, \hat{y}) = -y \log(\hat{y})$$

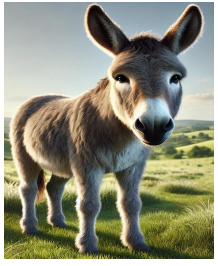
Encoding class labels as probability distributions for binary and multilabel classification





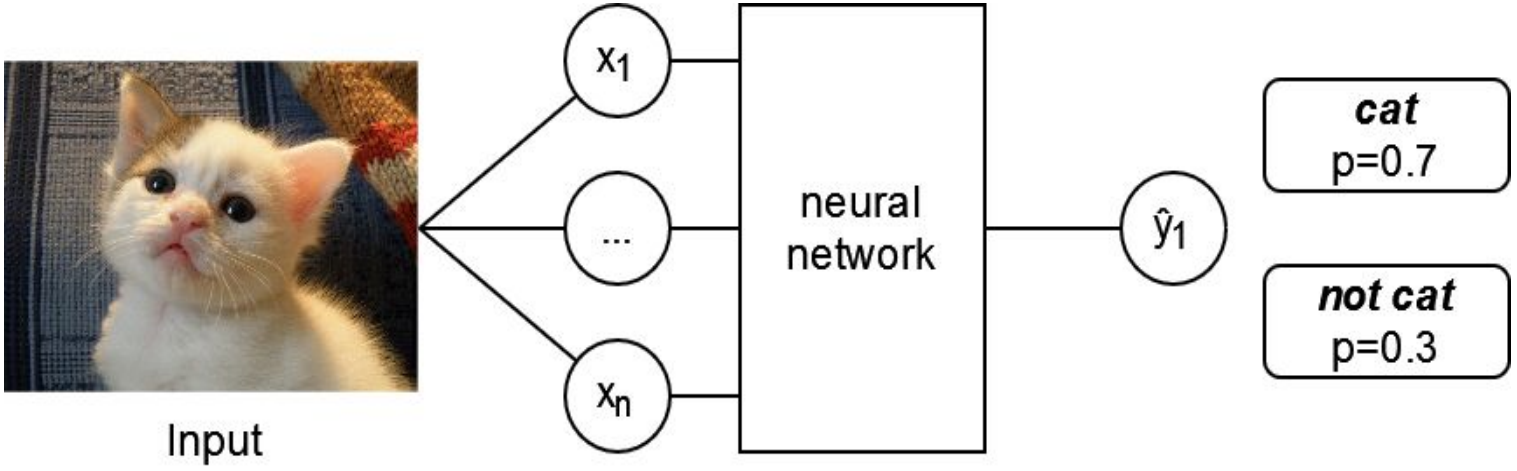




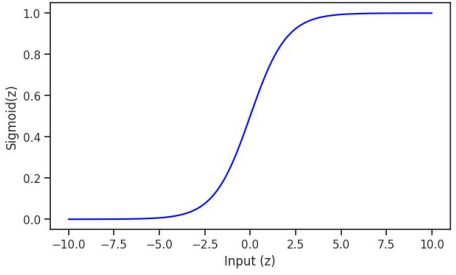


Single label binary classifiers

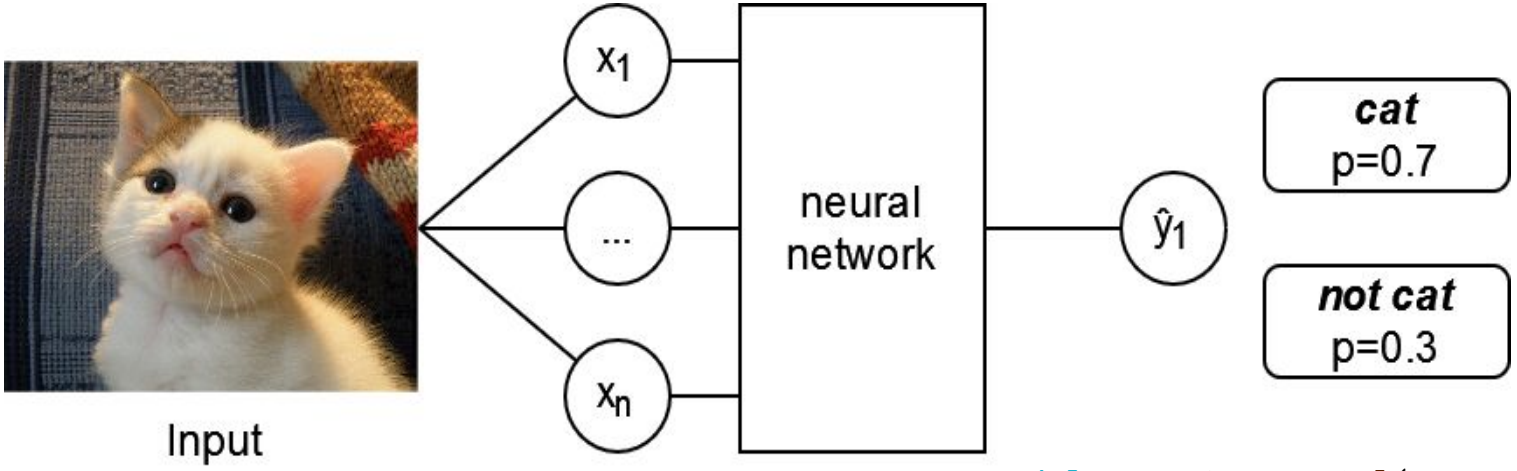
