Density Ratio Estimation for KL Divergence Minimization between Implicit Distributions

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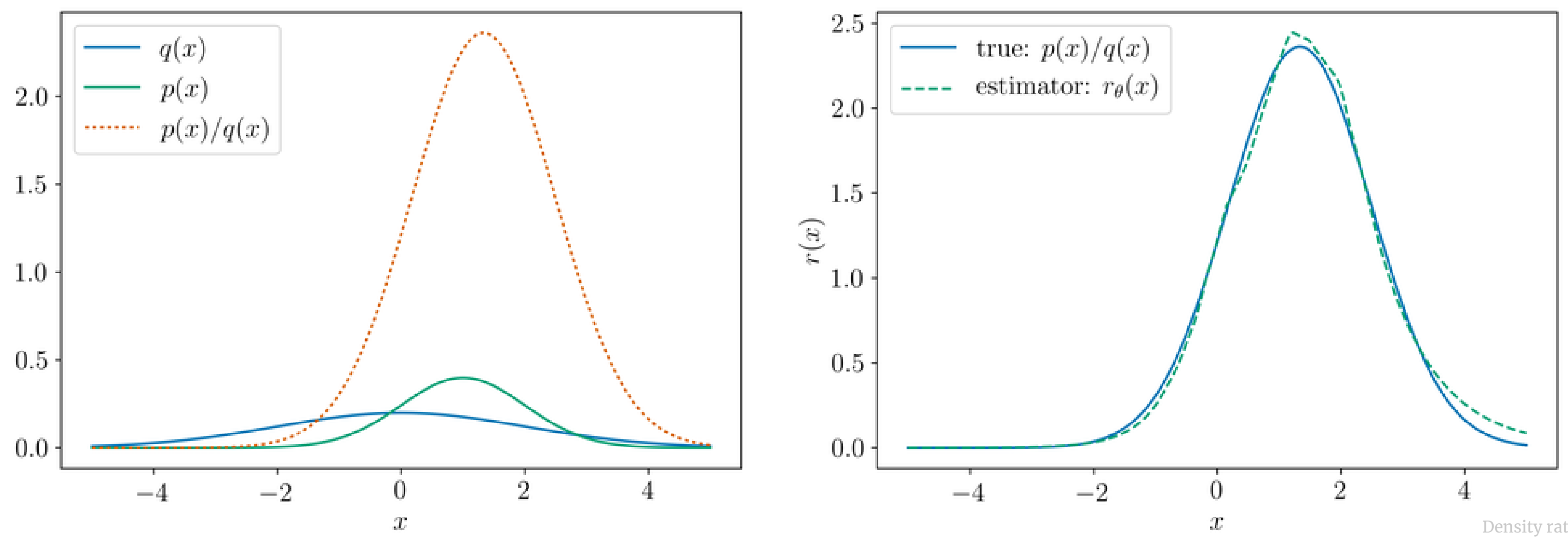
Project



Density ratio between Gaussians.

The Kullback-Leibler (KL) divergence between distributions p and q is defined as

$$\mathcal{D}_{\mathrm{KL}}[p(x)||q(x)] := \mathbb{E}_{p(x)}\left[\log\left(\frac{p(x)}{q(x)}\right)\right].$$

It can be expressed more succinctly as

$$\mathcal{D}_{\mathrm{KL}}[p(x)||q(x)] = \mathbb{E}_{p(x)}[\log r^*(x)],$$

where $r^*(x)$ is defined to be the ratio of between the densities $p(x)$ and $q(x)$,

$$r^*(x) := \frac{p(x)}{q(x)}.$$

This density ratio is crucial for computing not only the KL divergence but for all f-divergences, defined as[1]

$$\mathcal{D}_f[p(x)||q(x)] := \mathbb{E}_{q(x)}\left[f\left(\frac{p(x)}{q(x)}\right)\right].$$

Rarely can this expectation (i.e. integral) can be calculated analytically—in most cases, we must resort to Monte Carlo approximation methods, which explicitly requires the density ratio. In the more severe case where this density ratio is unavailable, because either or both $p(x)$ and $q(x)$ are not calculable, we must resort to methods for *density ratio estimation*. In this post, we illustrate how to perform density ratio estimation by exploiting its tight correspondence to *probabilistic classification*.

Example: Univariate Gaussians

Let us consider the following univariate Gaussian distributions as the running example for this post,

$$p(x) = \mathcal{N}(x \mid 1, 1^2), \qquad \text{and} \qquad q(x) = \mathcal{N}(x \mid 0, 2^2).$$

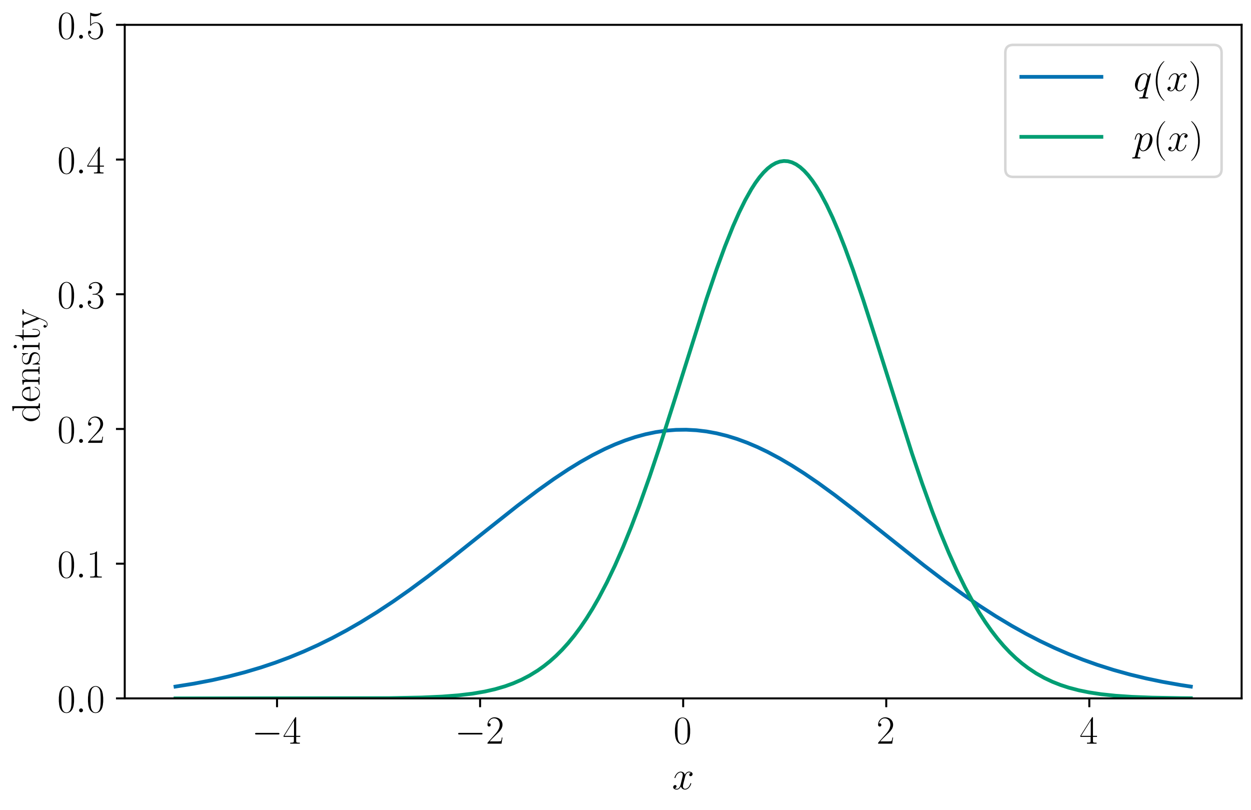
We will be using *TensorFlow*, *TensorFlow Probability*, and *Keras* in the code snippets throughout this post.

```
import tensorflow as tf
import tensorflow_probability as tfp
```

We first instantiate the distributions:

```
p = tfp.distributions.Normal(loc=1., scale=1.)
q = tfp.distributions.Normal(loc=0., scale=2.)
```

Their densities are shown below:



For any pair of distributions, we can implement their density ratio function r as follows:

