Bayesian Auto-Encoders Part Two

CS109B Data Science 2 Pavlos Protopapas, Mark Glickman, and Chris Tanner



- Motivation for Variational Autoencoders (VAE)
- Inference in Neural Networks
 - Bayesian Linear Regression
 - Bayesian Neural Networks
 - Introduction to Variational methods
 - Variational Autoencoder as an inference model
- Variational Autoencoders as generative model
 - Separability of VAE
 - Tips & tricks
 - Other generative models



Skulls of Bayesian Methods



MCMC will **not** work for NN's with more than a few dozens of parameters.

Why?

For each parameter (weight), we sample and calculate the likelihood 5 * *n* times, where *n* is the chain's length.

We also throw away a significant number of samples from the beginning of the chain.

The number of samples, *n*, necessary to adequately capture the distribution grows with the number of parameters and complexity of the posterior.

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Skulls of Bayesian Methods





Variational Approximations



Space of all distributions





Space of all distributions distributions

Let p(w|D) be the true posterior distribution.





Space of all distributions

True p(w|D)Space of all 'friendly' distributions, q(w)

Let p(w|D) be the true posterior distribution.

We want to find another distribution, which is easier to deal with, q(w), that is similar to p(w|D).





Let p(w|D) be the true posterior distribution.

Why KL: Because the maths work nicely

We want to find another distribution, which is easier to deal with, q(w), that is similar to p(w|D).

To do so we define the meaning of 'similar' to be some form of distance |between q(w) and p(w|D). We will use KL divergence for that:

 $D_{KL}[q|p] = \int q(w) \log \frac{q(w)}{p(w|D)} dw$

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Technically not a distance

Space of all distributions

True p(w|D)



$$D_{KL}[q|p] = \int q(w) \log \frac{q(w)}{p(w|D)} dx$$

By minimizing over all functions q(w)

$$q^* = argmin_q \int q(w) \log \frac{q(w)}{p(w|D)} dw,$$

we will discover q(w) that is the closest to p(w|D), namely $q^*(.)$.

If
$$q(.)$$
 is parametrized by ϕ , $q_{\phi}(.)$

$$\phi^* = argmin_{\phi} \int q_{\phi}(w) \log \frac{q_{\phi}(w)}{p(w|D)} dw$$

Space of We will always need to choose the prior of the parameters.

True p(W|D)

$$\phi^* = \operatorname{argmin}_{\phi} \int q_{\phi}(w) \log \frac{q_{\phi}(w)}{p(w|D)} dw$$

Doing a "little" of math that we will cover in the advanced section, we can derive a new loss function:

 $\mathcal{L} = KL(q_{\phi}(w)||p(w)) - E_{q_{\phi}}[\log p(D|w)]$

The important point is that we do not need to sample to discover the posterior distribution but, minimize this new loss function w.r.t. to ϕ .

This can be approached with gradient cs109B, PROT**CHESCENT** that stochastic gradient descent. 12



Variational Method in Action



RECAP: Bayesian Neural Network



Bayesian Neural Network

with MCMC FORWARD PASS ONLY

THAT'S IT?

VARIATIONAL METHOD

BACKWARD PASS

RECAP: Neural Network





Variational Neural Network



- In variational methods, we assume a weight distribution, $q_{\phi}(w)$, with distribution parameters, ϕ , which are to be optimized to best match the true posterior, p(W|D).
- However, for the **forward pass**, to compute the activations, we need values for the weights.
- Since we assume a distribution for the weights, we can take a sample from that distribution, $q_{\phi}(w)$, for some scaling parameters $\phi = \{\mu, \sigma\}$.

We will learn these parameters.

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This will double our trainable parameters, as we optimize for the μ & σ for each weight distribution.





Landscape of Inference Method for NN





• Dense Local Reparameterization



Quick Review





Quick Review





Quick Review





Building blocks of **probabilistic** machine learning









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Define training parameters
num_epochs = 15
train_dataset = X_train
eval_dataset= X_val





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Back to the same dataset from part one



Option #1 - Variational Approximation of the output








- We build a neural network like before, but instead of one output ŷ, we output two values, each representing the mean μ, and standard deviation σ.
- We introduce stochasticity by the equation $\hat{y} = \mu + \sigma \odot \epsilon$, thus for each input x, we have an output distribution given by $y \sim N(\mu, \sigma)$.
- We estimate (μ, σ) , by minimizing the Variational Loss as before and doing backpropagation.



Model Summary



'OUTPUT ONLY' ISSUES?

- Although easy to implement, the approximate posterior q(y|x) is not complex enough to capture the true posterior distribution p(y|x).
- As seen in the output on our sample dataset, the epistemic variance away from the dataset should be much higher, but the model still confidently predicts those regions.





