

# Density Ratio Estimation

Given two samples  $X^+ \sim \rho^+$  and  $X^- \sim \rho^-$ , how can we estimate their density ratio

$$r(x) = \frac{\rho^+(x)}{\rho^-(x)}?$$

We provide estimators for a more general rational ratio of the form

$$\frac{b_+\rho^+(x) - b_-\rho^-(x)}{a_+\rho^+(x) + a_-\rho^-(x)},$$

where  $a_\pm, b_\pm$  are constants.

## 1.1 Least Squares Estimators

The general idea is that we can recover information about the density ratio by fitting a function  $f$  to different targets for data drawn from different distributions. Consider the following objective:

$$\min_f a \mathbb{E}_{X^+ \sim \rho^+} [(f(X^+) - 1)^2] + b \mathbb{E}_{X^- \sim \rho^-} [(f(X^-) + 1)^2],$$

where  $a, b > 0$  are positive coefficients. Here, we regress  $f(X)$  to 1 if  $X \sim \rho^+$ , and to  $-1$  if  $X \sim \rho^-$ .

**Theorem 1.1.1.** *The minimizer of the objective above is*

$$f^*(x) = \frac{a\rho^+(x) - b\rho^-(x)}{a\rho^+(x) + b\rho^-(x)}.$$

*Proof.* Expanding the expectations as integrals, the loss can be written as

$$L(f) = \int (a\rho^+(x) + b\rho^-(x)) f(x)^2 - 2(a\rho^+(x) - b\rho^-(x)) f(x) dx + \text{const.}$$

It is clear that for each  $x$ , the value of  $f(x)$  minimizing  $L(f)$  is

$$f^*(x) = \frac{a\rho^+(x) - b\rho^-(x)}{a\rho^+(x) + b\rho^-(x)},$$

This completes the proof. □

**Remark** In general, we can fit  $f$  to  $m_+(x)$  for positive samples and to  $m_-(x)$  for negative samples:

$$\min_f a \mathbb{E}_{X^+ \sim \rho^+} [(f(X^+) - m_+(X^+))^2] + b \mathbb{E}_{X^- \sim \rho^-} [(f(X^-) - m_-(X^-))^2], \quad a + b > 0,$$

where  $m_+$  and  $m_-$  are given functions. The minimizer in this case is

$$f^*(x) = \frac{am_+(x)\rho^+(x) + bm_-(x)\rho^-(x)}{a\rho^+(x) + b\rho^-(x)}.$$

## 1.2 Convex $\phi$ Loss

We now extend the least squares loss to a more general form using a convex function  $\phi$  to replace the  $(\cdot)^2$  cost. Consider the objective:

$$\min_f \mathbb{E}_{X^+ \sim \rho^+} [a_+ \phi(f(X^+)) - b_+ f(X^+)] + \mathbb{E}_{X^- \sim \rho^-} [a_- \phi(f(X^-)) + b_- f(X^-)],$$

where  $\phi$  is a strictly convex function,  $a_+, a_- \geq 0$ , and  $b_+, b_- \in \mathbb{R}$ .

**Theorem 1.2.1.** *The optimal solution to the problem above satisfies*

$$\nabla \phi(f^*(x)) = \frac{b_+ \rho^+(x) - b_- \rho^-(x)}{a_+ \rho^+(x) + a_- \rho^-(x)}.$$

*Proof.* Expanding the expectations into integrals, the objective becomes

$$\int ((a_+ \rho^+(x) + a_- \rho^-(x)) \phi(f(x)) - (b_+ \rho^+(x) - b_- \rho^-(x)) f(x)) dx.$$

For each  $x$ , this is a pointwise convex optimization problem of the form

$$\min_{f(x)} A(x) \phi(f(x)) - B(x) f(x),$$

where  $A(x) = a_+ \rho^+(x) + a_- \rho^-(x)$  and  $B(x) = b_+ \rho^+(x) - b_- \rho^-(x)$ . The unique minimizer is given by

$$A(x) \nabla \phi(f^*(x)) = B(x).$$

This yields the results. □

**Cross Entropy Loss** Let  $\phi(x) = \log(\exp(x) + \exp(-x))$ , the softplus of  $|x|$ . Then,

$$\nabla \phi(x) = \frac{\exp(x) - \exp(-x)}{\exp(x) + \exp(-x)} = \tanh(x).$$

Therefore, the optimal solution satisfies

$$\frac{\exp(2f^*(x)) - 1}{\exp(2f^*(x)) + 1} = \frac{b_+ \rho^+(x) - b_- \rho^-(x)}{a_+ \rho^+(x) + a_- \rho^-(x)}.$$

In particular, taking  $a_+ = a_- = b_+ = b_- = 1$ , and matching the two sides we get

$$2f^*(x) = \log \frac{\rho^+(x)}{\rho^-(x)}.$$

This reduces to the typical logistic regression estimator of density ratio:

$$\max_f \mathbb{E}_{X^+ \sim \rho^+} [\log p_f(X^+)] + \mathbb{E}_{X^- \sim \rho^-} [\log(1 - p_f(X^-))],$$

where  $\log p_f(x) = f(x) - \log(\exp(f(x)) + \exp(-f(x)))$ , and  $\log(1 - p_f(x)) = -f(x) - \log(\exp(f(x)) + \exp(-f(x)))$ .