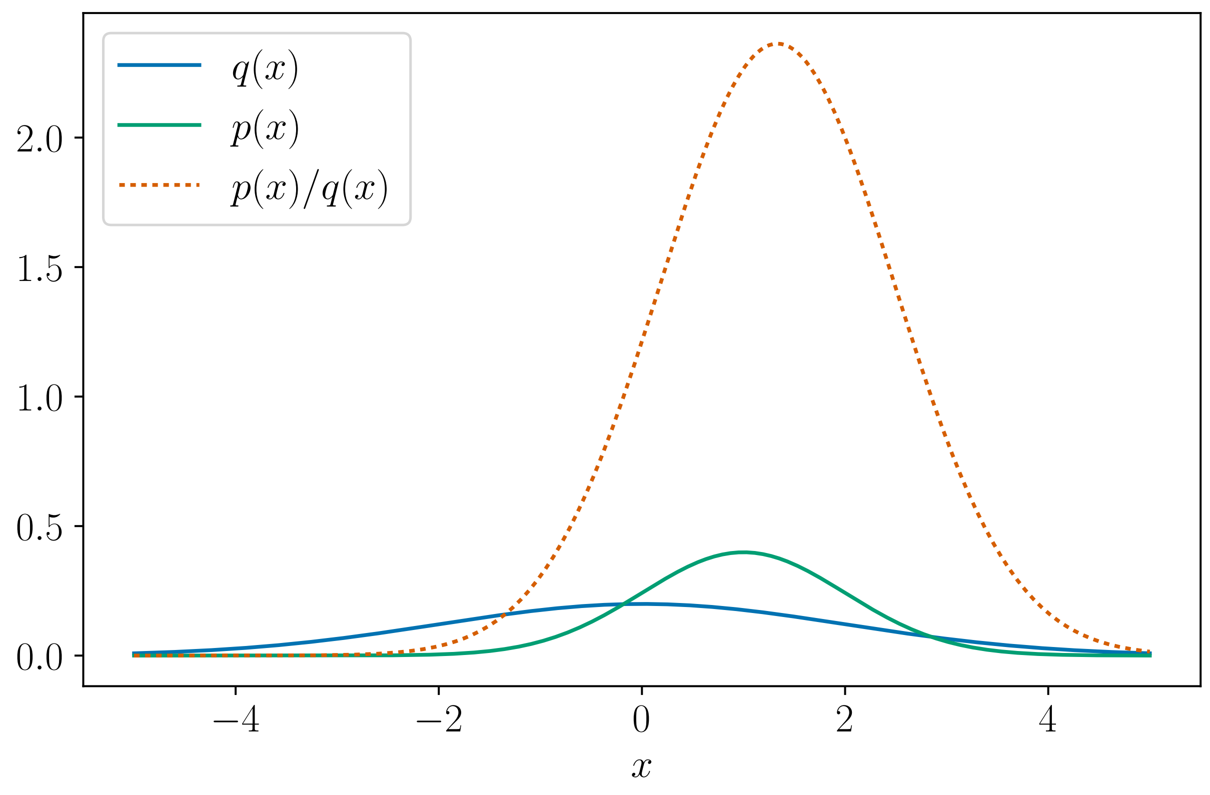
```
def log_density_ratio(p, q):

    def log_ratio(x):

        return p.log_prob(x) - q.log_prob(x)

    return log_ratio
```

```
def density_ratio(p, q):

    log_ratio = log_density_ratio(p, q)

    def ratio(x):

        return tf.exp(log_ratio(x))

    return ratio
```

Let’s create the density ratio function for the Gaussian distributions we just instantiated:

```
>>> r = density_ratio(p, q)
```

This density ratio function is plotted as the orange dotted line below, alongside the individual densities shown in the previous plot:



Analytical Form

For our running example, we picked $p(x)$ and $q(x)$ to be Gaussians so that it is possible to integrate out x and compute the KL divergence *analytically*. When we introduce the approximate methods later, this will provide us a “gold standard” to benchmark against.

In general, for Gaussian distributions

$$p(x) = \mathcal{N}(x \mid \mu_p, \sigma_p^2), \qquad \text{and} \qquad q(x) = \mathcal{N}(x \mid \mu_q, \sigma_q^2),$$

it is easy to verify that

$$\mathrm{KL}[p(x) || q(x)] = \log \sigma_q - \log \sigma_p - \frac{1}{2}\left[1 - \left(\frac{\sigma_p^2 + (\mu_p - \mu_q)^2}{\sigma_q^2}\right)\right].$$

This is implemented below:

```
def _kl_divergence_gaussians(p, q):

    r = p.loc - q.loc

    return (tf.log(q.scale) - tf.log(p.scale) -
            .5 * (1. - (p.scale**2 + r**2) / q.scale**2))
```

We can use this to compute the KL divergence between $p(x)$ and $q(x)$ *exactly*:

```
>>> _kl_divergence_gaussians(p, q).eval()
0.44314718
```

Equivalently, we could also use `kl_divergence` from *TensorFlow Probability–Distributions* (`tfp.distributions`), which implements the analytical closed-form expression of the KL divergence between distributions when such exists.

```
>>> tfp.distributions.kl_divergence(p, q).eval()
0.44314718
```

Monte Carlo Estimation — prescribed distributions

For distributions where their KL divergence is not analytically tractable, we may appeal to Monte Carlo (MC) estimation:

$$\begin{aligned}\mathcal{D}_{\mathrm{KL}}[p(x) || q(x)] &= \mathbb{E}_{p(x)}[\log r^*(x)] \\ &\approx \frac{1}{M}\sum_{i=1}^{M} \log r^*(x_p^{(i)}), \quad x_p^{(i)} \sim p(x).\end{aligned}$$

Clearly, this requires the density ratio $r^*(x)$ and, in turn, the densities $p(x)$ and $q(x)$ to be analytically tractable. Distributions for which the density function can be readily evaluated are sometimes referred to as **prescribed distributions**. As before, we *prescribed* Gaussians distributions in our running example so the Monte Carlo estimate can be later compared against. We approximate their KL divergence using $M = 5000$ Monte Carlo samples as follows:

```
>>> p_samples = p.sample(5000)
>>> true_log_ratio = log_density_ratio(p, q)
>>> tf.reduce_mean(true_log_ratio(p_samples)).eval()
0.44670376
```

Or equivalently, using the `expectation` function from *TensorFlow Probability–Monte Carlo* (`tfp.monte_carlo`):

```
>>> tfp.monte_carlo.expectation(f=true_log_ratio, samples=p_samples).eval()
0.4581419
```

More generally, we can approximate any f-divergence with MC estimation:

$$\begin{aligned}\mathcal{D}_f[p(x) || q(x)] &= \mathbb{E}_{q(x)}[f(r^*(x))] \\ &\approx \frac{1}{M}\sum_{i=1}^{M} f(r^*(x_q^{(i)})), \quad x_q^{(i)} \sim q(x).\end{aligned}$$

This can be done using the `monte_carlo_csiszar_f_divergence` function from *TensorFlow Probability–Variational Inference* (`tfp.vi`). One simply needs to specify the appropriate convex function f. The convex function that instantiates the (forward) KL divergence is provided in `tfp.vi` as `kl_forward`, alongside many other common f-divergences.

```
>>> tfp.vi.monte_carlo_csiszar_f_divergence(f=tfp.vi.kl_forward,
...                                         p_log_prob=p.log_prob, q=q,
...                                         num_draws=5000).eval()
0.4430853
```

Density Ratio Estimation — implicit distributions

When either density $p(x)$ or $q(x)$ is unavailable, things become more tricky. Which brings us to the topic of this post. Suppose we only have samples from $p(x)$ and $q(x)$—these could be natural images, outputs from a neural network with stochastic inputs, or in the case of our running example, i.i.d. samples drawn from Gaussians, etc. Distributions for which we are only able to observe their samples are known as **implicit distributions**, since their samples *imply* some underlying true density which we may not have direct access to.

Density ratio estimation is concerned with estimating the ratio of densities $r^*(x) = p(x)/q(x)$ given access only to samples from $p(x)$ and $q(x)$. Moreover, density ratio estimation usually encompass methods that achieve this without resorting to direct *density estimation* of the individual densities $p(x)$ or $q(x)$, since any error in the estimation of the denominator $q(x)$ is magnified exponentially.

