Risk Minimization for Classification

RISK MINIMIZATION FOR CLASSIFICATION

Let y be categorical with g classes, i. e. $\mathcal{Y} = \{1, ..., g\}$ and let $f : \mathcal{X} \to \mathbb{R}^g$. We assume our model f outputs a g-dimensional vector of scores or probabilities, one per class.

Note: In this section, we will consider loss for **binary classification** tasks, so $f(\mathbf{x})$ and $\pi(\mathbf{x})$ are univariate scalars.

We will (usually) encode labels as $y \in \{-1, 1\}$ for scoring classifiers $f(\mathbf{x})$, and as $y \in \{0, 1\}$ for probabilistic classifiers $\pi(\mathbf{x})$ unless explicitly stated differently.

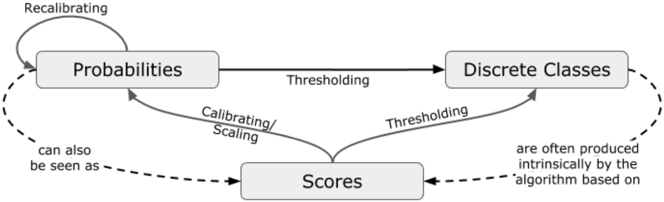
Goal: Find a model f that minimizes the expected loss over random observations $(\mathbf{x}, y) \sim \mathbb{P}_{xy}$

$$\arg\min_{f \in \mathcal{H}} \mathcal{R}(f) = \mathbb{E}_{xy}[L(y, f(\mathbf{x}))] = \int L(y, f(\mathbf{x}))\ d\mathbb{P}_{xy}.$$

RISK MINIMIZATION FOR CLASSIFICATION

- As for regression before, losses measure prediction errors **point-wise**.
- In classification, however, we need to distinguish the different types of prediction functions:
- Losses can either be defined on
  - hard labels $h(\mathbf{x})$ or
  - (class) scores $f(\mathbf{x})$ or
  - (class) probabilities $\pi(\mathbf{x})$.
- For multiclass classification, loss functions will be defined on vectors of scores $(f_1(\mathbf{x}), ..., f_g(\mathbf{x}))$ or on vectors of probabilities $(\pi_1(\mathbf{x}), ..., \pi_g(\mathbf{x}))$.

RISK MINIMIZATION FOR CLASSIFICATION



Note that for a **binary scoring classifier** $f(\mathbf{x})$,

$$h(\mathbf{x}) = \text{sign}(f(\mathbf{x})) \in \{-1, 1\}$$

and for a **probabilistic classifier** $\pi(\mathbf{x})$

$$h(\mathbf{x}) = \mathbb{1}_{\{\pi(\mathbf{x}) > c\}} \in \{0, 1\}$$

(e.g. $c = 0.5$) will be the corresponding label.

MARGINS

When considering scoring classifiers $f(\mathbf{x})$ we usually define loss functions on the so-called **margin**

$$r = y \cdot f(\mathbf{x}) = \begin{cases} > 0 & \text{if } y = \text{sign}(f(\mathbf{x})) \text{ (correct classification)}, \\ < 0 & \text{if } y \neq \text{sign}(f(\mathbf{x})) \text{ (misclassification)}, \end{cases}$$

$|f(\mathbf{x})|$ is called **confidence**.

POINT-WISE OPTIMUM

We can in general rewrite the risk as

$$\begin{aligned}\mathcal{R}(f) &= \mathbb{E}_{xy}\left[L\left(y, f(\mathbf{x})\right)\right] = \mathbb{E}_x\left[\mathbb{E}_{y|x}[L(y, f(\mathbf{x}))]\right] \\ &= \mathbb{E}_x\left[\sum_{k\in\mathcal{Y}} L(k, f(\mathbf{x}))\mathbb{P}(y = k \mid \mathbf{x} = \mathbf{x})\right],\end{aligned}$$

with $\mathbb{P}(y = k|\mathbf{x} = \mathbf{x})$ being the posterior probability for class k.

