Classification loss functions and metrics

COMP 4630 | Winter 2025

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Overview

- All the derivation thus far has been for mean squared error
- **Cross-entropy loss** is more appropriate for classification problems
- References and suggested reading:
  - Scikit-learn book: Chapter 4, training models
  - Scikit-learn docs: Log loss
  - Deep Learning Book: Sections 3.1, 3.8, and 6.2

Statistics review: Expected value

The **expected value** of some function $f(x)$ when x is distributed as $P(x)$ is given in discrete form as:

$$\mathbb{E}[f(x)] = \sum_x P(x) f(x)$$

where the sum is over all possible values of x.

In continuous form, this is an integral:

$$\mathbb{E}[f(x)] = \int p(x) f(x) dx$$

Binary case: Bernoulli distribution

- If a random variable x has a p probability of being 1 and a $1-p$ probability of being 0, then x is distributed as a **Bernoulli distribution**:

$$P(x) = p^x(1-p)^{1-x} = \begin{cases} p & \text{for } x = 1 \\ 1-p & \text{for } x = 0 \end{cases}$$

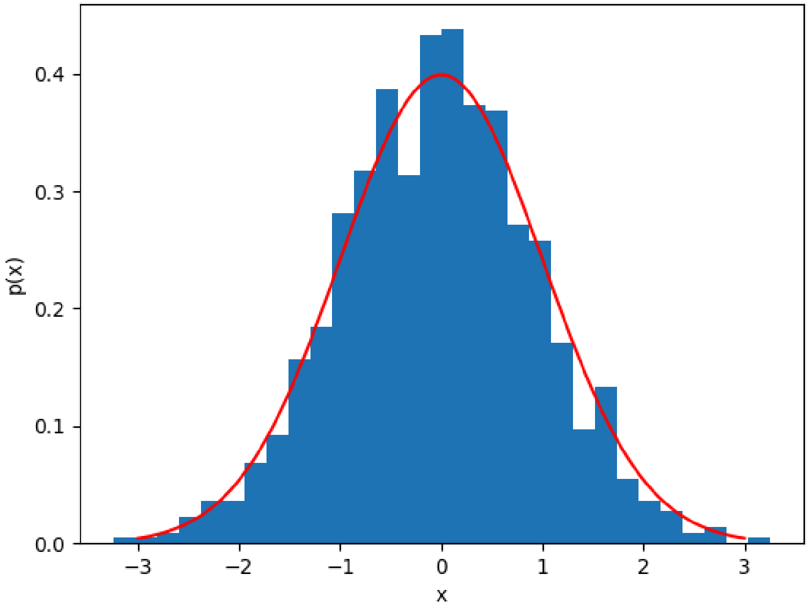
- The expected value of x is then:

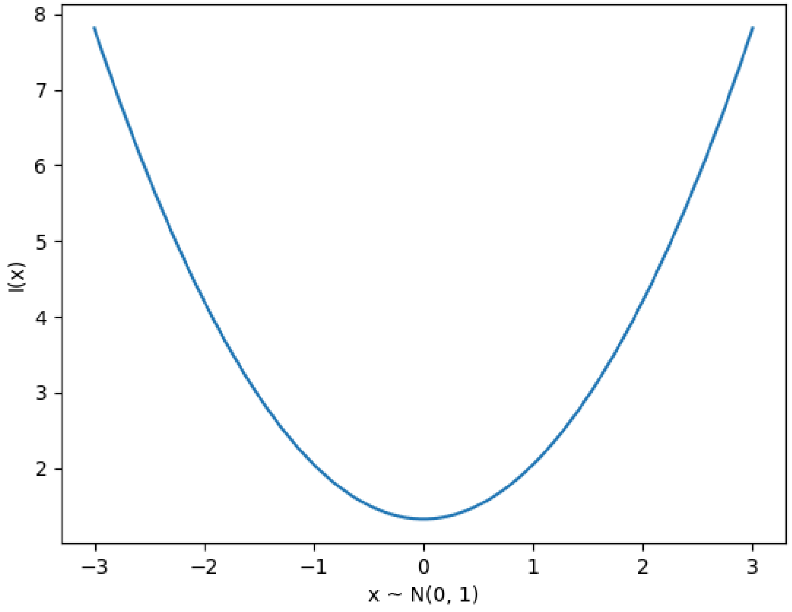
$$\mathbb{E}[x] = 0 \cdot (1-p) + 1 \cdot p = p$$