Option #2 – Variational Approximation of the weights







Variational BNN - Bayes by Backprop





- To perform variational approximation on the weights, instead of using a deterministic value for w, we let each $q_{\mu_i,\sigma_i}(w_i) = N(\mu_i,\sigma_i)$ and sample from these distributions.
- In the forward pass, we introduce stochasticity in the weights by using the equation $w = \mu + \sigma \odot \epsilon$, and thus the output $\hat{y} = NN_W(x)$ will have an output distribution.
- In order to perform backpropagation, we modify our equations to take the derivate $\frac{\partial L}{\partial \mu}, \frac{\partial L}{\partial \sigma}$ and update the $\mu \& \sigma$.



Variational BNN

'BAYES BY BACKPROP' ISSUES?

- Although the approximate posterior $q_{\phi}(w)$ adds sufficient complexity to the output posterior, it doubles the trainable parameters, which can be significant for very large neural networks.
- Since it is computationally prohibitive to sample a unique e in each forward pass, the implementation uses the same sample for all weights.
- This causes the gradients to be correlated, thereby preventing variance reduction during training.





- Like Bayes By Backprop, Flipout performs variational approximation on the weights $w \sim q_{\phi}(w_i) = N(\mu, \sigma)$.
- Unlike Bayes By Backprop, in the forward pass Flipout uses a different ϵ_i for each weight w_i . Like Bayes By Backprop, it introduces stochasticity in the weights by using the equation $w = \mu + \sigma \odot \epsilon$, and thus the output $\hat{y} = NN(w, x)$ will have an output distribution.
- Flipout overcomes the computational difficulty of a unique sampling by multiplying the sample
 e with a random sign matrix.

Flipout: Efficient Pseudo-Independent Weight Perturbations on Mini-Batches



Observation 1. Let q_{θ} be a perturbation distribution that satisfies the above assumptions, and let $\widehat{\Delta W} \sim q_{\theta}$. Let *E* be a random sign matrix that is independent of $\widehat{\Delta W}$. Then $\Delta W = \widehat{\Delta W} \circ E$ is identically distributed to $\widehat{\Delta W}$. Furthermore, the loss gradients computed using ΔW are identically distributed to those computed using $\widehat{\Delta W}$.





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Flipout Explained



Variational BNN – Output only

'FLIPOUT' ISSUES?

- Although Flipout is a significant improvement over Bayes By Backprop, Flipout still suffers from some degree of correlation between the stochastic gradients, and performance suffers from an increased number of weights.
- In order to get uncorrelated stochastic gradients, we will need to sample independently for each weight for each forward pass.





Option #3 – Variational Approximation on hidden units



Variational BNN - Stochastic Weights





Quick Review





Variational BNN – Stochastic hidden units

- Instead of using stochastic weights, we could approximate the true posterior
 p(z | x) with the approximate posterior
 q(z | x) with a known distribution such as a Gaussian.
- Since number of hidden units are an order of two lesser than the weights in a network, we can easier sample for each hidden unit in the forward pass.







Variational Auto-Encoders



Quick Review









Variational AutoEncoder



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ESTIMATED LOWER BOUND



ESTIMATED LOWER BOUND

heta are the decoder weights

entropy:

 $-\sum x^{(i)} \log \hat{x}^{(i)} + x^{(i)} \log \hat{x}^{(i)}$





- 1. Set priors: p(z) = N(0,1)
- 2. Forward pass with sampling: $z = \mu + \sigma \odot \epsilon$
- 3. Calculate the loss:

$$\mathcal{L}oss\left(\boldsymbol{\theta}, \boldsymbol{\phi}; \mathbf{x}^{(i)}\right) = KL\left(q_{\boldsymbol{\phi}}\left(\mathbf{z} \mid \mathbf{x}^{(i)}\right) \| p(\mathbf{z})\right) - \mathbb{E}_{q_{\boldsymbol{\phi}}\left(\mathbf{z} \mid \mathbf{x}^{(i)}\right)}\left[\log p_{\boldsymbol{\theta}}\left(\mathbf{x}^{(i)} \mid \mathbf{z}\right)\right]$$

4a. Update the decoder weights using backpropagation4b. Update the encoder weights using backpropagation

Note: If priors are N(0,1) and $q_{\phi}(z, x^{(i)})$ is also normal, the KL can be analytically calculated.





Inference Summary







Summary



RECAP: Variational AutoEncoder Paper

Let us consider some dataset $X = \{x^{(i)}\}_{i=1}^{N}$ consisting of N i.i.d. samples of some continuous or discrete variable x. We assume that the data are generated by some random process, involving an unobserved continuous random variable z.

We are interested in a general algorithm that works in case of:

- 1. Intractability: $p_{\theta}(x) = \int p_{\theta}(z)p_{\theta}(x|z)dz$ is intractable
- 2. Large Dataset: Sampling based solutions eg. Monte Carlo would be too slow

Auto-Encoding Variational Bayes (Diederik P. Kingma et al)



. . .