The optimal model for a loss function $L\left(y, f(\mathbf{x})\right)$ is

$$\hat{f}(\mathbf{x}) = \arg\min_{f\in\mathcal{H}} \sum_{k\in\mathcal{Y}} L(k, f(\boldsymbol{x}))\mathbb{P}(y = k|\mathbf{x} = \mathbf{x}).$$

POINT-WISE OPTIMUM

If we can estimate $\mathbb{P}_{xy}$ very well via $\pi_k(\mathbf{x})$ through a stochastic model, we can now compute the loss-optimal classifications point-wise.
But usually we directly adapt to the loss via **empirical risk minimization**.

$$\hat{f} = \underset{f \in \mathcal{H}}{\arg\min}\, \mathcal{R}_{\text{emp}}(f) = \underset{f \in \mathcal{H}}{\arg\min} \sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)}\right)\right).$$

0-1-Loss

0-1-LOSS

- Let us first consider a classifier $h(\mathbf{x})$ that outputs discrete classes directly.
- The most natural choice for $L(y, h(\mathbf{x}))$ is of course the 0-1-loss that counts the number of misclassifications

$$L(y, h(\mathbf{x})) = \mathbb{1}_{\{y \neq h(\mathbf{x})\}} = \begin{cases} 1 & \text{if } y \neq h(\mathbf{x}) \\ 0 & \text{if } y = h(\mathbf{x}) \end{cases} \quad .$$

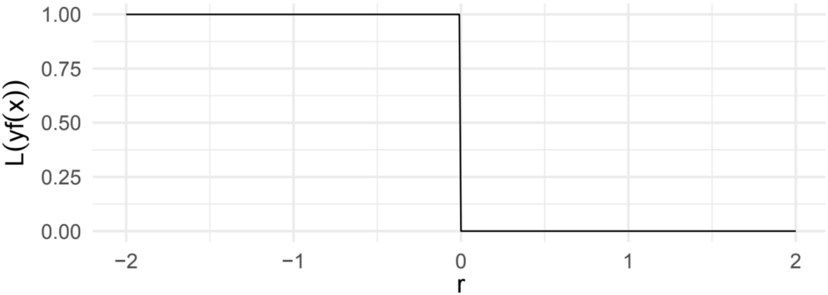
- We can express the 0-1-loss also for a scoring classifier $f(\mathbf{x})$ based on the margin r

$$L(r) = \mathbb{1}_{\{r<0\}} = \mathbb{1}_{\{yf(\mathbf{x})<0\}} = \mathbb{1}_{\{y \neq h(\mathbf{x})\}}.$$

0-1-LOSS

$$L(r) = \mathbb{1}_{\{r<0\}} = \mathbb{1}_{\{yf(\mathbf{x})<0\}} = \mathbb{1}_{\{y \neq h(\mathbf{x})\}}$$

- Intuitive, often what we are interested in.
- Analytic properties: Not continuous, even for linear f the optimization problem is NP-hard and close to intractable.



0-1-LOSS: POINT-WISE OPTIMUM

For an (unrestricted) classifier $h(\mathbf{x})$ and the 0-1-loss:

$$\min_{h \in \mathcal{H}} \mathcal{R}(h) = \mathbb{E}_{xy}[L(y, h(\mathbf{x}))].$$

The (point-wise) solution of the above minimization problem is

$$\begin{aligned}
\hat{h}(\mathbf{x}) &= \arg\min_{l \in \mathcal{Y}} \sum_{k \in \mathcal{Y}} L(k, l) \cdot \mathbb{P}(y = k \mid \mathbf{x} = \mathbf{x}) \\
&= \arg\min_{l \in \mathcal{Y}} \sum_{k \neq l} \mathbb{P}(y = k \mid \mathbf{x} = \mathbf{x}) = \arg\min_{l \in \mathcal{Y}} 1 - \mathbb{P}(y = l \mid \mathbf{x} = \mathbf{x}) \\
&= \arg\max_{l \in \mathcal{Y}} \mathbb{P}(y = l \mid \mathbf{x} = \mathbf{x})
\end{aligned}$$

which corresponds to predicting the most probable class.