Information theory

Originally developed for message communication, with the intuition that less likely events carry more **information**, defined for a single event as:

$$I(x) = -\log P(x)$$



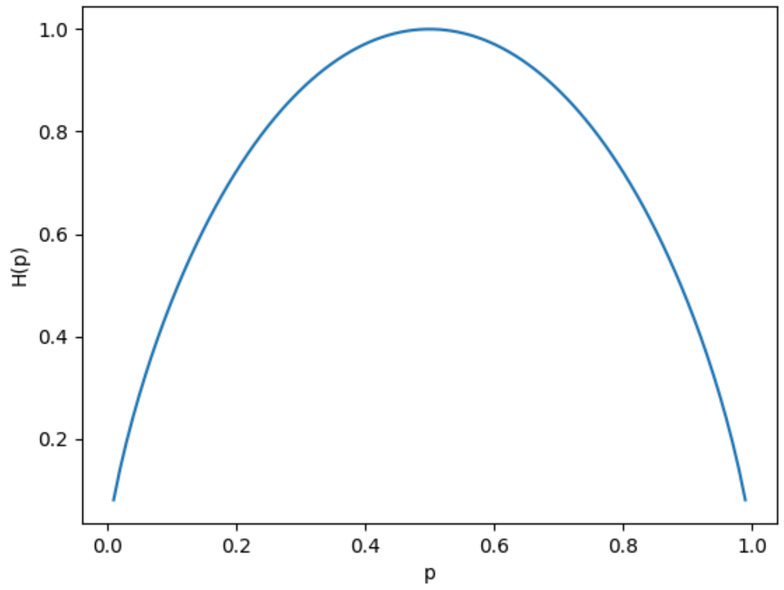


Entropy

- We can measure the **expected information** of a distribution $P(x)$ as:

$$H(X) = \mathbb{E}[I(x)] = -\mathbb{E}_{x \sim P}[\log P(x)]$$

- This is called the **Shannon entropy**
- Measured in bits (base 2) or nats (base e)
- 🧮 Find the entropy of a bernoulli distribution



Cross-entropy

- The **KL divergence** is a measure of the *extra* information needed to encode a message from a true distribution $P(x)$ using an approximate distribution $Q(x)$:

$$D_{KL}(P||Q) = \mathbb{E}_{x\sim P}\left[\log \frac{P(x)}{Q(x)}\right] = \mathbb{E}_{x\sim P}[\log P(x) - \log Q(x)]$$

- The **cross-entropy** is a simplification that drops the term $\log P(x)$:

$$H(P,Q) = -\mathbb{E}_{x\sim P}[\log Q(x)]$$

- Minimizing the cross-entropy is equivalent to minimizing the KL divergence
- If $P(x) = Q(x)$, then $D_{KL}(P||Q) = 0$ and $H(P,Q) = H(P)$

