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**:

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

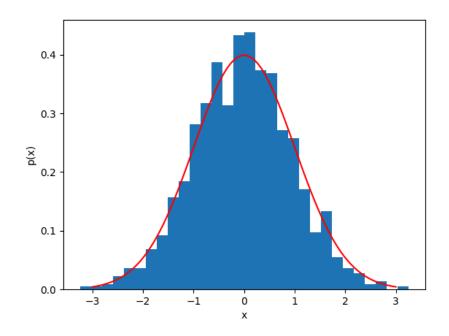
• The expected value of x is then:

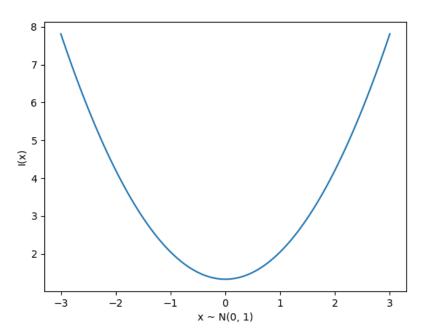
$$\mathbb{E}[x] = 0 \cdot (1-p) + 1 \cdot p = p$$

Information theory

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

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



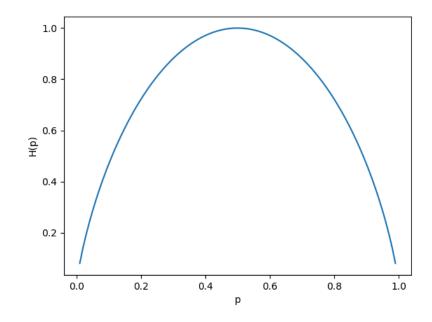


Entropy

• 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)
- Eind 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):

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

• 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
- ullet If P(x)=Q(x), then $D_{KL}(P||Q)=0$ and H(P,Q)=H(P)

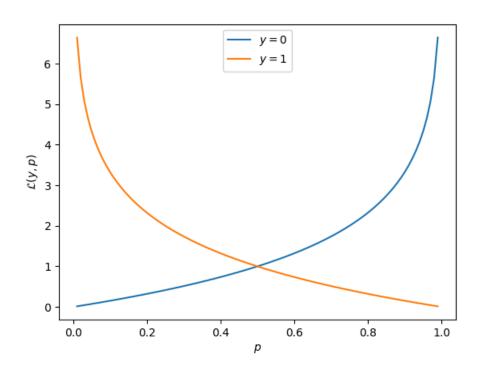
Cross-entropy loss

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

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

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

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

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

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

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

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:

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

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

ullet 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) \checkmark
- True negative: predicted negative, label was negative (TN) \checkmark
- False positive: predicted positive, label was negative $(FP) \times (type \ I)$
- False negative: predicted negative, label was positive $(FN) \times (type II)$
- Accuracy is the fraction of correct predictions, given as:

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

Precision and recall

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

$$ext{precision} = rac{TP}{TP + FP}$$

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

$$ext{recall} = rac{TP}{TP + FN}$$

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

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:

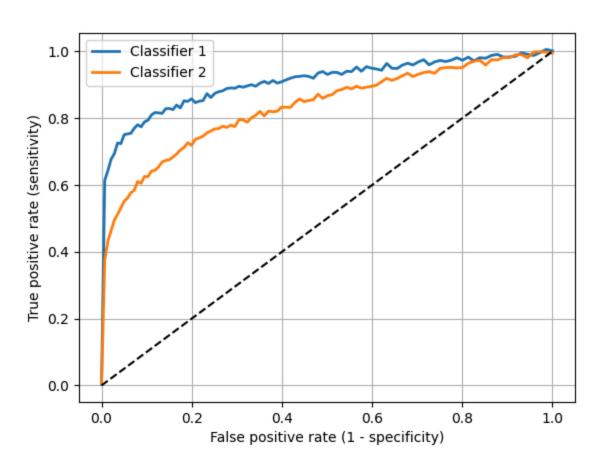
$$F1 = 2 \cdot rac{ ext{precision} \cdot ext{recall}}{ ext{precision} + ext{recall}}$$

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