Density Ratio Estimators in Variational Bayesian Machine Learning

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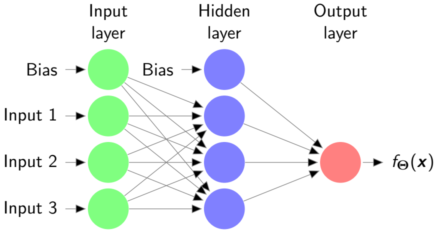
Outline

1. Background Info
   - Neural Networks
   - (Amortized) Variational Inference
   - Density Ratio Estimation
2. Activation Function Experiment
3. Optimal Estimator Experiment
4. Undertrained Estimator Experiment
   - Generation Experiment
5. Theory

Neural Networks

Overall Structure

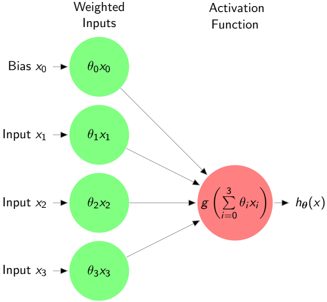
- Mathematical model based off human brain.
- Objective is to approximate a function f^* using mapping with parameters $\boldsymbol{\Theta}$: $\mathbf{f}_{\boldsymbol{\Theta}}(\boldsymbol{x})$.
- Universal Approximation Theorem states a neural network can approximate (almost) any function if it is complex enough.
- Consists of layers of nodes:



Neural Networks

Individual Node Structure

- Each node is a generalised linear model of preceding layer output.
- Weights θ are randomly initialised.
- Bias $x_0 = 1$ has role of intercept term in typical regression.
- $g(x)$ is activation function, e.g. ReLU is $g(x) = \max\{0, x\}$ in $[0, \infty)$, Sigmoid is $g(x) = (1 + \exp(-x))^{-1}$ in $(0, 1)$.



Neural Networks

Training

- Weights and biases trained such that (ideally convex) loss function is minimized e.g. Mean Squared Error: $\min_{\Theta} \frac{1}{2}||\boldsymbol{y} - \boldsymbol{f}_{\Theta}(\boldsymbol{x})||_2^2$.
- Back-propagation finds partial derivatives of loss function with respect to weights.
- Gradient descent uses these partial derivatives to optimize network.

(Amortized) Variational Inference

Bayesian Inference

- Fundamental problem in Bayesian computation is to estimate posterior densities $p(z|x)$.

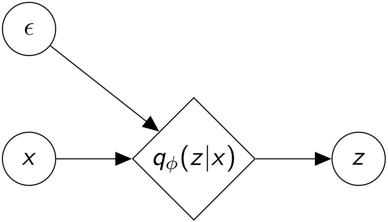
$$p(z|x) = \frac{p(z,x)}{p(x)} = \frac{p(z)p(x|z)}{\int_{\mathcal{Z}} p(z,x)dz}$$

- Problems arise when $\int_{\mathcal{Z}} p(z,x)dz$ is computationally intractable.
- Typical MCMC methods are slow with large datasets or high dimensional data.
- Variational Inference is a solution.

(Amortized) Variational Inference

Introduction

- Amortized variational inference approximates $p(z|x)$ with a different distribution $q_\phi(z|x)$.
- $q_\phi(z|x)$ is a neural network with parameters ϕ that takes in data x and random noise $\epsilon \sim \pi(\epsilon)$ and outputs samples $z \sim q_\phi(z|x)$.
- Typically $\pi(\epsilon) = \mathcal{N}(0, I_{n \times n})$.



(Amortized) Variational Inference

Network Training

- Minimize the **n**egative of the **e**vidence **l**ower **bo**und $NELBO(q)$:

  $$\min_{\phi} NELBO(q) = -\mathbb{E}_{q_\phi(z|x)q^*(x)}[\log p(x|z)] + \mathbb{E}_{q^*(x)}[KL(q_\phi(z|x)||p(z))].$$

- This is the same as minimizing the reverse KL divergence between the two distributions:

  $$\mathbb{E}_{q^*(x)}[KL(q(z|x)||p(z|x))] = \mathbb{E}_{q^*(x)q(z|x)}\left[\log\left(\frac{q(z|x)}{p(z|x)}\right)\right]$$

  .

- Taking expectation with respect to dataset distribution $q^*(x)$ allows model to work for different data points.