Of the many density ratio estimation methods that now flourish[2], the classical approach of *probabilistic classification* remains dominant, due in no small part to its simplicity.

Reducing Density Ratio Estimation to Probabilistic Classification

We now demonstrate that density ratio estimation can be reduced to probabilistic classification. We shall do this by highlighting the one-to-one correspondence between the density ratio of $p(x)$ and $q(x)$ and the optimal probabilistic classifier that discriminates between their samples. Specifically, suppose we have a collection of samples from both $p(x)$ and $q(x)$, where each sample is assigned a class label indicating which distribution it was drawn from. Then, from an estimator of the class-membership probabilities, it is straightforward to recover an estimator of the density ratio.

Suppose we have N_p and N_q samples drawn from $p(x)$ and $q(x)$, respectively,

$$x_p^{(1)}, \dots, x_p^{(N_p)} \sim p(x), \qquad \text{and} \qquad x_q^{(1)}, \dots, x_q^{(N_q)} \sim q(x).$$

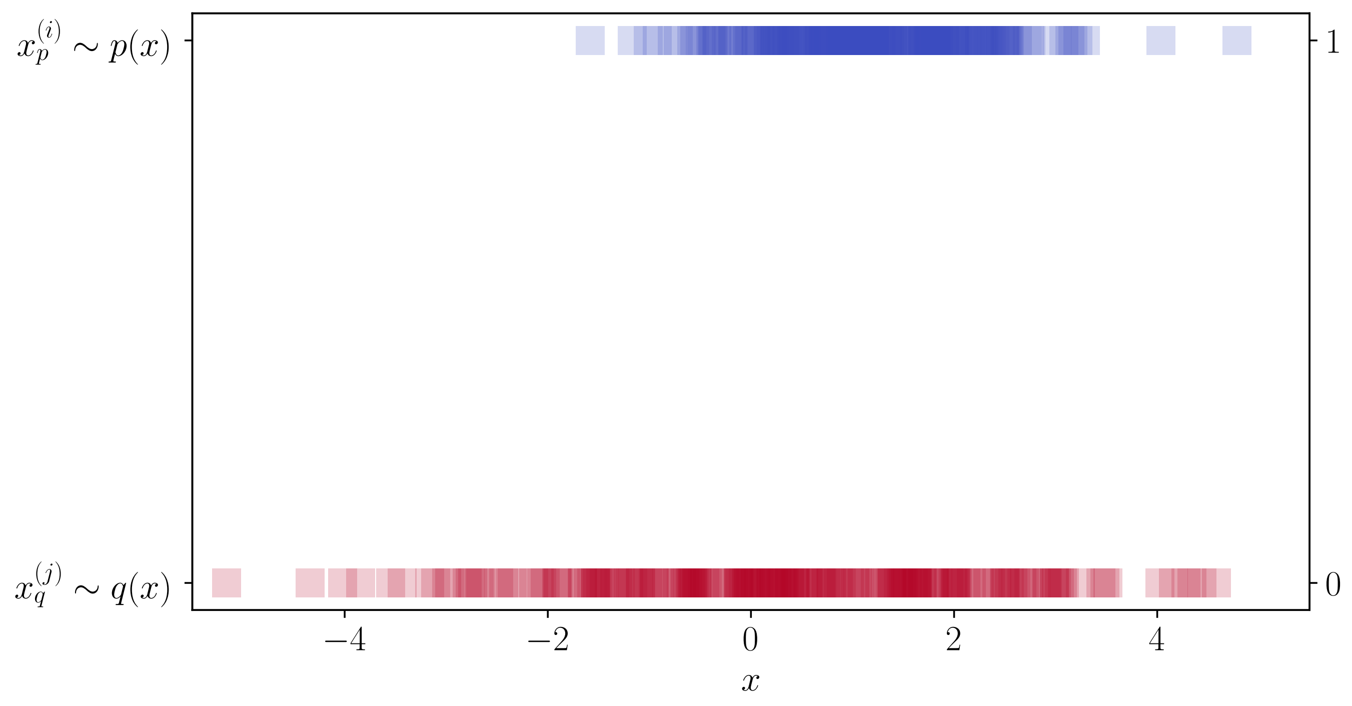
Then, we form the dataset $(x_n, y_n)_{n=1}^N$, where $N = N_p + N_q$ and

$$\begin{aligned}(x_1, \dots, x_N) &= (x_p^{(1)}, \dots, x_p^{(N_p)}, x_q^{(1)}, \dots, x_q^{(N_q)}), \\ (y_1, \dots, y_N) &= (\underbrace{1, \dots, 1}_{N_p}, \underbrace{0, \dots, 0}_{N_q}).\end{aligned}$$

In other words, we label samples drawn from $p(x)$ as 1 and those drawn from $q(x)$ as 0. In code, this looks like:

```
>>> p_samples = p.sample(sample_shape=(n_p, 1))
>>> q_samples = q.sample(sample_shape=(n_q, 1))
>>> X = tf.concat([p_samples, q_samples], axis=0)
>>> y = tf.concat([tf.ones_like(p_samples), tf.zeros_like(q_samples)], axis=0)
```

This dataset is visualized below. The blue squares in the top row are samples $x_p^{(i)} \sim p(x)$ with label 1; red squares in the bottom row are samples $x_q^{(j)} \sim q(x)$ with label 0.



Now, by construction, we have

$$p(x) = \mathcal{P}(x \mid y = 1), \qquad \text{and} \qquad q(x) = \mathcal{P}(x \mid y = 0).$$

Using Bayes' rule, we can write

$$\mathcal{P}(x \mid y) = \frac{\mathcal{P}(y \mid x)\mathcal{P}(x)}{\mathcal{P}(y)}.$$

Hence, we can express the density ratio $r^*(x)$ as

$$\begin{aligned} r^*(x) = \frac{p(x)}{q(x)} &= \frac{\mathcal{P}(x \mid y=1)}{\mathcal{P}(x \mid y=0)} \\ &= \left(\frac{\mathcal{P}(y=1 \mid x)\mathcal{P}(x)}{\mathcal{P}(y=1)}\right)\left(\frac{\mathcal{P}(y=0 \mid x)\mathcal{P}(x)}{\mathcal{P}(y=0)}\right)^{-1} \\ &= \frac{\mathcal{P}(y=0)}{\mathcal{P}(y=1)} \frac{\mathcal{P}(y=1 \mid x)}{\mathcal{P}(y=0 \mid x)}. \end{aligned}$$

Let us approximate the ratio of marginal densities by the ratio of sample sizes,

$$\frac{\mathcal{P}(y=0)}{\mathcal{P}(y=1)} \approx \frac{N_q}{N_p + N_q}\left(\frac{N_p}{N_p + N_q}\right)^{-1} = \frac{N_q}{N_p}.$$

To avoid notational clutter, let us assume from now on that $N_q = N_p$. We can then write $r^*(x)$ in terms of class-posterior probabilities,

$$r^*(x) = \frac{\mathcal{P}(y=1 \mid x)}{\mathcal{P}(y=0 \mid x)}.$$

Recovering the Density Ratio from the Class Probability

This yields a one-to-one correspondence between the density ratio $r^*(x)$ and the class-posterior probability $\mathcal{P}(y = 1 \mid x)$. Namely,

$$\begin{aligned} r^*(x) = \frac{\mathcal{P}(y=1 \mid x)}{\mathcal{P}(y=0 \mid x)} &= \frac{\mathcal{P}(y=1 \mid x)}{1-\mathcal{P}(y=1 \mid x)} \\ &= \exp\left[\log \frac{\mathcal{P}(y=1 \mid x)}{1-\mathcal{P}(y=1 \mid x)}\right] \\ &= \exp[\sigma^{-1}(\mathcal{P}(y=1 \mid x))], \end{aligned}$$

where σ^{-1} is the *logit* function, or inverse sigmoid function, given by $\sigma^{-1}(\rho) = \log\left(\frac{\rho}{1-\rho}\right)$

