Variational Auto-Encoder (VAE)

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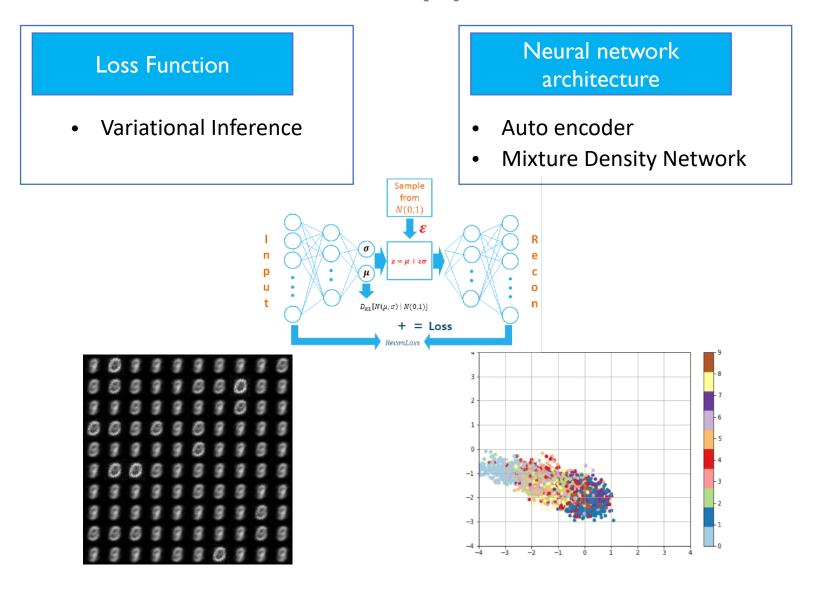
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Contents

- 1. Introduction
- 2. Preliminary
- 3. Auto-encoding variational bayes
- 4. Variational auto encoder
- 5. Experimental Result
- 6. What's Next



INTRODUCTION TO VAE (1)



INTRODUCTION TO VAE (2)

Characteristics

- Scalable generative model
 - Amortized variational inference
 - Simple network architecture
 - Stochastic gradient descent (Back-propagation)
 - Scales to huge datasets
- Inference based on probability graphical model
 - Continuous Latent Space
 - Data reduction / Data Imputation
 - Liable to noisy

THIS SEMINAR

- Paper "Auto-encoding variational bayes"
 - "VAE" is a example of experiment results in this paper.
- Introduce the rest of this paper without "VAE"
 - Stochastic Gradient Variational Bayes(SGVB) estimator
 - Auto-encoding Variational Bayes algorithm
 - Reparameterization trick
 - Appendix
 - Full Variational Bayes
 - Marginal Likelihood estimator
- Research trend of VAE

PRELIMINARY

TRADITIONAL VARIATIONAL INFERENCE

BAYESIAN INFERENCE

General expression

- A random variable $x \in X$
- A set $\{y_1, \dots, y_N\}$ of i.i.d observations

$$p(x, y_1, \dots, y_N) = p_0(x) \prod_{n=1}^{N} p(y_n | x)$$

• Given prior $p_{0(x)}$ and observations, posterior can be evaluated.

$$p(x \mid y_1, \dots, y_N) = \frac{p_0(x) \prod_{\{n=1\}}^N p(y_n \mid x)}{Z} \coloneqq \frac{\bar{p}(x)}{Z}$$

$$Z \coloneqq \int_{X} \bar{p}(x) dx$$

VARIATIONAL INFERENCE

Variational Inference

• Approximate the target distribution p(x) by using a tractable distribution q(x) in Q

$$q^* = argmin_{q \in Q} KL(q \mid \mid p)$$

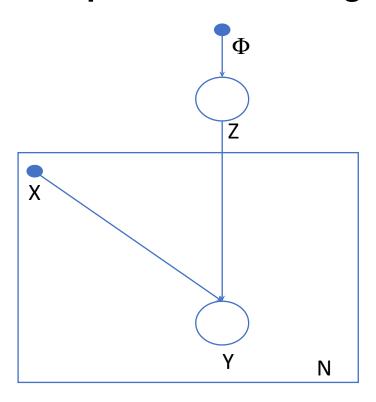
Variational Bound

$$log p(x) = \int log p(x) \cdot q(z) dz = \int log \frac{p(x, z)}{p(z \mid x)} \cdot q(z) dz$$

$$= \int log \frac{p(x,z)}{q(z)} \cdot q(z) dz - \int log \frac{q(z)}{p(z|x)} \cdot q(z) dz$$

