Density Ratio Estimation in Variational Bayesian Machine Learning

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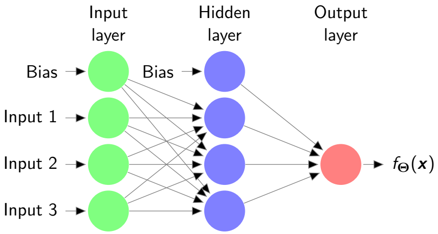
Outline

1. Background Information
   - Neural Networks
   - (Amortized) Variational Inference
   - Density Ratio Estimation
2. Undertrained Estimator Experiment
3. Autoencoder Experiment

- 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.
- Each node output is a transformed, weighted sum of previous node outputs.



Neural Networks

Training

- Weights 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.

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

$$p(z|x) \propto \underbrace{p(z)}_{\text{Prior}} \underbrace{p(x|z)}_{\text{Likelihood}} .$$

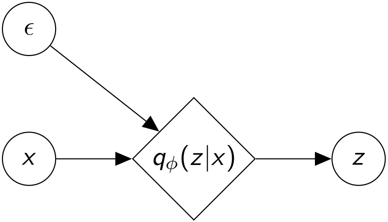
- Typical MCMC methods are slow with large datasets or high dimensional data.

- 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 $\epsilon \sim \mathcal{N}(0, I_{n\times n})$ and outputs samples $z \sim q_\phi(z|x)$.



- Train network by minimizing the (expected) reverse KL divergence between the two distributions:

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

.

- This is the same as solving the following minimization problem:

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

- We call this $NELBO(q)$ as it is the **n**egative of **e**vidence **l**ower **bo**und.

Consider our log density ratio term

$$KL(q_\phi(z|x)||p(z)) = \mathbb{E}_{q_\phi(z|x)}\left[\frac{q_\phi(z|x)}{p(z)}\right].$$

- $q_\phi(z|x)$ is an **implicit** distribution.
- Use density ratio estimation to evaluate $\frac{q_\phi(z|x)}{p(z)}$ in $KL(q_\phi(z|x)||p(z))$.
- Density ratio estimation only requires **samples** from the distributions.

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

1. Define discriminator network that finds probability that a sample u came from $q(u)$.

2. Train discriminator with Bernoulli loss:
$\min_\alpha -\mathbb{E}_{q(u)}[\log D_\alpha(u)] - \mathbb{E}_{p(u)}[\log(1 - D_\alpha(u))]$.

3. Optimal discriminator is $D_\alpha^*(u) = \frac{q(u)}{q(u)+p(u)}$.

$$\frac{q(u)}{p(u)} = \frac{D_\alpha^*(u)}{1 - D_\alpha^*(u)}$$

Density Ratio Estimation

Divergence Minimisation

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 letting $r_\alpha(u) \simeq \frac{q(u)}{p(u)}$ we have:

$$KL[q(u)||p(u)] \geq \sup_{\alpha} \{\mathbb{E}_{q(u)}[1 + \log r_\alpha(u)] - \mathbb{E}_{p(u)}[r_\alpha(u)]\}$$

- Actually, upper bound f-divergence of $\underbrace{2JS(p(u)\|q(u)) - \log 4}_{\text{GAN Divergence}}$ and $D(u) = \frac{r(u)}{r(u)+1}$ leads to class probability estimation loss function.

- Choose either reverse KL or GAN ***f*-divergence 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 $T_\alpha(u) \simeq \log \frac{q(u)}{p(u)}$.

Recap

To train a variational posterior network:

1. Train estimator network until convergence.
2. Use estimator network to calculate intractable term in *NELBO*.
3. Take one optimisation step of posterior network.
4. Repeat until posterior convergence.

Undertrained Estimator Experiment

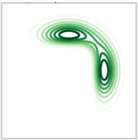
Experiment Outline

$$p(z_1, z_2) \sim \mathcal{N}(0, \sigma^2 I_{2\times 2})$$
$$p(x|\boldsymbol{z}) \sim Exp(3 + \max(0, z_1)^3 + \max(0, z_2)^3)$$

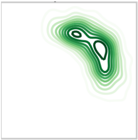
- Posterior is flexible and bimodal.
- Use Gaussian KDE to find 'true' KL divergence for $q_\phi(z|x = 0, 5, 8, 12, 50)$.