Recovering the Class Probability from the Density Ratio

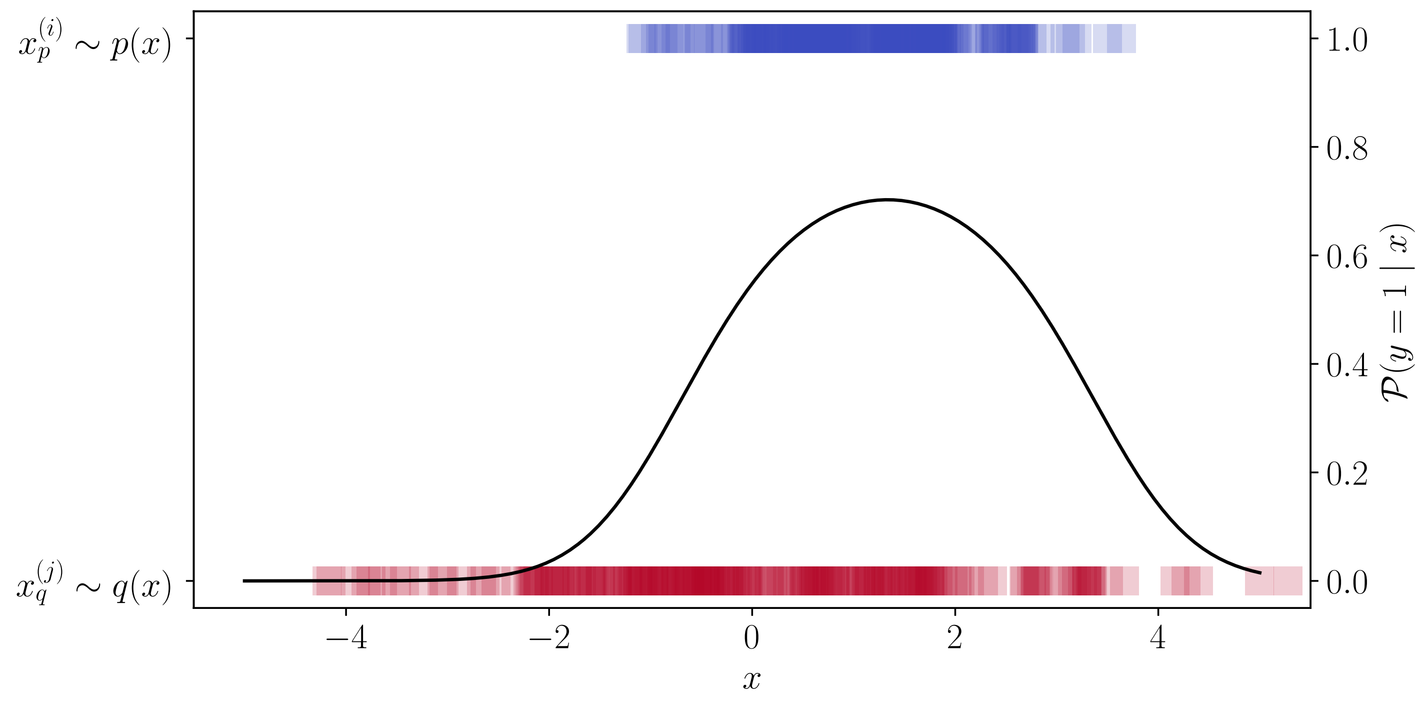
By simultaneously manipulating both sides of this equation, we can also recover the exact class-posterior probability as a function of the density ratio,

$$\mathcal{P}(y=1 \mid x) = \sigma(\log r^*(x)) = \frac{p(x)}{p(x)+q(x)}.$$

This is implemented below:

```
def optimal_classifier(p, q):

    def classifier(x):

        return tf.truediv(p.prob(x), p.prob(x) + q.prob(x))

    return classifier
```

In the figure below, The class-posterior probability $\mathcal{P}(y=1 \mid x)$ is plotted against the dataset visualized earlier.



Probabilistic Classification with Logistic Regression

The class-posterior probability $\mathcal{P}(y=1 \mid x)$ can be approximated using a parameterized function $D_\theta(x)$ with parameters θ. This functions takes as input samples from $p(x)$ and $q(x)$ and outputs a *score*, or probability, in the range $[0, 1]$ that it was drawn from $p(x)$. Hence, we refer to $D_\theta(x)$ as the probabilistic classifier.

From before, it is clear to see how an estimator of the density ratio $r_\theta(x)$ might be constructed as a function of probabilistic classifier $D_\theta(x)$. Namely,

$$\begin{aligned} r_\theta(x) &= \exp[\sigma^{-1}(D_\theta(x))] \\ &\approx \exp[\sigma^{-1}(\mathcal{P}(y=1 \mid x))] = r^*(x), \end{aligned}$$

and *vice versa*,

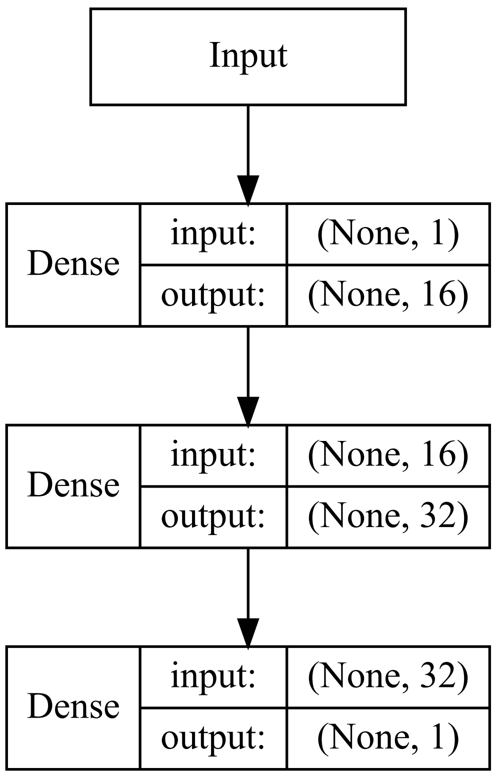
$$\begin{aligned} D_\theta(x) &= \sigma(\log r_\theta(x)) \\ &\approx \sigma(\log r^*(x)) = \mathcal{P}(y=1 \mid x). \end{aligned}$$

Instead of $D_\theta(x)$, we usually specify the parameterized function $\log r_\theta(x)$. This is also referred to as the *log-odds*, or *logits*, since it is equivalent to the unnormalized output of the classifier before being fed through the logistic sigmoid function.

We define a small fully-connected neural network with two hidden layers and ReLU activations:

```
log_ratio = Sequential([
    Dense(16, input_dim=1, activation='relu'),
    Dense(32, activation='relu'),
    Dense(1),
])
```

This simple architecture is visualized in the diagram below:



We learn the optimal class probability estimator by optimizing it with respect to a *proper scoring rule*[3] that yields well-calibrated probabilistic predictions, such as the *binary cross-entropy loss*,

$$\begin{aligned}\mathcal{L}(\theta) &:= -\mathbb{E}_{p(x)}[\log D_\theta(x)] - \mathbb{E}_{q(x)}[\log(1 - D_\theta(x))] \\ &= -\mathbb{E}_{p(x)}[\log \sigma(\log r_\theta(x))] - \mathbb{E}_{q(x)}[\log(1 - \sigma(\log r_\theta(x)))].\end{aligned}$$

An implementation optimized for numerical stability is given below:

```
def _binary_crossentropy(log_ratio_p, log_ratio_q):

    loss_p = tf.nn.sigmoid_cross_entropy_with_logits(
        logits=log_ratio_p,
        labels=tf.ones_like(log_ratio_p)
    )

    loss_q = tf.nn.sigmoid_cross_entropy_with_logits(
        logits=log_ratio_q,
        labels=tf.zeros_like(log_ratio_q)
    )

    return tf.reduce_mean(loss_p + loss_q)
```

Now we can build a multi-input/multi-output model, where the inputs are fixed with stochastic tensors—samples from $p(x)$ and $q(x)$, respectively.

```
>>> x_p = Input(tensor=p_samples)
>>> x_q = Input(tensor=q_samples)
>>> log_ratio_p = log_ratio(x_p)
>>> log_ratio_q = log_ratio(x_q)
```