(Amortized) Variational Inference

Prior-Contrastive

$$\min_{\phi} \underbrace{-\mathbb{E}_{q_\phi(z|x)q^*(x)}[\log p(x|z)]}_{\text{Likelihood}} + \underbrace{\mathbb{E}_{q^*(x)}[KL(q_\phi(z|x)||p(z))]}_{\text{Log Density Ratio}}.$$

- $q_\phi(z|x)$ is a neural network so extremely difficult to evaluate density function but easy to draw samples, we therefore say that it is **implicit**.
- Use density ratio estimation to evaluate $\frac{q_\phi(z|x)}{p(z)}$ in $KL(q_\phi(z|x)||p(z))$.
- The prior $p(z)$ can also be implicit.
- We call this the "prior-contrastive" formulation.

(Amortized) Variational Inference

Joint-Contrastive

- If the likelihood $p(x|z)$ is implicit, then our optimization problem is

$$\min_{\phi} KL(q(z,x)||p(z,x)) = \mathbb{E}_{q^*(x)q_\phi(z|x)} \log \frac{q^*(x)q_\phi(z|x)}{p(z)p(x|z)}.$$

- Use density ratio estimation to evaluate $\frac{q(z,x)}{p(z,x)}$.
- For consistency, $NELBO(q) = KL(q(z,x)||p(z,x))$.
- We call this the “joint-contrastive” formulation.

Density Ratio Estimation

Class Probability Estimation

We want to estimate $\frac{q(u)}{p(u)}$.

1. Define discriminator function that finds probability that a sample u came from $q(u)$: $D_\alpha(u) \simeq P(u \sim q(u))$, so that $\frac{q(u)}{p(u)} \simeq \frac{D_\alpha(u)}{1-D_\alpha(u)}$.
2. $D_\alpha(u)$ is neural network parametrised by α, sigmoid activation function used for output layer
3. Train discriminator with Bernoulli loss: $\min_\alpha -\mathbb{E}_{q(u)}[\log D_\alpha(u)] - \mathbb{E}_{p(u)}[\log(1 - D_\alpha(u))]$.
4. Optimal discriminator is $D^*_\alpha(u) = \frac{q(u)}{q(u)+p(u)}$.

Density Ratio Estimation

Class Probability Estimation

Prior-Contrastive Application:

$$\min_{\alpha} -\mathbb{E}_{q^*(x)q_\phi(z|x)}[\log D_\alpha(z,x)] - \mathbb{E}_{q^*(x)p_\theta(z)}[\log(1 - D_\alpha(z,x))]$$

$$\min_{\phi} \underbrace{-\mathbb{E}_{q^*(x)q_\phi(z|x)}[\log p(x|z)]}_{\text{Likelihood}} + \underbrace{\mathbb{E}_{q^*(x)q_\phi(z|x)}\left[\log \frac{D_\alpha(z,x)}{1 - D_\alpha(z,x)}\right]}_{\text{Log Density Ratio}}$$

Joint-Contrastive Application:

$$\min_{\alpha} -\mathbb{E}_{q^*(x)q_\phi(z|x)}[\log D_\alpha(z,x)] - \mathbb{E}_{p(z)p(x|z)}[\log(1 - D_\alpha(z,x))]$$

$$\min_{\phi} \mathbb{E}_{q^*(x)q_\phi(z|x)} \log \frac{D_\alpha(z,x)}{1 - D_\alpha(z,x)}$$

Program alternates between several optimisation steps of discriminator and one optimisation step of posterior.

Theorem

If f is a convex function with derivative f' and convex conjugate f^*, and $\mathscr{R}$ is a class of functions with codomains equal to the domain of f', then we have the lower bound for the f-divergence between distributions $p(u)$ and $q(u)$:

$$D_f[p(u)||q(u)] \geq \sup_{r \in \mathscr{R}} \{\mathbb{E}_{q(u)}[f'(r(u))] - \mathbb{E}_{p(u)}[f^*(f'(r(u)))]\},$$

with equality when $r(u) = q(u)/p(u)$.

For the reverse KL divergence, $f(u) = u \log u$ so we have

$$KL[q(u)||p(u)] \geq \sup_{r \in \mathscr{R}} \{\mathbb{E}_{q(u)}[1 + \log r(u)] - \mathbb{E}_{p(u)}[r(u)]\}$$

Density Ratio Estimation

Divergence Minimisation

- Let our ratio estimator be a neural network parametrised by α: $r_\alpha(u) \simeq \frac{q(u)}{p(u)}$.
- Maximise the lower bound w.r.t. α until equality, which is when $r_\alpha(u) = \frac{q(u)}{p(u)}$. The optimisation problem for this is

$$\min_\alpha -\mathbb{E}_{q(u)}[\log r_\alpha(u)] + \mathbb{E}_{p(u)}[r_\alpha(u)].$$

- Obviously our optimal ratio estimator is $r^*_\alpha(u) = \frac{q(u)}{p(u)}$.

