Density Ratio Estimation in Variational Bayesian Machine Learning

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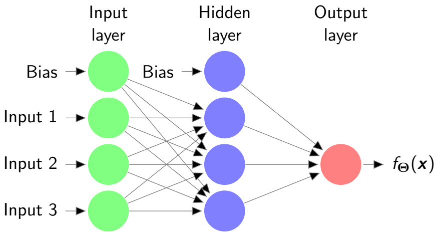
Outline

Neural Networks

Overall Structure

- Objective is to approximate a function f^* using mapping with parameters $\mathbf{\Theta}$: $\mathbf{f}_{\mathbf{\Theta}}(\boldsymbol{x})$.
- Universal Approximation Theorem states a neural network can approximate (almost) any function if it is complex enough.
- Each node output is a weighted sum of previous node outputs, passed through an activation function.



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.

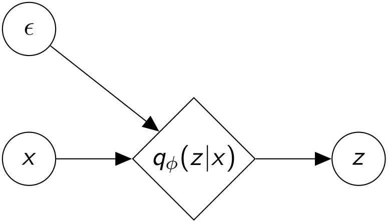
- Fundamental problem in Bayesian computation is to estimate posterior densities $p(z|x)$:

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

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

- Variational Inference is a solution.

- Amortized variational inference 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 $\pi(\epsilon) = \mathcal{N}(0, I_{n\times n})$.



- Minimize the **n**egative of **e**vidence **l**ower **bo**und $NELBO(q)$ w.r.t. ϕ:

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

- 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

Problems with Implicit Distributions

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

- $q_\phi(z|x)$ is an **implicit** distribution.
- Use density ratio estimation to evaluate $\frac{q_\phi(z|x)}{p(z)}$ in $KL(q_\phi(z|x)||p(z))$.
- We call this the "prior-contrastive" formulation.
- "Joint-contrastive" formulation used with implicit likelihood minimizes $NELBO(q) = \underbrace{KL(q(z,x)\|p(z,x))}_{\text{Log Density Ratio}}$.

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

1. Define discriminator network 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. 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 $D^*_\alpha(u) = \frac{q(u)}{q(u)+p(u)}$.

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 $r^*_\alpha(u) = \frac{q(u)}{p(u)}$.

Prior-Contrastive Application:

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

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

Joint-Contrastive Application:

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

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

- 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.

- 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 $T_\alpha(u) \simeq \log \frac{q(u)}{p(u)}$.

Optimal Estimator Experiment

Experiment Outline

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

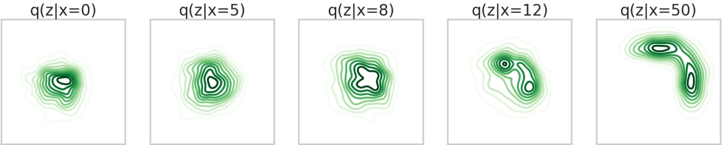
$$p(x|\boldsymbol{z}) \sim Exp(3 + \max(0, z_1)^3 + \max(0, z_2)^3)$$

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

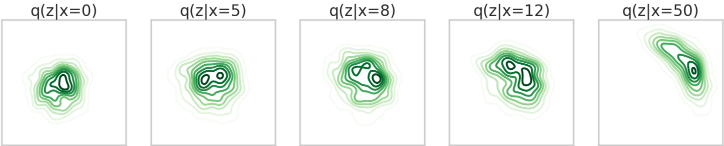
Optimal Estimator Experiment

Experiment Outline

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



(a) Average KL Divergence of 1.3288



(b) Average KL Divergence of 1.3963

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.

- 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

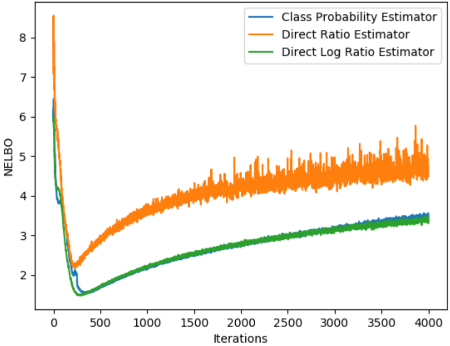
Results

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

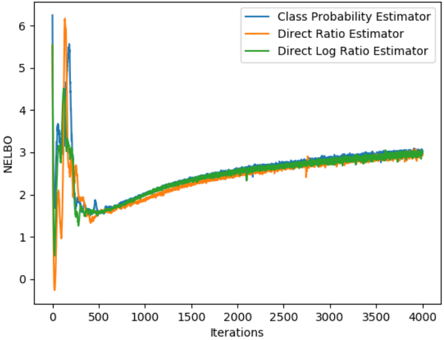
- Reverse KL divergence significantly better than GAN divergence.
- $D_\alpha(z, x) < r_\alpha(z, x) < T_\alpha(z, x)$

Undertrained Estimator Experiment

Joint-Contrastive NELBO Plots



(a) GAN Divergence

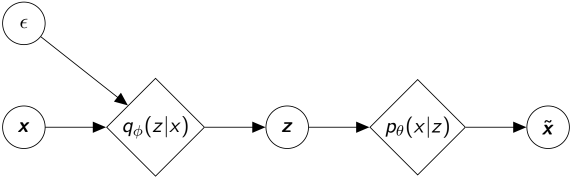


(b) Reverse KL Divergence

- Unclear why direct ratio estimator has unusual NELBO plot: posterior convergence was not affected.
- 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 $p(z)$.



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

Autoencoder Experiment

Experiment Outline

- MNIST dataset - 28×28 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

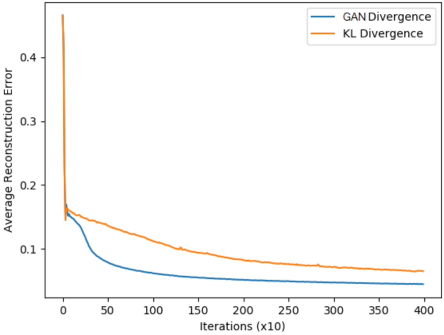
Results - high dimensional latent space

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

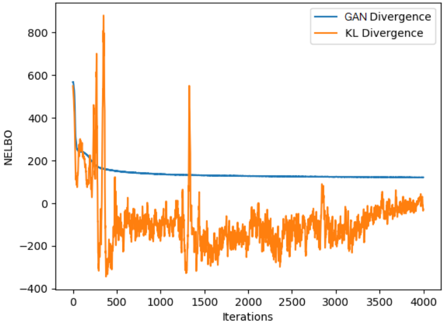
- Direct ratio and direct log ratio estimators attempted to store numbers exceeding float64(max).
- Exponential of $T_\alpha(z,x)$ taken in loss function.
- $D_\alpha(z,x)$ ranges in $(0,1)$.
- Value before sigmoid activation function for $D_\alpha(z,x)$ is log density ratio.

Autoencoder 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.

- 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 the highest 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.