The model can now be compiled and finalized. Since we're using a custom loss that take the two sets of log-ratios as input, we specify `loss=None` and define it instead through the `add_loss` method.

```
>>> m = Model(inputs=[x_p, x_q], outputs=[log_ratio_p, log_ratio_q])
>>> m.add_loss(_binary_crossentropy(log_ratio_p, log_ratio_q))
>>> m.compile(optimizer='rmsprop', loss=None)
```

As a sanity-check, the loss evaluated on a random batch can be obtained like so:

```
>>> m.evaluate(x=None, steps=1)
1.3765026330947876
```

We can now fit our estimator, recording the loss at the end of each epoch:

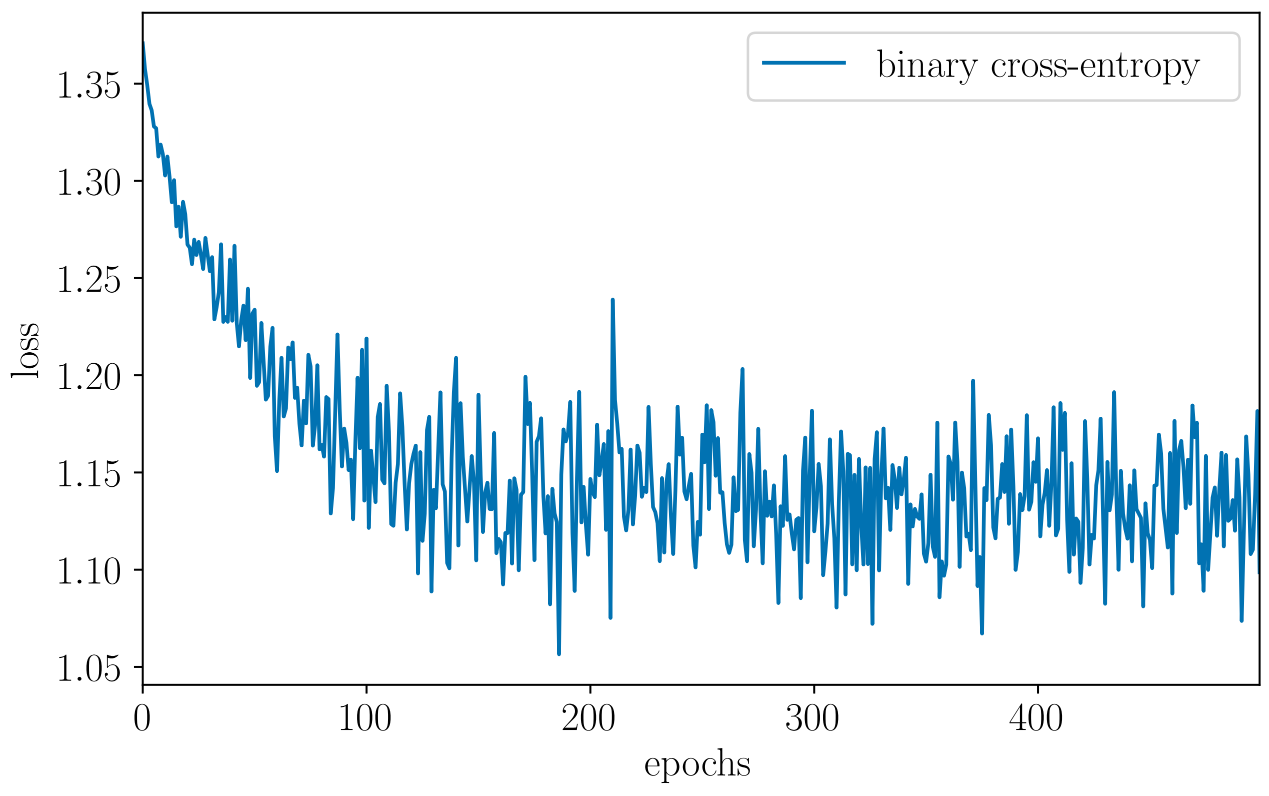
```
>>> hist = m.fit(x=None, y=None, steps_per_epoch=1, epochs=500)
```

The following animation shows how the predictions for the probabilistic classifier, density ratio, log density ratio, evolve after every epoch:

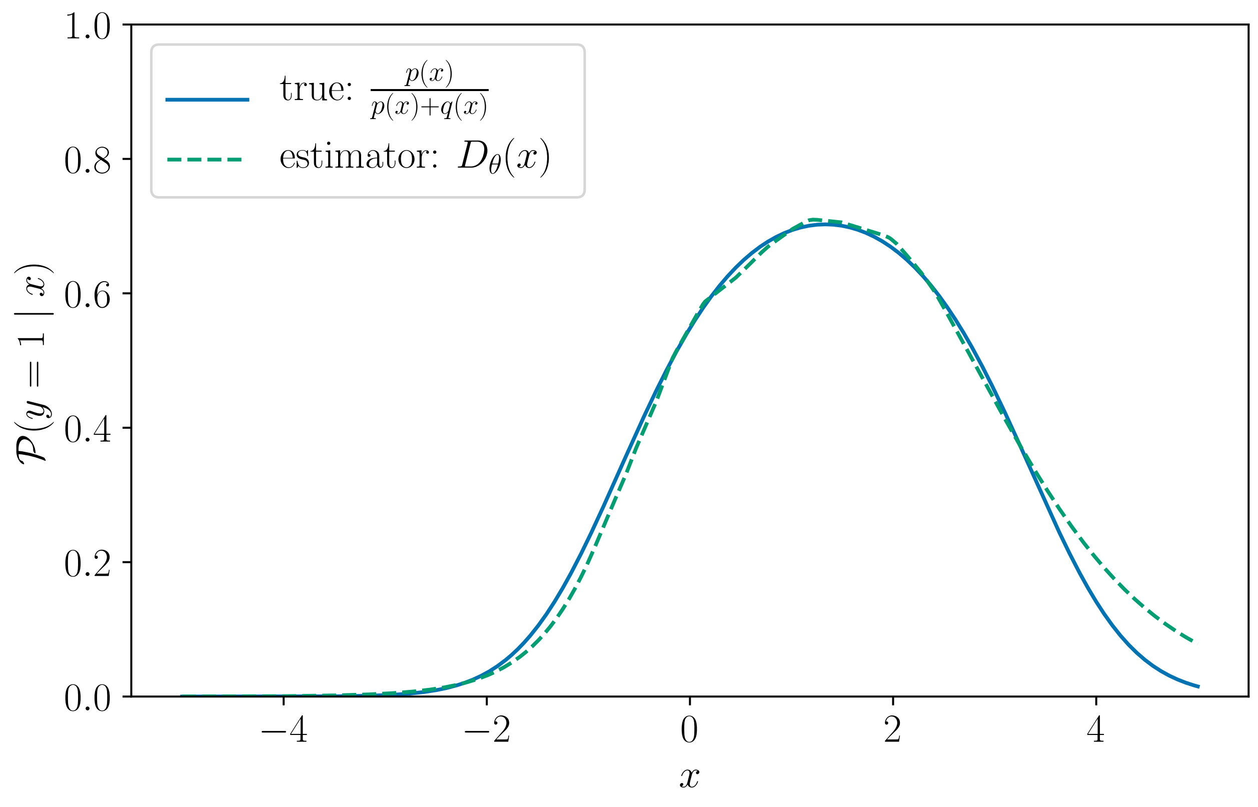
0:30 / 0:30

It is overlaid on top of their exact, analytical counterparts, which are only available since we prescribed them to be Gaussian distribution. For implicit distributions, these won't be accessible at all.