Density Ratio Estimation

Divergence Minimisation

Prior-Contrastive Application:

$$\min_{\alpha} -\mathbb{E}_{q^*(x)q_\phi(z|x)}[\log r_\alpha(z,x)] + \mathbb{E}_{q^*(x)p(z)}[r_\alpha(z,x)]$$

$$\min_{\phi} \underbrace{-\mathbb{E}_{q^*(x)q_\phi(z|x)}\,[\log p(x|z)]}_{\text{Likelihood}} + \underbrace{E_{q^*(x)q_\phi(z|x)}[\log r_\alpha(z,x)]}_{\text{Log Density Ratio}}$$

Joint-Contrastive Application:

$$\min_{\alpha} -\mathbb{E}_{q^*(x)q_\phi(z|x)}[\log r_\alpha(z,x)] + \mathbb{E}_{p(z)p(x|z)}[r_\alpha(z,x)]$$

$$\min_{\phi} \mathbb{E}_{q^*(x)q_\phi(z|x)}[\log r_\alpha(z,x)]$$

Density Ratio Estimation

Algorithm Generalisation

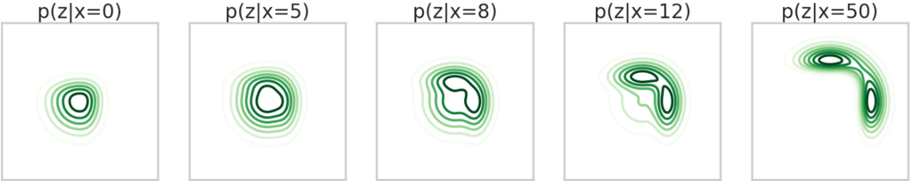
- Actually, $f(u) = u \log u - (u+1)\log(u+1)$ and $D(u) = \frac{r(u)}{r(u)+1}$ leads to class probability estimation equations.
- The upper bound f-divergence is $2JS(p(u)\|q(u)) - \log 4$, we call this the GAN divergence.
- To formulate optimisation problems for density ratio estimation, choose either reverse KL or GAN f-divergence upper bound and estimator parametrisation:
  - Class Probability Estimator $D_\alpha(u) \simeq \frac{q(u)}{q(u)+p(u)}$
  - Direct Ratio Estimator $r_\alpha(u) \simeq \frac{q(u)}{p(u)}$
  - Direct Log Ratio Estimator $T_\alpha(u) \simeq \log \frac{q(u)}{p(u)}$.

Activation Function Experiment

Experiment Outline

$$p(z_1, z_2) \sim \mathcal{N}(0, \sigma^2 I_{2\times 2})$$

$$p(x|\boldsymbol{z}) \sim EXP(3 + \max(0, z_1)^3 + \max(0, z_2)^3)$$



- Posterior is flexible and bimodal.
- Use Gaussian KDE to find 'true' KL divergence for $q_\phi(z|x = 0, 5, 8, 12, 50)$.

Activation Function Experiment

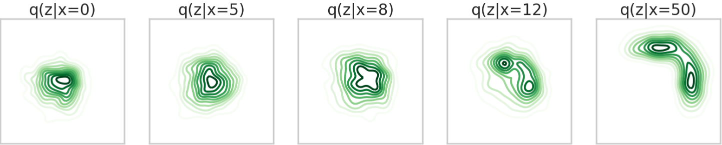
Experiment Outline

- Common to use ReLU $g(x) = \max\{0, x\}$ as activation function for output layer of direct ratio estimator $r_\alpha(u) \simeq \frac{q(u)}{p(u)}$.
- Experiences ‘dying ReLU problem’.
- Linearity of ReLU activation causes imbalance between ratios in $(0, 1)$ and $(1, \infty)$.
- We propose exponential activation function $g(x) = e^x$.
- Compare them for $r_\alpha(u)$ with reverse KL divergence upper bound.
- Low training rate, high iterations.
- Use Gaussian kernel density estimator to estimate ‘true’ KL divergence.