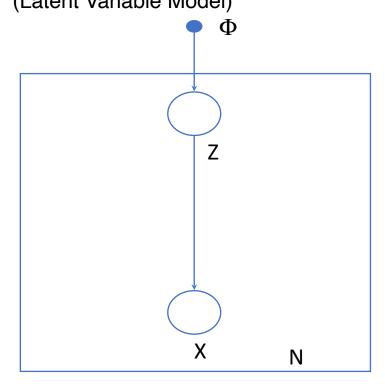
PROBABILITY GRAPHICAL MODEL

Supervised Learning



e.g) Bayesian Logistic regression

• Unsupervised Learning (Latent Variable Model)



e.g) EM algorithm for Gaussian Mixture Model

PROBABILITY GRAPHICAL MODEL

Supervised learning

e.g) Bayesian logistic regression

$$p(x | w, y) \cdot p(w) \propto p(w, x | y)$$

$$p(x \mid w, y) : \prod_{i=1}^{n} \sigma(w^{T}x)^{y_i} \cdot (1 - \sigma(w^{T}x)^{1-y_i}) \Rightarrow$$
 Approximate Gaussian Dist.

Latent Variable Model

e.g) Gaussian Mixture Model (EM algorithm)

 \rightarrow tractable conditional pdf : $p(z \mid x)$

$$q(z) \approx p(z \mid x, \theta^{old})$$

$$\theta^* = argmax_{\theta} \sum p(z \mid x, \theta^{old}) \cdot lnp(x, z \mid \theta)$$

TRADITIONAL VARIATIONAL INFERENCE

Mean field assumption

• If p(z|x) is intractable ?

$$q(\mathbf{z}) = \prod_i q_i(z_i)$$

$$lnq_{j}^{*}(z_{j}) = E_{i\neq j}[lnp(x, z)] + const$$

$$q_j^* \left(z_j \right) = \frac{\exp(E_{i \neq j}[lnp(\mathbf{x}, \mathbf{z})])}{\int \exp(E_{i \neq j}[lnp(\mathbf{x}, \mathbf{z})] d\mathbf{z})}$$

- Under specific probabilistic graphical model, approximate distribution can be evaluated by expectation of $E_{i\neq j}[lnp(x,z)]$
- Depending on each problem, we have to derive the form of $E_{i\neq j}[lnp(x,z)]$
- Through sequential optimization, All of $q_i(z_i)$ can be updated in order until converged.

TRADITIONAL VARIATIONAL INFERENCE (2)

VI with Stochastic gradient descent

$$L = \int log \frac{p(x, z)}{q_{\phi}(z)} \cdot q_{\phi}(z) dz$$

$$\nabla_{\phi} L = \int lnp(x, z) \cdot \nabla_{\phi} lnq(z) \cdot q(z) dz = E_{x \sim q} [lnp(x, z) \cdot \nabla_{\phi} lnq(z)]$$

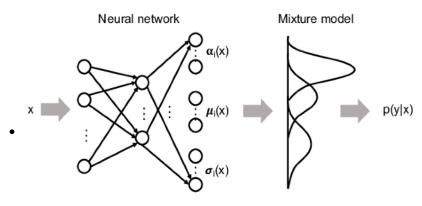
$$\nabla_{\phi} L = E_{x \sim q} \Big[lnp(x, z) \cdot \nabla_{\phi} lnq(z) \Big] \approx \frac{1}{n} \sum_{i} lnp(x_{i}, z) \cdot \nabla_{\phi} lnq(z)$$

- In order to avoid exact derivation of expectation and sequential optimization, stochastic gradient descent method was introduced.
- This method only requires log p(x, z), $q_{\phi}(z)$ and its derivative
- All components can be easily handed
 - log p(x, z) can be derived from probabilistic graphical model
 - $q_{\phi}(z)$ and $\nabla_{\phi}q_{\phi}(z)$ are decided by users.
- However, since this estimator has a huge variance, it also requires many samples.