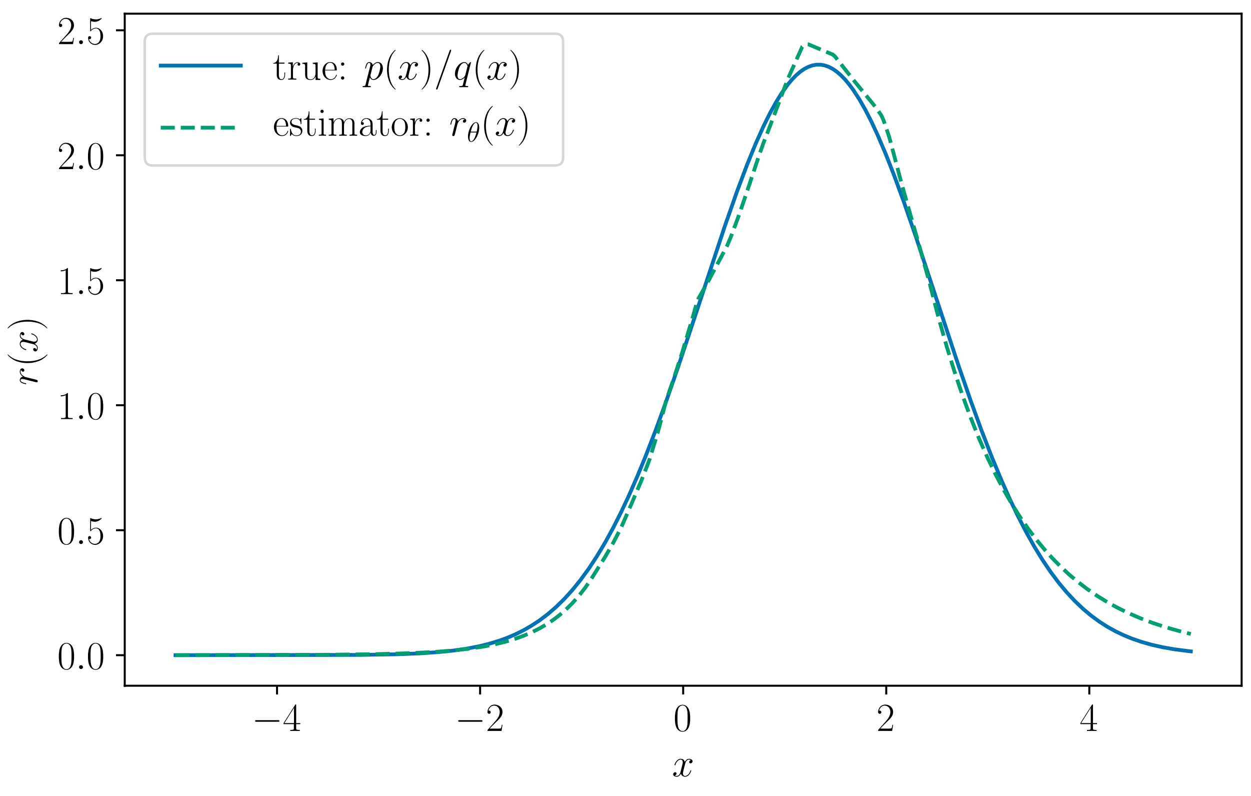
Below is the final plot of how the binary cross-entropy loss converges:



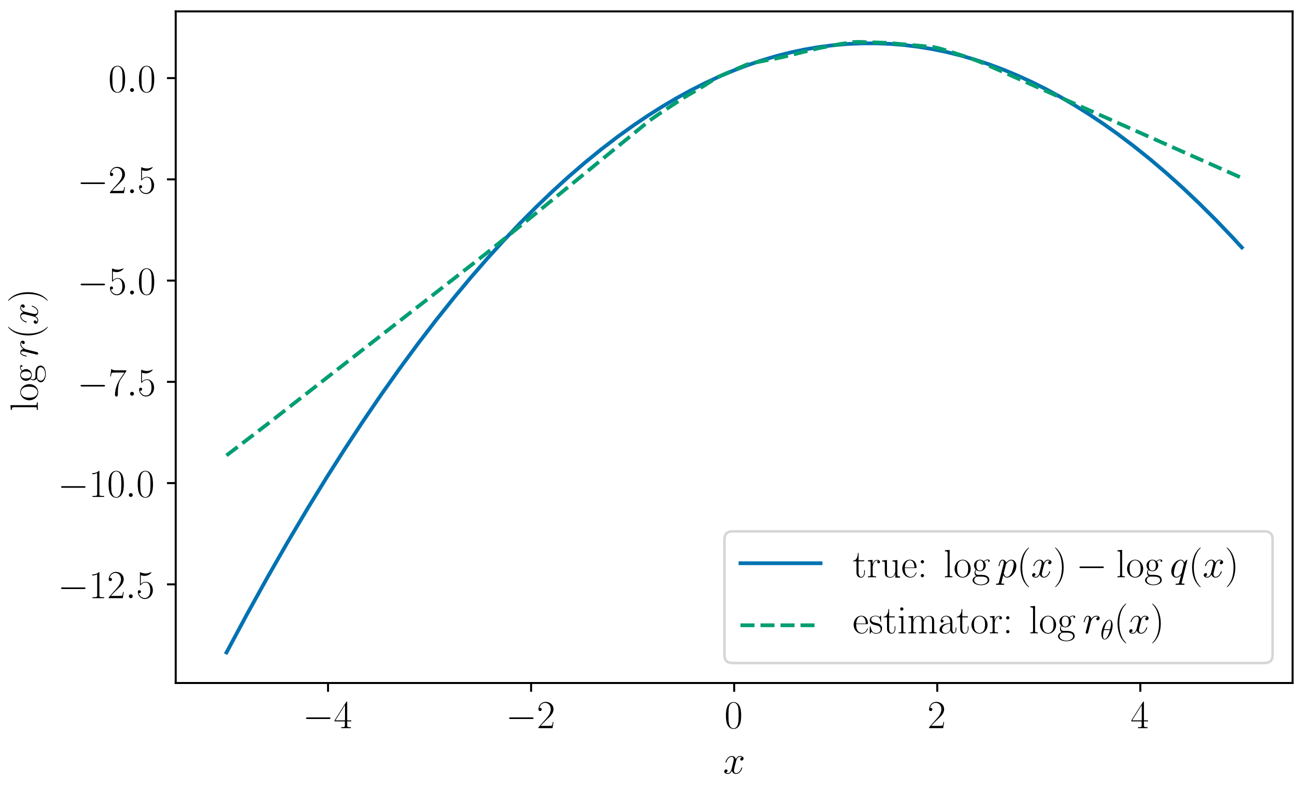
Below is a plot of the probabilistic classifier $D_\theta(x)$ (*dotted green*), plotted against the optimal classifier, which is the class-posterior probability $\mathcal{P}(y=1 \mid x) = \frac{p(x)}{p(x)+q(x)}$ (*solid blue*):



Below is a plot of the density ratio estimator $r_\theta(x)$ (*dotted green*), plotted against the exact density ratio function $r^*(x) = \frac{p(x)}{q(x)}$ (*solid blue*):



And finally, the previous plot in logarithmic scale:



While it may appear that we are simply performing regression on the latent function $r^*(x)$ (which is not wrong—we are), it is important to emphasize that we do this without ever having observed values of $r^*(x)$. Instead, we only ever observed samples from $p(x)$ and $q(x)$ This has profound implications and potential for a great number of applications that we shall explore later on.

Back to Monte Carlo estimation

Having an obtained an estimate of the log density ratio, it is now feasible to perform Monte Carlo estimation:

$$\begin{aligned}\mathcal{D}_{\mathrm{KL}}[p(x)||q(x)] &= \mathbb{E}_{p(x)}[\log r^*(x)] \\ &\approx \frac{1}{M}\sum_{i=1}^{M} \log r^*(x_p^{(i)}), \quad x_p^{(i)} \sim p(x) \\ &\approx \frac{1}{M}\sum_{i=1}^{M} \log r_\theta(x_p^{(i)}), \quad x_p^{(i)} \sim p(x).\end{aligned}$$

```
>>> tf.squeeze(tfp.monte_carlo.expectation(f=log_ratio, samples=p_samples)).eval()
0.4570999
```

In other words, we draw MC samples from $p(x)$ as before. But instead of taking the mean of the function $\log r^*(x)$ evaluated on these samples (which is unavailable for implicit distributions), we do so on a proxy function $\log r_\theta(x)$ that is estimated through probabilistic classification as described above.