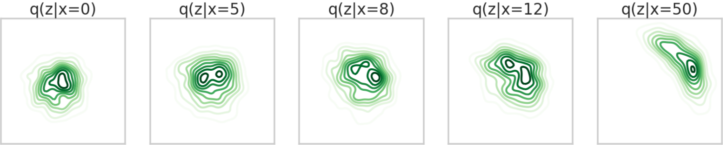
Activation Function Experiment

Results

Algorithm	Mean KL Divergence	Standard Deviation
Prior Contrastive - ReLU	1.3807	0.0391
Prior Contrastive - Exp	1.3265	0.0045
Joint-Contrastive - ReLU	1.6954	0.4337
Joint-Contrastive - Exp	1.3397	0.0066



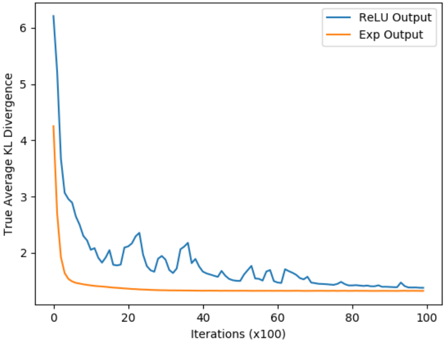
(a) Average KL Divergence of 1.3288



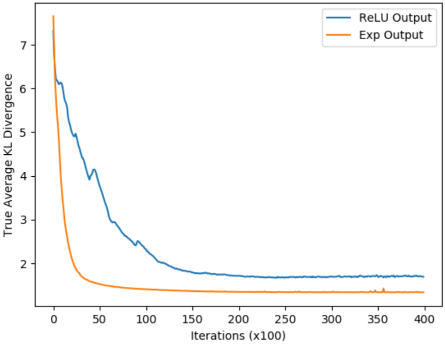
(b) Average KL Divergence of 1.3963

Inference Experiment - Activation Function

KL Divergence Plots



(a) Prior-Contrastive

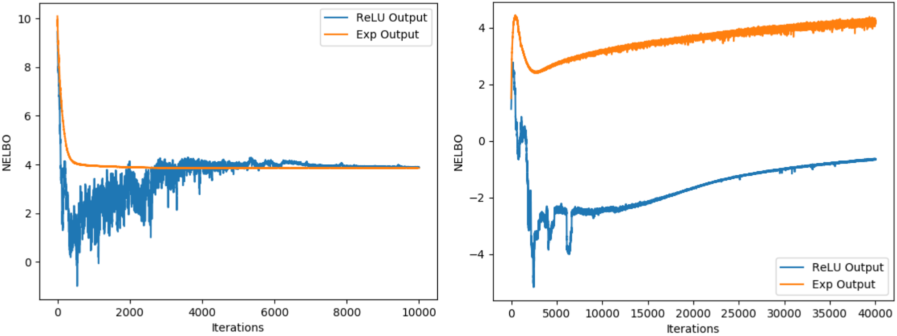


(b) Joint-Contrastive

- Exponential output has smoother and faster convergence.

Inference Experiment - Activation Function

NELBOs



(a) Prior-Contrastive

(b) Joint-Contrastive

- More stable NELBO estimation by exponential output.
- Variance of exponential output in joint-contrastive case increases over time.

Optimal Estimator Experiment

Experiment Outline

- Same inference problem as before.
- Aim of this experiment is to verify that choice of estimator does not matter as long as it reaches equality.
- Low training rate with high estimator to posterior optimisation ratio (100:1).
- High posterior iterations.

Optimal Estimator Experiment

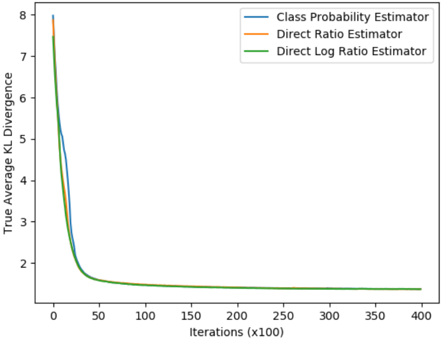
Results

Algorithm	Mean KL Divergence	Standard Deviation
JC Reverse KL - $D_\alpha(z,x)$	1.3416	0.0068
JC Reverse KL - $r_\alpha(z,x)$	1.3397	0.0066
JC Reverse KL - $T_\alpha(z,x)$	1.3446	0.0108
JC GAN - $D_\alpha(z,x)$	1.3648	0.0242
JC GAN - $r_\alpha(z,x)$	1.3657	0.0302
JC GAN - $T_\alpha(z,x)$	1.3670	0.0387