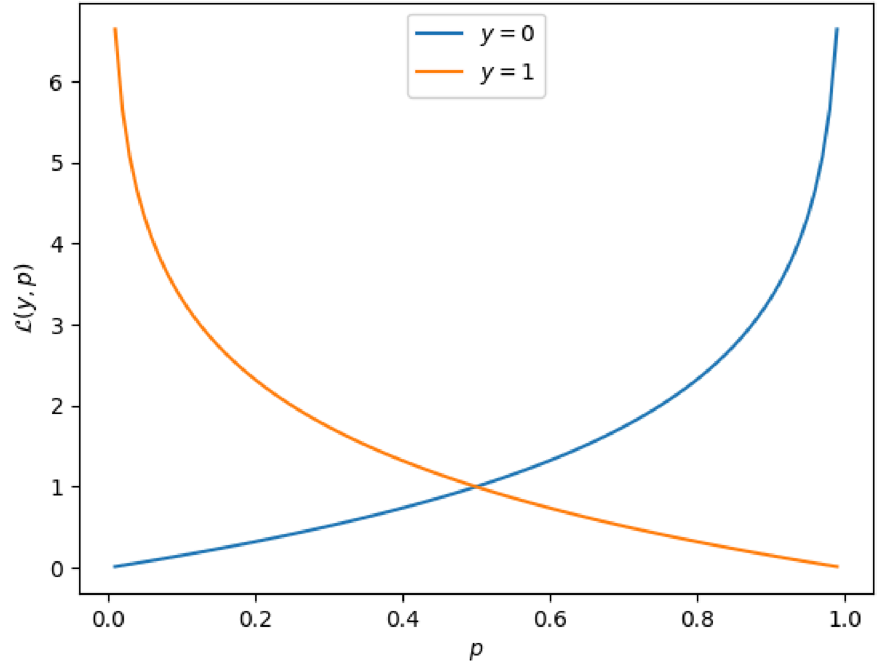
Cross-entropy loss

For a true label $y \in \{0, 1\}$ and predicted $\hat{p} \in [0, 1]$, the cross-entropy loss is:

$$\begin{aligned}\mathcal{L}(y, \hat{p}) &= -\mathbb{E}_y[\log P(x)] \\ &= -y \log \hat{p} - (1-y) \log(1-\hat{p})\end{aligned}$$

where $\hat{p} = \sigma(\mathbf{w}^T \mathbf{h} + b)$ is the output of the final layer of a neural network (thresholded to obtain the prediction $\hat{y}$)

> *This is also called **log loss** or **binary cross-entropy***



Multiclass case

- For K classes, the output is a vector $\hat{\mathbf{p}}$ with $\hat{p}_i = P(y = i|\mathbf{x})$
- The cross-entropy loss is then:

$$\mathcal{L}(\mathbf{y}, \hat{\mathbf{p}}) = -\sum_{i=1}^{K} y_i \log \hat{p}_i$$

- For a one-hot encoded vector $\mathbf{y}$, this simplifies to:

$$\mathcal{L}(\mathbf{y}, \hat{\mathbf{p}}) = -\log \hat{p}_k$$

where k is the index of the true class

The softmax function

- For binary classification, the sigmoid function $\sigma(z) = \frac{1}{1+e^{-z}}$ is used to predict the probability of the positive class
- For multiclass classification, the **softmax function** is used:

$$\hat{p}_i = \frac{e^{z_i}}{\sum_{j=1}^{K} e^{z_j}}$$

  where $z_i = \mathbf{w}_i^T \mathbf{h} + b_i$ is the output of neuron i in the final layer before the activation function is applied
- This means that K neurons are needed in the final layer, one for each class

Terminology for evaluation

- **True positive**: predicted positive, label was positive (TP) ✓
- **True negative**: predicted negative, label was negative (TN) ✓
- **False positive**: predicted positive, label was negative (FP) ✗ (type I)
- **False negative**: predicted negative, label was positive (FN) ✗ (type II)

- **Accuracy** is the fraction of correct predictions, given as:

$$\text{accuracy} = \frac{TP + TN}{TP + TN + FP + FN}$$

Precision and recall

- **Precision**: Out of all the positive **predictions**, how many were correct?

$$\text{precision} = \frac{TP}{TP + FP}$$

- **Recall**: Out of all the positive **labels**, how many were correct?

$$\text{recall} = \frac{TP}{TP + FN}$$

- **Specificity**: Out of all the negative **labels**, how many were correct?

