



# SURROGATED ASSISTED BAYESIAN NEURAL NETWORK FOR GEOLOGICAL MODELS

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By far the greatest thanks must go to my supervisor for the guidance, care and support they provided.

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Thanks go to Fred Flintstone and Robert Taggart for allowing his thesis style to be shamelessly copied.

Sean Luo, Day Month Year.



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## Abstract

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This thesis is an investigation of the ??????????





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## CHAPTER 1

### Introduction (Currently a collection of messy up notes)

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In the past decade there has been some progression in the field of bayesian deep learning. Bayesian deep learning offers an intrinsic way to ensemble models that helps to quantify the posterior uncertainty in model parameters and prediction. Applying traditional bayesian inference techniques such as Monte Carlo sampling in deep neural networks have multiple challenges, mainly revolving around computational expenses due to the evaluation speed of large dataset, exponentially increasing rejection rate in MCMC sampler as the parameter space dimensions grows with large model, difficulty to evaluate uncertainty in realtime data, efficient proposal convergence and others. Variational bayesian inference methods are faster than sampling, but it does not offer an exact approximation of the target distribution.

Ideas explored:

Pure Bayesian:

1. Using stochastic mini batches with Langevin dynamic by Welling et al [6].
2. Using langevin dynamic Dynamic as proposal to predict time series by chandra et al [2]
3. Using parallel tempering to speed up exploration and exploitation by chandra [3]
4. Using surrogate models to simulate the posterior likelihood  $p(D|\theta)$  to speed up evaluation, by chandra. [4]
5. Surrogate models are selected from variational inference category, including, GAN, VAE, and Normalizing Flow.

Modification to frequentist models that turns into bayesian:

1. Using dropout as intrinsic ensemble (bayesian?).
2. Using stochastic weight averaging with gaussian noise (SWAG) - Wilson et al

This paper proposes to have the surrogate to generate weight and its corresponding numerator and denominator during accept reject to avoid all the extra forward pass and backward loss compare to normal DNN training. The input would be a window of past model parameters and a random vector from normal distribution, The output would be a new set of model parameters, the corresponding numerator and denominator of accept reject step.

#### 1.1 Generative Models

The target loss function for generative model in continuous case (we care for continuous case only as we plan to use it to generate the weights) in unsupervised setting is  $L(D) \approx \frac{1}{N} \sum_{i=1}^N -\log(p_{\theta}(\tilde{x}^{(i)})) + c$ . Where  $\tilde{x}^{(i)} = x^i + u$  with  $u \sim U(0, a)$  and

$c = -M \times \log a$ ,  $a$  is dependent on data discretization and  $M$  is the dimension of  $x$ . This loss function encourages the network to learn to distribute data across the domain of the standard normal distribution. When there is an underlying distribution to approximate, we need to utilize distance/divergence measures in loss function to have convergent distribution.

VAE is a shrinkage training model that has two shrinker that trains to a latent space of mean and variance of normal distribution. from the two latent vector it then trains to simulate a proper input.

GAN have discriminator and generator, generator samples from standard normal and maps it via a network to output space, discriminator compare the overall generated result to dataset. The training is conducted via a maximizing loss for discriminator and minimizing loss on generator.

Normalizing Flow is composed of multiple inversible layers that helps to provide a tractable posterior likelihood on weights. Specifically the GLOW model proposed by OpenAI [5] uses 1x1 convolution to simulate channel switching to boost training performance. Another paper from USTC improves upon this by using matrix exponentials (no idea what it means at the moment)

In flow and autoencoder we are dealing with distributions directly in the latent space (flow is autoencoder with only one network) and Arjovsky (NYU) [1] et al proposed in 2017 to simulate the Wasserstein distance (in general Earth Mover Distance) instead as a loss measure when training GAN.(maybe it can be applied to VAE or NF? Or maybe it already is, base on how I see the implementation).