NETWORK FOR LEARNING PARAMETERS

Mixture density network

 $\{n=1\}$



[Structure of Mixture density Network]

 $\{k=1\}$

 $E(w) = -\sum_{n} \ln \{\sum_{n} \pi_k(x_n, w) N(t_n | u_k(x_n, w), \sigma_k^2(x_n, w))\}$

[Data point and result by Mixture Density Network]

Mixture density network presents that artificial neural network trains hyperparameters for learning parameters of distributions

CHAPTER SUMMARY

Variational Inference

- It provide the evidence in which mathematical analysis can be conducted
- Before emerging amortized VI, Most researches had a interest in efficient usage of VI using stochastic gradient descent and improving performance of approximate distribution for classification model
 - : Basic example : Bayesian logistic regression.
- Especially, VI with stochastic gradient descent influenced that "Auto-encoding variational bayes" were published.

Mixture Density Network

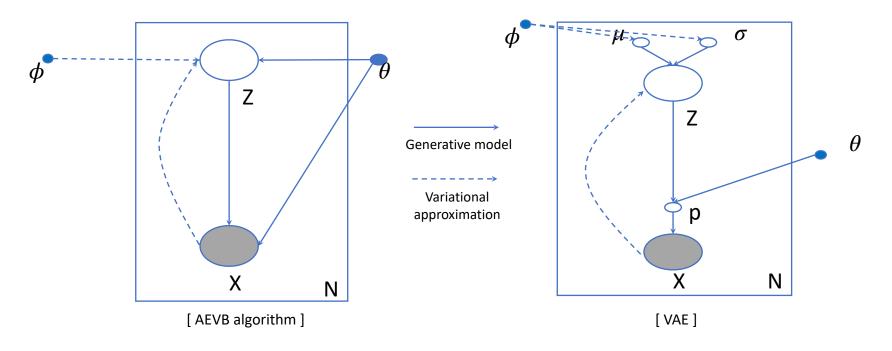
- Mixture Density Network is known to learn parameters of specific distributions using NN
- It is starting point to derive an approach to bayesian neural network

AUTO-ENCODING VARIATIONAL BAYES

PROBABILISTIC GRAPHICAL MODEL
STOCHASTIC VARIATIONAL GRADIENT BAYES ESTIMATOR

PROBABILISTIC GRAPHICAL MODEL

Amortized generative model



- ϕ : hyper-parameters in recognition network
- θ : hyper-parameters in generative network

PROBLEMS SCENARIO

Traditional Latent variable model

- Intractable : p(z|x)
- A large data set: Sampling based EM algorithm → Too slow

This paper has interested in

- Using stochastic gradient descent
- Efficient approximate posterior inference of latent variable z
- This paper introduce (The reason why this method referred "Variational")
 - $q_{\theta}(z \mid x)$: recognition model / approximate posterior distribution to $p_{\theta}(z \mid x)$
 - Figure out parameters of approximate distribution
 - $p_{\theta}(x \mid z)$: generative model (defined as graphical model)
 - Learning the recognition model parameter ϕ with generative model parameter θ using reparameterization trick