Learning in Implicit Generative Models

Now let's take a look at where these ideas are being used in practice. Consider a collection of natural images, such as the MNIST handwritten digits shown below, which are assumed to be samples drawn from some implicit distribution $q(\mathbf{x})$:

MNIST hand-written digits

Directly estimating the density of $q(\mathbf{x})$ may not always be feasible—in some cases, it may not even exist. Instead, consider defining a parametric function $G_\phi : \mathbf{z} \mapsto \mathbf{x}$ with parameters ϕ, that takes as input $\mathbf{z}$ drawn from some fixed distribution $p(\mathbf{z})$. The outputs $\mathbf{x}$ of this generative process are assumed to be samples following some implicit distribution $p_\phi(\mathbf{x})$. In other words, we can write

$$\mathbf{x} \sim p_\phi(\mathbf{x}) \quad \Leftrightarrow \quad \mathbf{x} = G_\phi(\mathbf{z}), \quad \mathbf{z} \sim p(\mathbf{z}).$$

By optimizing parameters ϕ, we can make $p_\phi(\mathbf{x})$ close to the real data distribution $q(\mathbf{x})$. This is a compelling alternative to density estimation since there are many situations where being able to generate samples is more important than being able to calculate the numerical value of the density. Some examples of these include *image super-resolution* and *semantic segmentation*.

One approach might be to introduce a classifier D_θ that discriminates between real and synthetic samples. Then we optimize G_ϕ to synthesize samples that are indistinguishable, to classifier D_θ, from the real samples. This can be achieved by simultaneously optimizing the binary cross-entropy loss, resulting in the saddle-point objective,

$$\begin{aligned}&\min_\phi \max_\theta \mathbb{E}_{q(\mathbf{x})}[\log D_\theta(\mathbf{x})] + \mathbb{E}_{p_\phi(\mathbf{x})}[\log(1 - D_\theta(\mathbf{x}))] \\ &= \min_\phi \max_\theta \mathbb{E}_{q(\mathbf{x})}[\log D_\theta(\mathbf{x})] + \mathbb{E}_{p(\mathbf{z})}[\log(1 - D_\theta(G_\phi(\mathbf{z})))].\end{aligned}$$

This is, of course, none other than the groundbreaking *generative adversarial network (GAN)*[4]. You can read more about the density ratio estimation perspective of GANs in the paper by Uehara et al. 2016[5]. For an even more general and complete treatment of learning in implicit models, I recommend the paper from Mohamed and Lakshminarayanan, 2016[6], which partially inspired this post.

For the remainder of this section, I want to highlight a variant of this approach that specifically aims to minimize the KL divergence w.r.t. parameters ϕ,

$$\min_\phi \mathcal{D}_{\mathrm{KL}}[p_\phi(\mathbf{x}) || q(\mathbf{x})].$$

To overcome the fact that the densities of both $p_\phi(\mathbf{x})$ and $q(\mathbf{x})$ are unknown, we can readily adopt the density ratio estimation approach outlined in this post. Namely, by maximizing the following objective,

$$\begin{aligned}&\max_\theta \mathbb{E}_{q(\mathbf{x})}[\log D_\theta(\mathbf{x})] + \mathbb{E}_{p(\mathbf{z})}[\log(1 - D_\theta(G_\phi(\mathbf{z})))] \\ &= \max_\theta \mathbb{E}_{q(\mathbf{x})}[\log \sigma(\log r_\theta(\mathbf{x}))] + \mathbb{E}_{p(\mathbf{z})}[\log(1 - \sigma(\log r_\theta(G_\phi(\mathbf{z}))))],\end{aligned}$$

which attains its maximum at

$$r_\theta(\mathbf{x}) = \frac{q(\mathbf{x})}{p_\phi(\mathbf{x})}.$$

Concurrently, we also minimize the current best estimate of the KL divergence,

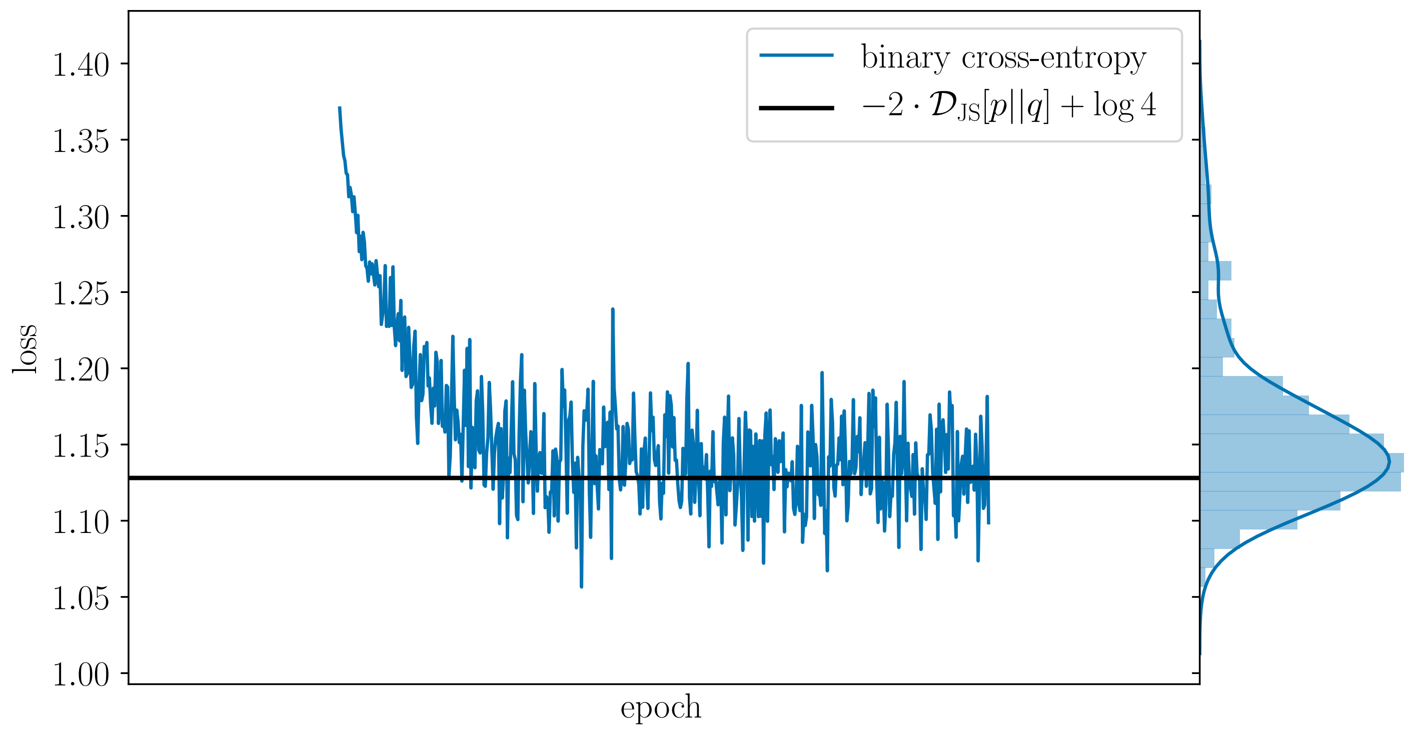
$$\begin{aligned}\min_\phi \mathcal{D}_{\mathrm{KL}}[p_\phi(\mathbf{x}) || q(\mathbf{x})] &= \min_\phi \mathbb{E}_{p_\phi(\mathbf{x})}\left[\log \frac{p_\phi(\mathbf{x})}{q(\mathbf{x})}\right] \\ &\approx \min_\phi \mathbb{E}_{p_\phi(\mathbf{x})}[-\log r_\theta(\mathbf{x})] \\ &= \min_\phi \mathbb{E}_{p(\mathbf{z})}[-\log r_\theta(G_\phi(\mathbf{z}))].\end{aligned}$$

In addition to being more stable than the vanilla GAN approach (alleviates saturating gradients), this is especially important in contexts where there is a specific need to minimize the KL divergence, such as in *variational inference (VI)*.

This was first used in *AffGAN* by Sønderby et al. 2016[7], and has since been incorporated in many papers that deal with implicit distributions in variational inference, such as (Mescheder et al. 2017[8], Huszar 2017[9], Tran et al. 2017[10], Pu et al. 2017[11], Chen et al. 2018[12], Tiao et al. 2018[13]), and many others.

Bound on the Jensen-Shannon Divergence

Before we wrap things up, let us take another look at the plot of the binary-cross entropy loss recorded at the end of each epoch. We see that it converges quickly to some value. It is natural to wonder: what is the significance, if any, of this value?