VAE as a generative model



Variational Autoencoders – Generative models













Separability is not only between classes, but we also want similar items in the same class to be near each other.

For example, there are different ways of writing "2"; we want similar styles to end up near each other.

Let us examine VAE; there is something magical happening once we add stochasticity in the latent space.







Latent Space

Encode the first sample (a "2") and find μ_1, σ_1 . Sample $z_1 \sim N(\mu_1, \sigma_1)$ and decode to \hat{x}_1



Latent Space







Latent Space

Encode the second sample (a "3") find μ_2, σ_2 . Sample $z_2 \sim N(\mu_2, \sigma_2)$ where \hat{x}_2 and decode to \hat{x}_2



Latent Space

Train with the first sample (a "2") again and find μ_1, σ_1 . However $z_1 \sim N(\mu_1, \sigma_1)$ will not be the same.




Latent Space

Train with the first sample (a "2") again and find μ_1, σ_1 . However $z_1 \sim N(\mu_1, \sigma_1)$ will not be the same. It happens to be close to the "3" in latent space.





Latent Space

Train with 1st sample again.





Latent Space

Keep doing this multiple times with 2's and 3's





Soon images belonging to different classes are separated and images within a class are clustered together within a class are clustered together



Variational AutoEncoder



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Variational AutoEncoder as a generative model

Generative model





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Training VAE

Traditional AE:

Input Image:

Output Images:



Variational AE:

Input Image:

Output Images:

Difference:





Generative model in action: The Famous plots







Latent space of VAE

- More separable than AE
- Because of the prior
 N(0,1) everything is center at
 (0,0) with spread of approximately one.



 Blending is more continuous because latent space is continuous



Exercise: Variational Auto-Encoder From scratch

The goal of this exercise is to build a VAE from scratch to reconstruct images of the MNIST dataset. We will use the decoder to generate blended images like on the right.

Note: Here we show you one way of doing VAE. During section we show a slightly different way.



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Generative model applications





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- Deep Nostalgia from MyHeritage is a generative model based on the ideas mentioned before.
- All generative models are in some way inference models.
- We will study other types of generative models in the upcoming lecture.

https://www.myheritage.com/deep-nostalgia





Bonus Material



What else could work?







Local reparametrization trick

arxiv.org > stat 💌

Auto-Encoding Variational Bayes

by DP Kingma · 2013 · Cited by 13215 — From: Diederik P Kingma M.Sc. [view email 20 Dec 2013 20:58:10 UTC (3,884 KB) [v2] Mon, 23 Dec 2013 13:19:52 UTC (7,549 K

Cite as: arXiv:1312.6114

Cited 13,215 times

Variational Dropout and the Local Reparameterization Trick

by DP Kingma · 2015 · Cited by 711 — We investigate a **local** reparameterizaton technique for greatly reducing the variance of stochastic gradients for **variational** Bayesian inference (SGVB) of a posterior over model parameters, while retaining parallelizability.

Cited only 711 times

Everybody talks about my first paper, but the magic is in the second paper!



DP Kingma



• Reformulate weight perturbations as activation perturbations and sample (Applicable only on fully connected neural networks with no weight sharing)

$$B = XW$$

$$q_{\theta} (W_{i,j}) = \mathcal{N} \left(\mu_{i,j}, \sigma_{i,j}^2 \right) \quad \forall W_{i,j} \in W \Longrightarrow q_{\theta} \left(b_{m,j} \mid X \right) = \mathcal{N} \left(\gamma_{m,j}, \delta_{m,j} \right)$$
$$\gamma_{m,j} = \sum_{i=1} x_{m,i} \mu_{i,j}, \quad \text{and} \quad \delta_{m,j} = \sum_{i=1} x_{m,i}^2 \sigma_{i,j}^2$$

• Inspired from the above idea, Variational dropout works on other



Distribution over the weights instead of hidden state

- How about we use *Flipout* layers instead
- Do we still get a similar output distribution?
- How does it compare to stochastic hidden units?



Quick Review



Variational Autoencoder - Weight distributions





Variational AutoEncoder - Weight distributions



Probabilistic Encoder



Deterministic Decoder





Test Input Reconstructio



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Other methods for uncertainty quantification

Here are the other popular types of inference variants other than the vanilla version:

- BBB Bayes by Backprop
- PBP Probabilistic Backprop
- MVG Matrix Variate Gaussian
- BBH Bayes by Hypernet
- BB- α Black-box α divergence
- SGLD Stochastic Gradient LD
- Dropout
- Ensemble



Please refer to the paper <u>Quality Uncertainty Quantification</u> for a thorough Versis of all the variants CS109B, PROTOPAPAS, GLICKMAN, TANNER

Uncertainty Quantification - Weiwei Pan Research