$$\text{specificity} = \frac{TN}{TN + FP}$$

Confusion matrix

	Predicted Positive	**Predicted Negative**
True Positive	TP	FN
True Negative	FP	TN

- The axes might be reversed, but a good predictor will have strong diagonals
- There's also the **F1 score**, or harmonic mean of precision and recall:

$$F1 = 2 \cdot \frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}}$$

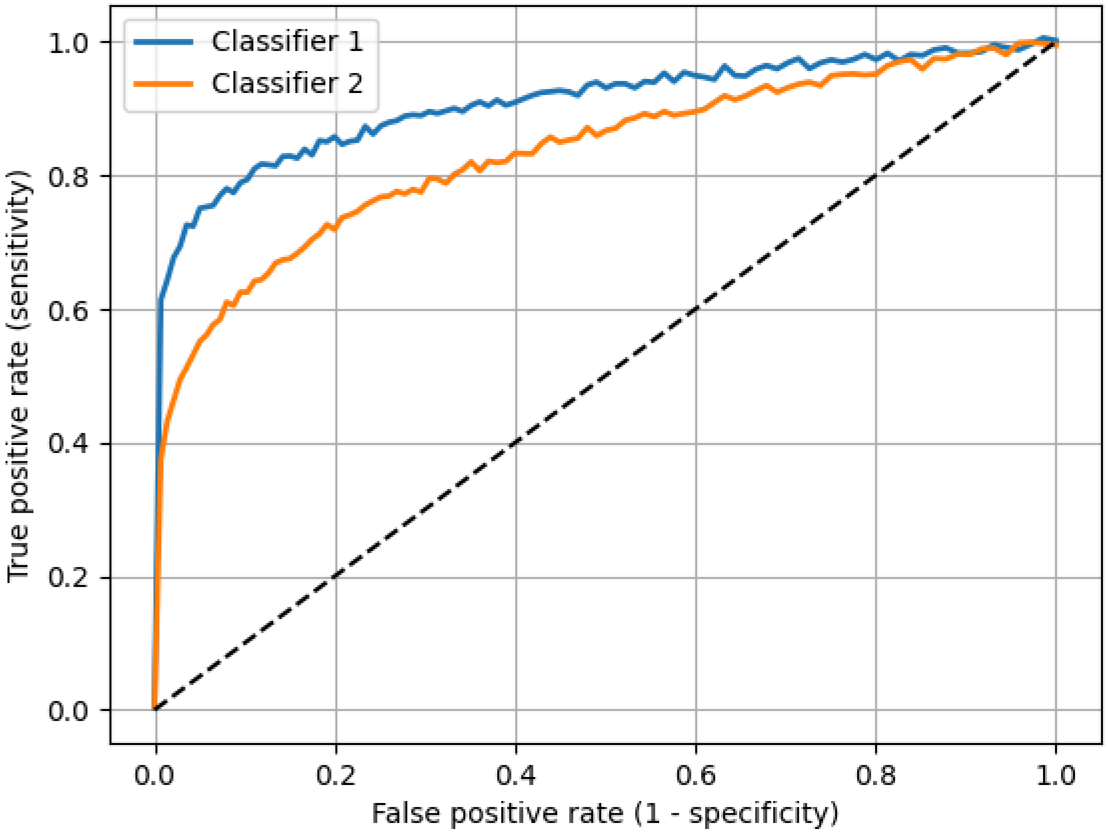
Check out the Wikipedia page for more ways of describing the same information

ROC Curves

- The receiver operating characteristic curve is a plot of the **true positive rate** (recall or sensitivity) vs. **false positive rate** (1 - specificity) as the detection threshold changes
- The diagonal is the same as random guessing
- A perfect classifier would hug the top left corner

> *Fun fact: the name comes from WWII radar operators, where true positives were airplanes and false positives were noise*

Which classifier is better?



Next up: Convolution and NN frameworks