$\hat{h}(\mathbf{x})$ is called the **Bayes optimal classifier**. The expected loss is called **Bayes loss** or **Bayes error rate** for the 0-1-loss.

0-1-LOSS: OPTIMAL CONSTANT MODEL

The optimal constant model (featureless predictor) under 0-1 loss, with $y \in \{-1, +1\}$, either for hard classifiers $h(\mathbf{x})$ or scoring classifiers $f(\mathbf{x})$

$$L(y, h(\mathbf{x})) = \mathbb{1}_{y \neq h(\mathbf{x})}$$

is the classifier that predicts the most frequent class in the data

$$h(\mathbf{x}) = \text{mode}\left\{y^{(i)}\right\} \qquad \text{or} \qquad f(\mathbf{x}) = \text{mode}\left\{y^{(i)}\right\}.$$

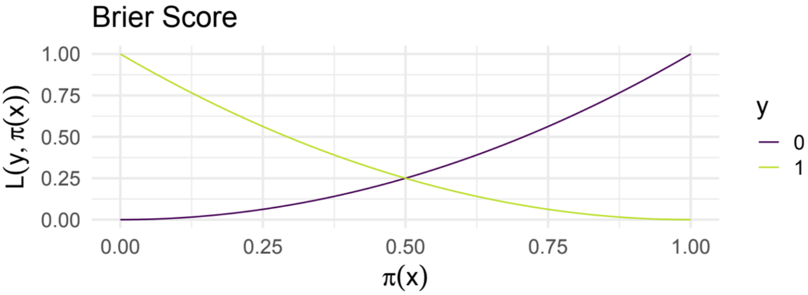
Proof: Exercise / Trivial.

Brier Score

BRIER SCORE

The binary Brier score is defined on probabilities $\pi(\mathbf{x}) \in [0, 1]$ and 0-1-encoded labels $y \in \{0, 1\}$ and measures their squared distance (L2 loss on probabilities).

$$L(y, \pi(\mathbf{x})) = (\pi(\mathbf{x}) - y)^2$$



BRIER SCORE: POINT-WISE OPTIMUM

The minimizer of the (theoretical) risk $\mathcal{R}(f)$ for the Brier score

$$\hat{\pi}(\mathbf{x}) \quad = \quad \mathbb{P}(y \mid \mathbf{x} = \mathbf{x}),$$

which means that the Brier score would reach its minimum if the prediction equals the “true” probability of the outcome.

Proof: We have seen that the (theoretical) optimal prediction c for an arbitrary loss function at fixed point $\mathbf{x}$ is

$$\arg\min_{c} \sum_{k \in \mathcal{Y}} L(y, c) \mathbb{P}(y = k | \mathbf{x} = \mathbf{x}) \,.$$

BRIER SCORE: POINT-WISE OPTIMUM

We plug in the Brier score

$$
\begin{aligned}
& \arg\min_c L(1, c) \underbrace{\mathbb{P}(y = 1|\mathbf{x} = \mathbf{x})}_{p} + L(0, c) \underbrace{\mathbb{P}(y = 0|\mathbf{x} = \mathbf{x})}_{1-p} \\
= \quad & \arg\min_c \quad (c - 1)^2 p + c^2 (1 - p) \\
= \quad & \arg\min_c \quad (c - p)^2.
\end{aligned}
$$

The expression is minimal if $c = p = \mathbb{P}(y = 1 \mid \mathbf{x} = \mathbf{x})$.