It is in fact the (negative) Jensen-Shannon (JS) divergence, up to constants,

$$-2 \cdot \mathcal{D}_{\text{JS}}[p(x)||q(x)] + \log 4.$$

Recall the Jensen-Shannon divergence is defined as

$$\mathcal{D}_{\text{JS}}[p(x)||q(x)] = \frac{1}{2}\mathcal{D}_{\text{KL}}[p(x)||m(x)] + \frac{1}{2}\mathcal{D}_{\text{KL}}[q(x)||m(x)],$$

where m is the mixture density

$$m(x) = \frac{p(x) + q(x)}{2}.$$

With our running example, this cannot be evaluated exactly since the KL divergence between a Gaussian and a mixture of Gaussians is analytically intractable. However, like the KL, we can still estimate their JS divergence with Monte Carlo estimation[14]:

```
>>> js = - tfp.vi.monte_carlo_csiszar_f_divergence(f=tfp.vi.jensen_shannon,
...                                                p_log_prob=p.log_prob,
...                                                q=q, num_draws=5000)
```

This value is shown in the horizontal black line in the plot above. Along the right margin, we also plot the a histogram of the binary cross-entropy loss values over epochs. We can see that this value indeed coincides with the mode of this histogram.

It is straightforward to show that we have the upper bound

$$\inf_{\theta} \mathcal{L}(\theta) \geq -2 \cdot \mathcal{D}_{\text{JS}}[p(x)||q(x)] + \log 4.$$

Firstly, we have

$$\begin{aligned}
&\sup_{\theta} \mathbb{E}_{p(x)}[\log D_\theta(x)] + \mathbb{E}_{q(x)}[\log(1 - D_\theta(x))] \\
&\quad = \mathbb{E}_{p(x)}[\log \mathcal{P}(y = 1 \mid x)] + \mathbb{E}_{q(x)}[\log \mathcal{P}(y = 0 \mid x)] \\
&\quad = \mathbb{E}_{p(x)}\left[\log \frac{p(x)}{p(x) + q(x)}\right] + \mathbb{E}_{q(x)}\left[\log \frac{q(x)}{p(x) + q(x)}\right] \\
&\quad = \mathbb{E}_{p(x)}\left[\log \frac{1}{2}\frac{p(x)}{m(x)}\right] + \mathbb{E}_{q(x)}\left[\log \frac{1}{2}\frac{q(x)}{m(x)}\right] \\
&\quad = \mathbb{E}_{p(x)}\left[\log \frac{p(x)}{m(x)}\right] + \mathbb{E}_{q(x)}\left[\log \frac{q(x)}{m(x)}\right] - 2\log 2 \\
&\quad = 2 \cdot \mathcal{D}_{\text{JS}}[p(x)||q(x)] - \log 4.
\end{aligned}$$

Therefore,

$$2 \cdot \mathcal{D}_{\text{JS}}[p(x)||q(x)] - \log 4 \geq \sup_{\theta} \mathbb{E}_{p(x)}[\log D_\theta(x)] + \mathbb{E}_{q(x)}[\log(1 - D_\theta(x))].$$

Negating both sides, we get

$$\begin{aligned}-2\cdot\mathcal{D}_{\mathrm{JS}}[p(x)||q(x)]+\log 4 &\leq -\sup_{\theta}\mathbb{E}_{p(x)}[\log D_\theta(x)]+\mathbb{E}_{q(x)}[\log(1-D_\theta(x))]\\ &=\inf_{\theta}-\mathbb{E}_{p(x)}[\log D_\theta(x)]-\mathbb{E}_{q(x)}[\log(1-D_\theta(x))]\\ &=\inf_{\theta}\mathcal{L}(\theta),\end{aligned}$$

as required.

In short, this tells us that the binary cross-entropy loss is *itself* an approximation (up to constants) to the Jensen-Shannon divergence. This begs the question: is it possible to construct a more general loss that bounds any given f-divergence?

Teaser: Lower Bound on any f-divergence

Using convex analysis, one can actually show that for any f-divergence, we have the lower bound[15]

$$\mathcal{D}_f[p(x)||q(x)]\geq\sup_{\theta}\mathbb{E}_{p(x)}[f'(r_\theta(x))]-\mathbb{E}_{q(x)}[f^{\star}(f'(r_\theta(x)))],$$

with equality exactly when $r_\theta(x)=r^*(x)$. Importantly, this lower bound can be computed without requiring the densities of $p(x)$ or $q(x)$—only their samples are needed.

In the special case of $f(u)=u\log u-(u+1)\log(u+1)$, we recover the binary cross-entropy loss and the previous result, as expected,

$$\begin{aligned}\mathcal{D}_f[p(x)||q(x)] &= 2\cdot\mathcal{D}_{\mathrm{JS}}[p(x)||q(x)]-\log 4\\ &\geq\sup_{\theta}\mathbb{E}_{p(x)}[\log\sigma(\log r_\theta(x))]+\mathbb{E}_{q(x)}[\log(1-\sigma(\log r_\theta(x)))]\\ &=\sup_{\theta}\mathbb{E}_{p(x)}[\log D_\theta(x)]+\mathbb{E}_{q(x)}[\log(1-D_\theta(x))].\end{aligned}$$

Alternately, in the special case of $f(u)=u\log u$, we get

$$\begin{aligned}\mathcal{D}_f[p(x)||q(x)] &= \mathcal{D}_{\mathrm{KL}}[p(x)||q(x)]\\ &\geq\sup_{\theta}\mathbb{E}_{p(x)}[\log r_\theta(x)]-\mathbb{E}_{q(x)}[r_\theta(x)-1].\end{aligned}$$

This gives us *yet* another way to estimate the KL divergence between implicit distributions, in the form of a direct lower bound on the KL divergence itself. As it turns out, this lower bound is closely-related to the objective of the *KL Importance Estimation Procedure (KLIEP)*[16], and will be the topic of our next post in this series.

Summary

This post covered how to evaluate the KL divergence, or any f-divergence, between implicit distributions—distributions which we can only sample from. First, we underscored the crucial role of the density ratio in the estimation of f-divergences. Next, we showed the correspondence between the density ratio and the optimal classifier. By exploiting this link, we demonstrated how one can use a trained probabilistic classifier to construct a proxy for the exact density ratio, and use this to enable estimation of any f-divergence. Finally, we provided some context on where this method is used, touching upon some recent advances in implicit generative models and variational inference.

To receive updates on more posts like this, follow me on Twitter and GitHub!

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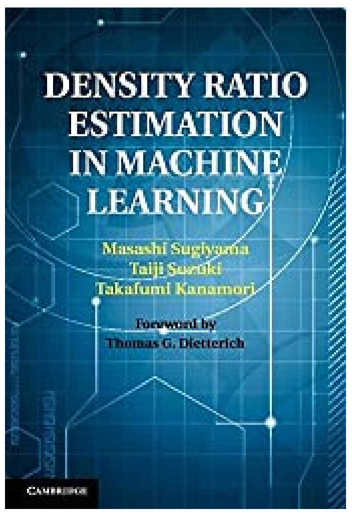
Links and Resources

- The notebook used to generate the figures in this post, which you can try out in Colaboratory.
- The very readable textbook on Density Ratio Estimation in Machine Learning[2], which I highly recommend. (Note: the Gaussian distributions example was borrowed from this book.)



- Shakir Mohamed's blog post Machine Learning Trick of the Day: Density Ratio Trick.
- The paper by Menon and Ong, 2016[17], which gives a generalized treatment of the theoretical link between density ratio estimation and probabilistic classification.

1. The (forward) KL divergence can be recovered with

$$f_{\mathrm{KL}}(u) := u \log u.$$

This is easy to verify,

$$\begin{aligned}\mathcal{D}_{\mathrm{KL}}[p(x) \| q(x)] &:= \mathbb{E}_{p(x)}\left[\log\left(\frac{p(x)}{q(x)}\right)\right] \\ &= \mathbb{E}_{q(x)}\left[\frac{p(x)}{q(x)}\log\left(\frac{p(x)}{q(x)}\right)\right] \\ &= \mathbb{E}_{q(x)}\left[f_{\mathrm{KL}}\left(\frac{p(x)}{q(x)}\right)\right].\end{aligned}$$

↩

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Density Ratio Estimation Machine Learning Implicit Distributions Information Theory

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CV

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