y = [1]



$$\hat{y} = \sigma(z) = \frac{1}{1 + e^{-z}}, \quad \text{where } z = w^T x + b$$



Single label binary classifiers in PyTorch

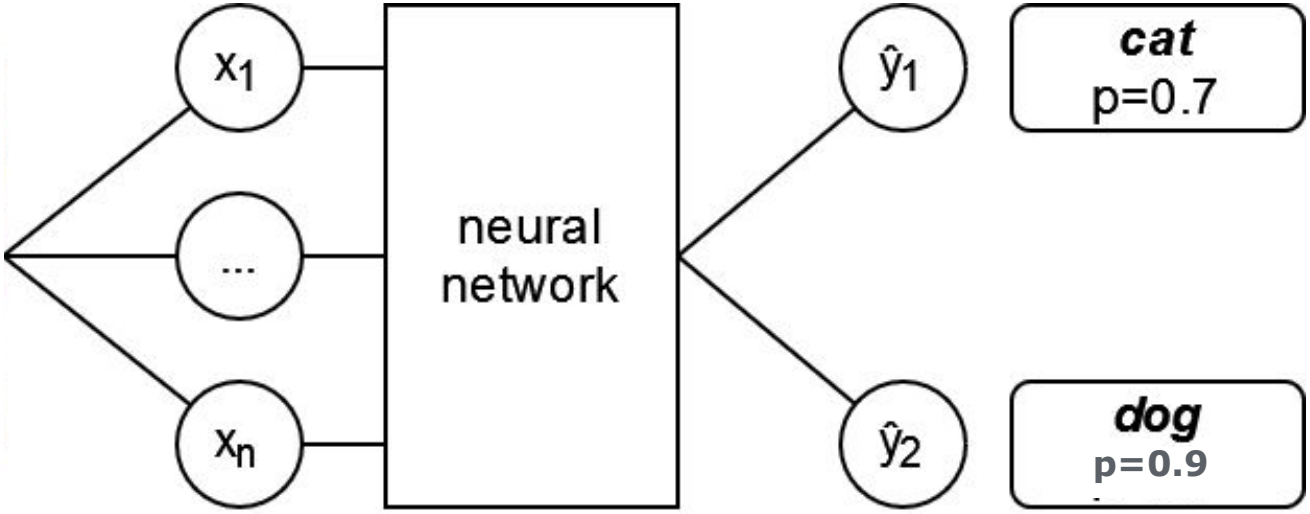



```
model = nn.Sequential(
     # Raw logits output
    nn.Linear(input_size, 1) )

criterion = nn.BCEWithLogitsLoss()
loss = criterion(logits, targets)
```