It is stated that divergence measures such as Jensen or KL fails to pickup the low dimensional manifold of a lot of problems' distributions (Q: are the distribution of weights of DNN parameters supported by low dimensional manifolds?), further in practice, other measures when training GAN produces in saturated discriminator that fails to provided any sensible gradient afterwards, that leads to mode collapse. WGAN resolves this as further training of critic/(score based discriminator instead of class based discriminator) still provides reasonable gradient. WGAN's weakness include failure when using momentum based optimizer (use RMSProp instead), and the clamping of hyperparameters to maintain lipschitz (what does this mean?) seems to be troublesome as it is problem specific. This might've being addressed in a later paper co-authored by Arjovsky.

More info here [blog](#)

## 1.2 low dimensional manifold

(Imagine your patterned bedsheets. They've got a nice plaid grid look to them, very easy to predict what the next few centimeters of material look like.

Now imagine someone tied them in a knot, tore them a little, balled them up, and made them a crumpled mess, then handed them to you. Now if you were to look at the plaid pattern, it would be very difficult to discern how the pattern is, or predict what will be the color of any point of the arbitrary 3D ball of mess you've got. But if you untangled it, you could clearly see the pattern again.

The data is a bunch of colors in an arbitrary 3D ball of mess with very difficult to discern patterns. But the data lies on a low dimensional manifold (the 2D bedsheet). If you could figure out the manifold (flatten the bedsheet), the data will be easy to model.) *explanation on reddit*

(stil have problem understanding the math behind it, but implementation wise i think it just removes the bounded final activation and uses the score as a loss)

### 1.3 Notes:

Swag : approximates local loss distribution (posterior?) using standard normal momentum distribution. Propose -; Accept Reject: replacing forward pass for proposal Surrogate by Chandra et al: evaluate proposal and spit out its posterior likelihood i.e.

$$\min(1, p(w * |x) / p(wi|x) * q(wi|w*) / q(w * |wi))$$

$$\min(1, p(x|w*) / p(x|wi) * p(w * |x) / p(wi|x) * q(wi|w*) / q(w * |wi))$$

$p(w|x)$  and  $q(wi|w*)$  are both easy to compute, the first is a loss, the second is proposal distribution (using tractable distribution like normal that s easy to evaluate)  $p(x|w)$  requires forward pass, so we evaluate it using surrogate

[https : //www.lpsm.paris/pageperso/merle/slides3.1.TV.pdf](https://www.lpsm.paris/pageperso/merle/slides3.1.TV.pdf) stuff for distance understanding

Packages of interest include pymc, pyro, pytorch, (maybe sydney-machine-learning/pingala?)

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## CHAPTER 2

### Sampling

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## CHAPTER 3

### Method

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## CHAPTER 4

### Experiment

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## CHAPTER 5

### Analysis

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## CHAPTER 6

### Discussion

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## CHAPTER 7

### Conclusion

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## References

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- [1] Martin Arjovsky, Soumith Chintala, and Léon Bottou. Wasserstein generative adversarial networks. In Doina Precup and Yee Whye Teh, editors, *Proceedings of the 34th International Conference on Machine Learning*, volume 70 of *Proceedings of Machine Learning Research*, pages 214–223. PMLR, 06–11 Aug 2017.
- [2] Rohitash Chandra, Lamiae Azizi, and Sally Cripps. Bayesian neural learning via langevin dynamics for chaotic time series prediction. In *ICONIP*, 2017.
- [3] Rohitash Chandra, Konark Jain, Ratneel Vikash Deo, and Sally Cripps. Langevin-gradient parallel tempering for bayesian neural learning. *CoRR*, abs/1811.04343, 2018.
- [4] Rohitash Chandra, Konark Jain, and Arpit Kapoor. Surrogate-assisted parallel tempering for bayesian neural learning. *CoRR*, abs/1811.08687, 2018.
- [5] Durk P Kingma and Prafulla Dhariwal. Glow: Generative flow with invertible 1x1 convolutions. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 31. Curran Associates, Inc., 2018.
- [6] Max Welling and Yee Whye Teh. Bayesian learning via stochastic gradient langevin dynamics. In *ICML*, 2011.