- In a previous experiment we found that all three estimator parametrisations lead to similar results when optimised effectively.
- What if they are poorly optimised?
- Training parameters:
  - High posterior training rate.
  - Low estimator training rate.
  - Low estimator to posterior iteration ratio (11:1).

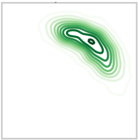
Algorithm	Mean KL Divergence	Standard Deviation
Reverse KL - $D_\alpha(z,x)$	**1.3786**	**0.0286**
Reverse KL - $r_\alpha(z,x)$	1.3934	0.0410
Reverse KL - $T_\alpha(z,x)$	1.4133	0.0597
GAN - $D_\alpha(z,x)$	1.4017	**0.0286**
GAN - $r_\alpha(z,x)$	1.4086	0.0555
GAN - $T_\alpha(z,x)$	1.4214	0.0518



True



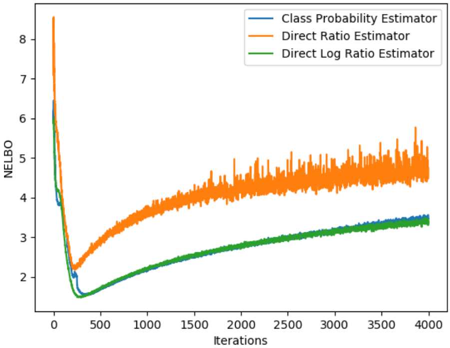
Reverse KL



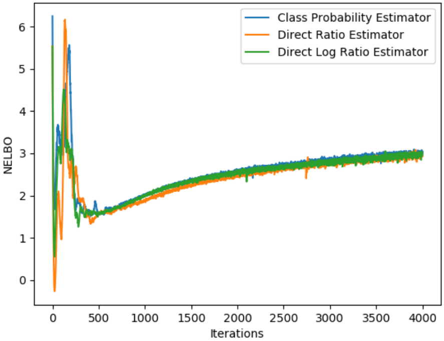
GAN

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

Undertrained Estimator Experiment
NELBO Plots



(a) GAN Divergence

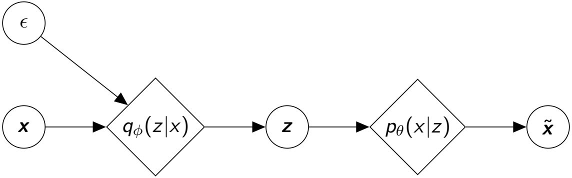


(b) Reverse KL Divergence

- Unclear why direct ratio estimator has unusual NELBO plot: posterior convergence was not affected.
- Reverse KL Divergence has initial instability.

Autoencoder Experiment

- 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 $p(z)$.



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

Autoencoder Experiment

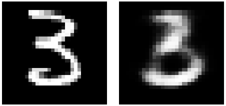
Experiment Outline

- MNIST dataset - 28 $\times$ 28 grey-scale images of handwritten digits
- 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).

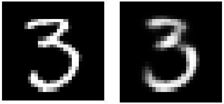
Generation Experiment

Results - high dimensional latent space

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

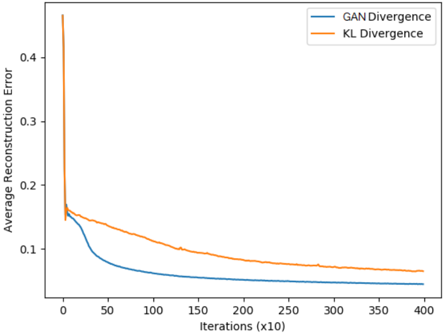


Reverse KL

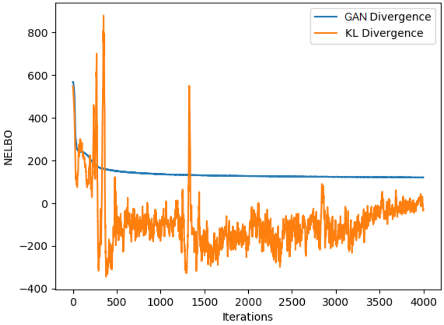


GAN

- 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 $(0, 1)$.



(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.

Summary

- The class probability estimator $D_\alpha(u) \simeq \frac{q(u)}{q(u)+p(u)}$ is the 'best' parametrisation as it can store the highest density ratios.
- Reverse KL divergence upper bound may be unstable but leads to faster convergence when stable.
- 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.