BRIER SCORE: OPTIMAL CONSTANT MODEL

The optimal constant probability model $\pi(\mathbf{x}) = \theta$ w.r.t. the Brier score for labels from $\mathcal{Y} = \{0, 1\}$ is:

$$
\begin{aligned}
\min_{\theta} \mathcal{R}_{\text{emp}}(\theta) &= \min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left(y^{(i)} - \theta\right)^2 \\
\Leftrightarrow \frac{\partial \mathcal{R}_{\text{emp}}(\theta)}{\partial \theta} &= -2 \cdot \sum_{i=1}^{n} (y^{(i)} - \theta) = 0 \\
\hat{\theta} &= \frac{1}{n} \sum_{i=1}^{n} y^{(i)}.
\end{aligned}
$$

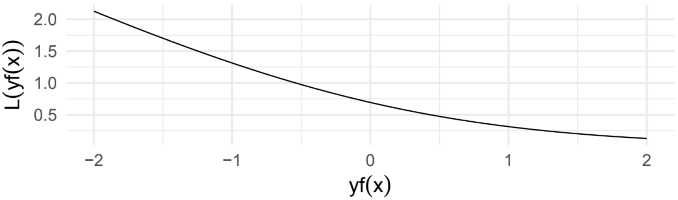
This is the fraction of class-1 observations in the observed data.
(This also directly follows from our $L2$-proof for regression).

Bernoulli Loss

BERNOULLI LOSS

$$
\begin{aligned}
L_{-1,+1}(y, f(\mathbf{x})) &= \ln(1 + \exp(-yf(\mathbf{x}))) \\
L_{0,1}(y, f(\mathbf{x})) &= -y \cdot f(\mathbf{x}) + \log(1 + \exp(f(\mathbf{x}))).
\end{aligned}
$$

- Two equivalent formulations: Labels $y \in \{-1, 1\}$ or $y \in \{0, 1\}$
- Negative log-likelihood of Bernoulli model, e.g., logistic regression
- Convex, differentiable
- Pseudo-Residuals (0,1 case): $\tilde{r} = y - \frac{1}{1+\exp(-f(\mathbf{x}))}$
  Interpretation: $L1$ distance between 0/1-labels and posterior prob!



BERNOULLI LOSS: POINT-WISE OPTIMUM

The theoretical point-wise optimum for scores under Bernoulli loss is actually the point-wise log-odds:

$$\hat{f}(\mathbf{x}) \quad = \quad \ln\left(\frac{\mathbb{P}(y \mid \mathbf{x} = \mathbf{x})}{1 - \mathbb{P}(y \mid \mathbf{x} = \mathbf{x})}\right).$$

The function is undefined when $P(y \mid \mathbf{x} = \mathbf{x}) = 1$ or $P(y \mid \mathbf{x} = \mathbf{x}) = 0$, but predicts a smooth curve which grows when $P(y \mid \mathbf{x} = \mathbf{x})$ increases and equals 0 when $P(y \mid \mathbf{x} = \mathbf{x}) = 0.5$.

Proof: We consider the case $\mathcal{Y} = \{-1, 1\}$. We have seen that the (theoretical) optimal prediction c for an arbitrary loss function at fixed point $\mathbf{x}$ is

$$\arg\min_{c} \sum_{k \in \mathcal{Y}} L(y, c)\mathbb{P}(y = k | \mathbf{x} = \mathbf{x})\,.$$

BERNOULLI LOSS: POINT-WISE OPTIMUM

We plug in the Bernoulli loss

$$
\begin{aligned}
& \arg\min_c L(1, c) \underbrace{\mathbb{P}(y = 1 | \mathbf{x} = \mathbf{x})}_{p} + L(-1, c) \underbrace{\mathbb{P}(y = -1 | \mathbf{x} = \mathbf{x})}_{1-p} \\
= \quad & \arg\min_c \ln(1 + \exp(-c))p + \ln(1 + \exp(c))(1 - p).
\end{aligned}
$$