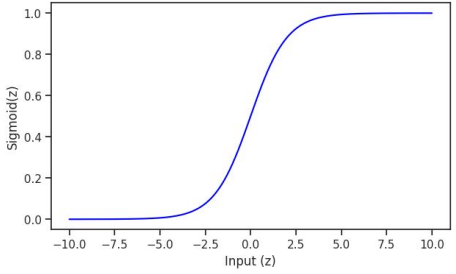
```
model = nn.Sequential(
    nn.Linear(input_size, 1),
    # Convert to probabilities
    nn.Sigmoid()
)

criterion = nn.BCELoss()
loss = criterion(predictions, targets)
```

Multilabel classifiers

Input



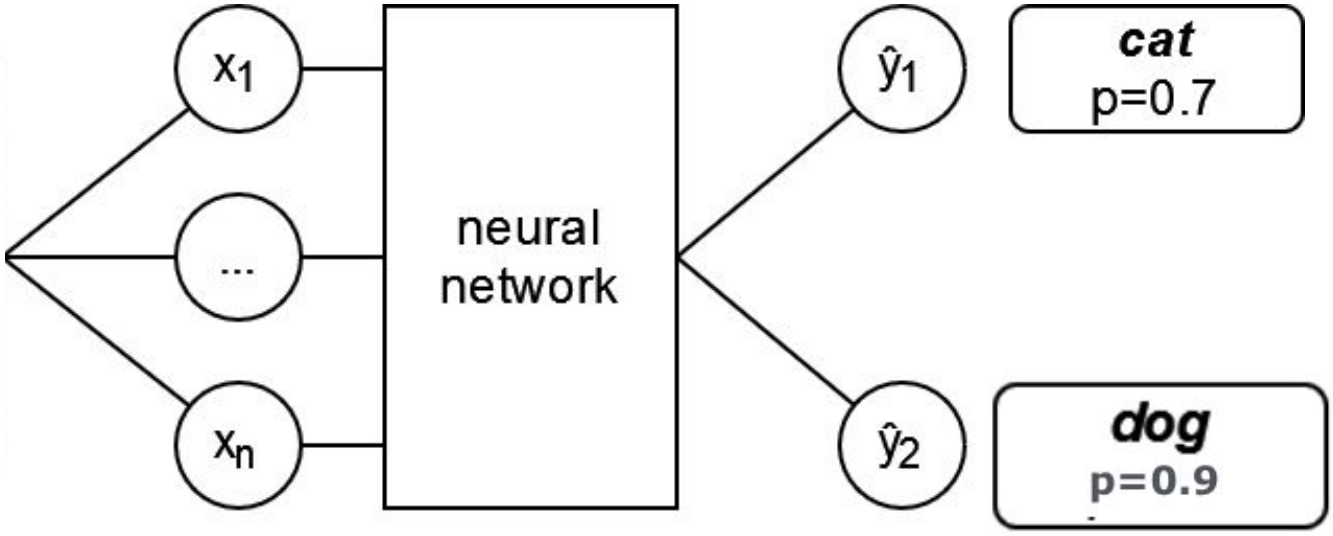
$$\hat{y} = \sigma(z) = \frac{1}{1 + e^{-z}}, \quad \text{where } z = w^T x + b$$



Multilabel classifiers in PyTorch

y = [1, 1, 0]

Input




```
model = nn.Sequential(
    nn.Linear(input_size, num_classes),
    # Convert to probabilities
    nn.Sigmoid()
)

criterion = nn.BCELoss()
loss = criterion(predictions, targets)
```

```
model = nn.Sequential(
    # Raw logits
    nn.Linear(input_size, num_classes),

criterion = nn.BCEWithLogitsLoss()
loss = criterion(predictions, targets)
```