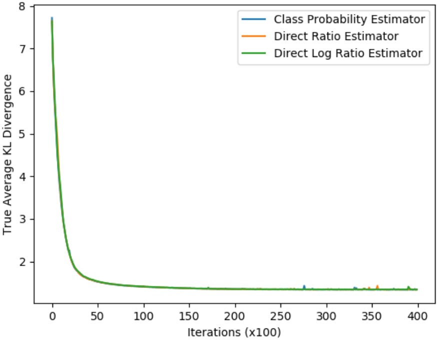
- Prior-contrastive posteriors fully converged at ≈ 1.325.
- No significant difference in convergence between estimators in each f-divergence.
- Reverse KL converged faster in joint-contrastive context.

Optimal Estimator Experiment

Joint-Contrastive KL Divergence Plots



(a) GAN Divergence

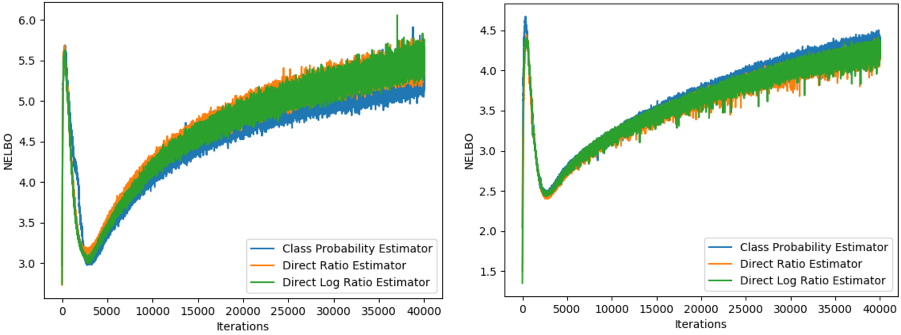


(b) Reverse KL Divergence

- Plots almost indistinguishable with exception of class probability estimator outlier in GAN divergence.

Optimal Estimator Experiment

Joint-Contrastive NELBO Plots



(a) GAN Divergence

(b) Reverse KL Divergence

- Again very similar plots.
- NELBO estimation smooth but has increasing variance over time.

Undertrained Estimator Experiment

Experiment Outline

- Estimators are similar when they are optimal but what if they are not optimal?
- Same inference experiment again.
- Significantly reduce amount of estimator training between posterior iterations.
- Increased posterior training rate.

Undertrained Estimator Experiment

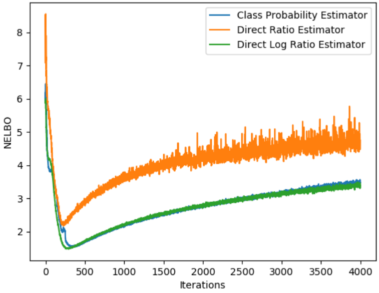
Results

Algorithm	Mean KL Divergence	Standard Deviation
JC Reverse KL - $D_\alpha(z,x)$	1.3786	0.0286
JC Reverse KL - $r_\alpha(z,x)$	1.3934	0.0410
JC Reverse KL - $T_\alpha(z,x)$	1.4133	0.0597
JC GAN - $D_\alpha(z,x)$	1.4017	0.0286
JC GAN - $r_\alpha(z,x)$	1.4086	0.0555
JC GAN - $T_\alpha(z,x)$	1.4214	0.0518

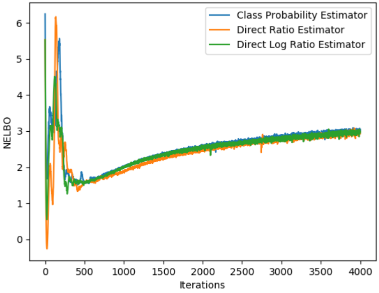
- Reverse KL divergence significantly better than GAN divergence.
- $D_\alpha(z,x) < r_\alpha(z,x) < T_\alpha(z,x)$

Undertrained Estimator Experiment

Joint-Contrastive NELBO Plots



(a) GAN Divergence



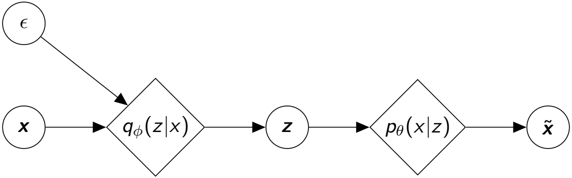
(b) Reverse KL Divergence

- Unclear why direct ratio estimator has unusual NELBO plot: posterior convergence was not affected.