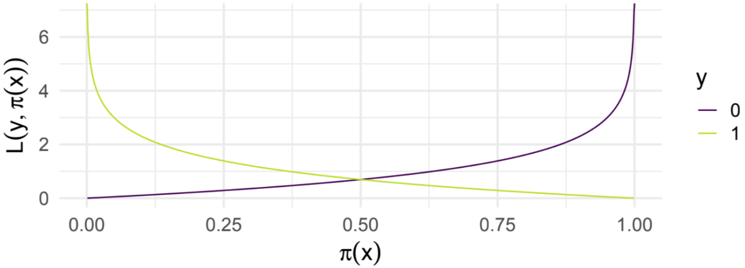
Setting the derivative w.r.t. c to zero yields

$$
\begin{aligned}
0 \quad &= \quad -\frac{\exp(-c)}{1 + \exp(-c)} p + \frac{\exp(c)}{1 + \exp(c)} (1 - p) \\
&= \quad -\frac{\exp(-c)}{1 + \exp(-c)} p + \frac{1}{1 + \exp(-c)} (1 - p) \\
&= \quad -p + \frac{1}{1 + \exp(-c)} \\
\Leftrightarrow p \quad &= \quad \frac{1}{1 + \exp(-c)} \\
\Leftrightarrow c \quad &= \quad \ln\left(\frac{p}{1 - p}\right)
\end{aligned}
$$

BERNOULLI LOSS ON PROBABILITIES

If scores are transformed into probabilities by the logistic function $\pi(\mathbf{x}) = (1 + \exp(-f(\mathbf{x})))^{-1}$, we arrive at another equivalent formulation of the loss

$$L_{0,1}(y, \pi(\mathbf{x})) = -y \log\left(\pi(\mathbf{x})\right) - (1-y)\log\left(1 - \pi(\mathbf{x})\right).$$



Via this form it is easy to show that the point-wise optimum for probability estimates is $\hat{\pi}(\mathbf{x}) = \mathbb{P}(y \mid \mathbf{x} = \mathbf{x})$.

BERNOULLI: OPTIMAL CONSTANT MODEL

The optimal constant probability model $\pi(\mathbf{x}) = \theta$ w.r.t. the Bernoulli loss for labels from $\mathcal{Y} = \{0, 1\}$) is:

$$\hat{\boldsymbol{\theta}} = \arg\min_{\theta} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} y^{(i)}$$

Again, this is the fraction of class-1 observations in the observed data. We can simply prove this again by setting the derivative of the risk to 0 and solving for θ.

BERNOULLI: OPTIMAL CONSTANT MODEL

The optimal constant score model $f(\mathbf{x}) = \theta$ w.r.t. the Bernoulli loss labels from $\mathcal{Y} = \{-1, +1\}$ or $\mathcal{Y} = \{0, 1\}$ is:

$$\hat{\boldsymbol{\theta}} = \arg\min_{\theta} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \ln \frac{n_{+1}}{n_{-1}} = \ln \frac{n_{+1}/n}{n_{-1}/n}$$

where n_{-1} and n_{+1} are the numbers of negative and positive observations, respectively.

This again shows a tight (and unsurprising) connection of this loss to log-odds.

Proving this is also a (quite simple) exercise.

BERNOULLI-LOSS: NAMING CONVENTION

We have seen three loss functions that are closely related. In the literature, there are different names for the losses:

$$
\begin{aligned}
L_{-1+1}(y, f(\mathbf{x})) &= \ln(1 + \exp(-yf(\mathbf{x}))) \\
L_{0,1}(y, f(\mathbf{x})) &= -y \cdot f(\mathbf{x}) + \log(1 + \exp(f(\mathbf{x}))).
\end{aligned}
$$

are referred to as Bernoulli, Binomial or logistic loss.

$$
L_{0,1}(y, \pi(\mathbf{x})) = -y \log\left(\pi(\mathbf{x})\right) - (1 - y) \log\left(1 - \pi(\mathbf{x})\right).
$$

is referred to as cross-entropy or log-loss.

For simplicity, we will call all of them **Bernoulli loss**, and rather make clear whether they are defined on labels $y \in \{0, 1\}$ or $y \in \{-1, 1\}$ and on scores $f(\mathbf{x})$ or probabilities $\pi(\mathbf{x})$.

Summary