Multilabel classification on satellite images

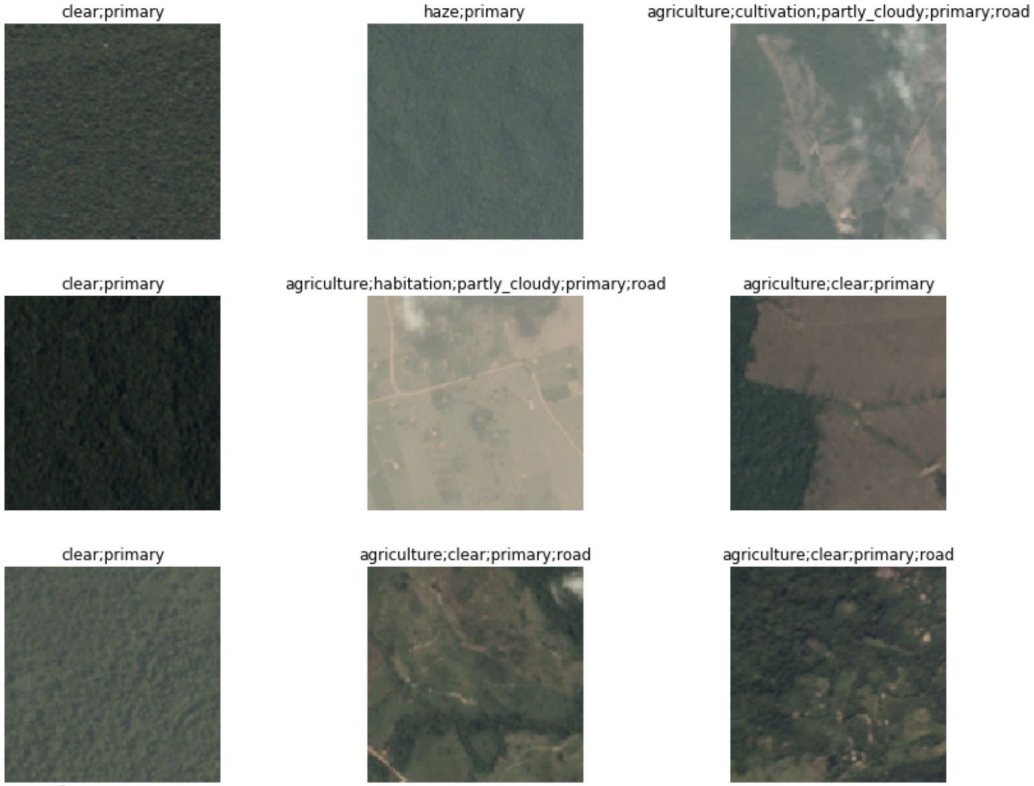
PLANET · FEATURED PREDICTION COMPETITION · 7 YEARS AGO

Planet: Understanding the Amazon from Space

Use satellite data to track the human footprint in the Amazon rainforest

https://www.kaggle.com/c/planet-understanding-the-amazon-from-space/

Multilabel classification on satellite images



https://www.kaggle.com/c/planet-understanding-the-amazon-from-space/

Summary

Cross entropy and the final activation function

- Cross entropy measures the mismatch between predicted and true distributions
- Softmax handles single-label problems with multiple classes
- Sigmoid handles both binary and multi-label cases

Network design

- Match output layer size to number of classes
- Consider single-label vs multi-label requirements for final layer
- Choose activation function based on classification type (e.g. single label vs multi-label)

Different tasks require different variants of cross entropy loss

- Use `nn.BCELoss` or nn.`BCEWithLogitsLoss` for binary or multi-label classification tasks
- Use `nn.CrossEntropyLoss` for single label tasks

Further reading

LogSoftmax vs Softmax

- https://discuss.pytorch.org/t/logsoftmax-vs-softmax/21386

Resources

- Github Repository
- YouTube playlist
- Discord channel
  #practical-computer-vision-workshops