Generation Experiment

Autoencoders

- Likelihood $p_\theta(x|z)$ is now a neural network.
- Posterior $q_\phi(z|x)$ represents data x as lower dimensional latent z.
- Likelihood $p_\theta(x|z)$ reconstructs data $\tilde{x}$ from z.
- Generate new data $\tilde{x}$ using z from $p(z)$.



$$\min_{\theta,\phi} -\mathbb{E}_{q_\phi(z|x)q^*(x)}[\log p_\theta(x|z)] + \mathbb{E}_{q^*(x)}[KL(q_\phi(z|x)||p(z))]$$

Generation Experiment

Experiment Outline

- MNIST dataset - 28 × 28 grey-scale images of handwritten digits
- Joint-contrastive context not tested here.
- Again use undertrained estimator.
- Use reconstruction error $\|x - \tilde{x}\|^2$ as metric.
- Perform experiment with low dimensional latent space (2 dimensions) and high dimensional latent space (20 dimensions).
- Low dimensional case had similar results to previous experiment.

Generation Experiment

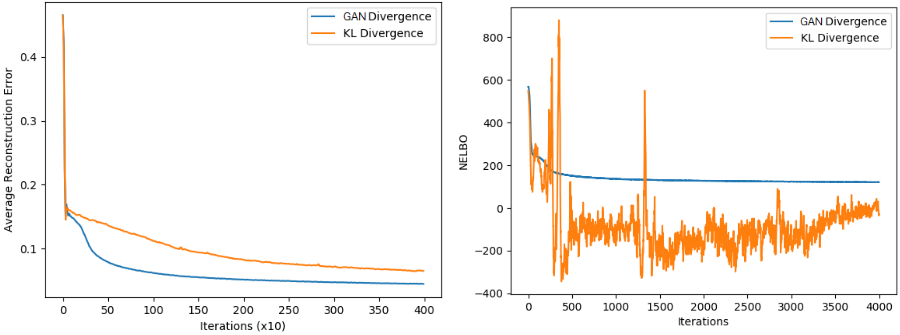
Results - high dimensional latent space

Algorithm	Mean Reconstruction Error	Standard Deviation
PC GAN - $D_\alpha(z,x)$	0.0444	0.0017
PC Reverse KL - $D_\alpha(z,x)$	0.0647	0.0019

- Direct ratio and direct log ratio estimators attempted to store numbers exceeding float64(max).
- Exponential of $T_\alpha(z,x)$ taken in loss function.
- $D_\alpha(z,x)$ ranges in $(0,1)$.
- Value before sigmoid activation function for $D_\alpha(z,x)$ is log density ratio.
- This time GAN divergence leads to better convergence than reverse KL.

Generation Experiment

Results - high dimensional latent space



(a) Reconstruction Error

(b) NELBO

- As before, GAN divergence is more stable.
- Recall reverse KL divergence is initially unstable but stabilizes later.
- In this case it fails to stabilise by the end of the program runtime.

Theory

Choice of f-divergence

- Nowozin's f-GAN paper shows empirically that the reverse KL divergence is superior when it is additionally used to optimize the posterior.
- Intuitive that the f-divergence used to optimize posterior is the best upper bound for estimator.

Further Estimator Loss Function Analysis

Estimator Parametrisation

- $D_\alpha(u)$ has smallest bound of $(0, 1)$, followed by $r_\alpha(u) \in \mathbb{R}^+$ and $T_\alpha(u) \in \mathbb{R}$.
- The density ratio changes every time the posterior is optimised, and the estimator must catch up.
- $D_\alpha(u)$ has a strictly lower displacement than $r_\alpha(u)$, that is, $|D_\alpha^{(n+1)}(u) - D_\alpha^{(n)}(u)| < |r_\alpha^{(n+1)}(u) - r_\alpha^{(n)}(u)|$.

Summary

- The class probability estimator $D_\alpha(u) \simeq \frac{q(u)}{q(u)+p(u)}$ is the ‘best’ parametrisation as it can store thehighest density ratios.
- Reverse KL divergence upper bound demonstrates initial instability (especially when estimator is undertrained) but leads to faster convergence when it stabilizes.
- Outlook
    - Still unclear exactly why reverse KL divergence is more unstable but more accurate when stable.
    - Several more f-divergences exist which have unknown stability when undertrained.