VARIATIONAL BOUND

Developing variational Bound

$$\int log \frac{p(x,z)}{q(z)} \cdot q(z) dz = \int log \frac{p(x \mid z) \cdot p(z)}{q(z)} \cdot q(z) dz$$

$$\int (\log p(x \mid z) + \log p(z) - \log q(z)) \cdot q(z) dz$$

$$= \int log p(x \mid z) \cdot q(z) dz + \int log p(z) - log q(z) dz$$

$$= \int log p(x \mid z) \cdot q(z) dz - D_{KL}(q(z) \mid |p(z)|)$$

STOCHASTIC GRADIENT VARIATIONAL BAYES ESTIMATOR (1)

Reparametrization Trick

- Random variable z → Function of variables (Deterministic)
 - Capable of using neural network
 - $z \sim q(z \mid x) \rightarrow \bar{z} = g_{\phi}(x, \epsilon), \epsilon \sim p(\epsilon)$
 - Assume that $p(\epsilon)$ is defined $(p(\epsilon) \sim N(0,1))$
 - The function g_{θ} is determined depending on $q(z \mid x)$ (In subsequent chapter, the forms of function g_{θ} is represented)
- Form of function g_{θ}
 - Tractable inverse CDF: similar to finding PDF

•
$$F(x) = p$$
, $F^{-1}(p) = x$ (unique x) / $g_{\phi}(\epsilon, x) = F_{\phi}^{-1}(\epsilon; x) = \bar{Z}$

- Location Scale Model :
 - $g_{\phi}(\epsilon, x) = \text{location} + \text{scale } \cdot \epsilon$

STOCHASTIC GRADIENT VARIATIONAL BAYES ESTIMATOR (2)

SGVB Estimator

$$E_{q_{\phi_{(z|x^i)}}}\big[f(z)\big] = E_{p(\epsilon)}\bigg[f\Big(g_{\phi}\big(\epsilon,x^i\big)\Big)\bigg] \approx \frac{1}{L}\sum_i f\Big(g_{\phi}\big(\epsilon^l,x^i\big)\Big) where, \; \epsilon^l \sim p(\epsilon)$$

- $f(z) = log p(x \mid z) + q(z) p(z)$
 - Given x, ϵ sampled from $p(\epsilon)$, $z \approx \bar{z} = g_{\phi}(\epsilon, x^i)$, f(z) can be evaluated.
- The form of $\frac{1}{L}\sum_i f\Big(g_\phi\big(\epsilon^l,x^i\big)\Big)$
 - Stochastic gradient method can be introduced w.r.t ϕ , θ (Back propagation)

STOCHASTIC GRADIENT VARIATIONAL BAYES ESTIMATOR (3)

SGVB Estimator A

$$\widetilde{L}^{A}(\theta, \phi; x^{i}) = \frac{1}{L} \sum_{l} log p_{\theta}(x^{i}, z^{i, l}) - log q_{\phi}(z^{i, l} | x^{i}) where, \ g_{\phi}(\epsilon, x^{i}), \ \epsilon^{l} \sim p(\epsilon)$$

- $log p_{\theta}(x^{i}, z^{i,l})$ is defined by probabilistic graphical model
- $log q_{\phi}(z^{i,l} | x^i)$ can be determined $g_{\phi}(\epsilon, x^i)$, $\epsilon^l \sim p(\epsilon)$

SGVB Estimator B

$$\widetilde{L}^{B}(\theta, \, \phi; x^{i}) = \frac{1}{L} \sum_{l} \log p_{\,\theta} (x^{i} | z^{i,l}) - D_{KL}(q_{\phi}(z | x^{i}) | | p_{\theta}(z))$$

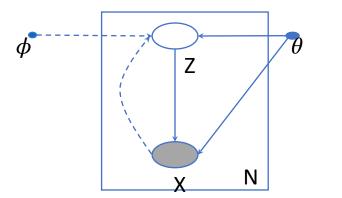
where,
$$g_{\phi}(\epsilon, x^i)$$
, $\epsilon^l \sim p(\epsilon)$

- $D_{KL}(q_{\phi}(z\,|\,x^i)\,|\,|\,p_{\theta}(z))$ is analytically evaluated (Gaussian Dist.)
- $D_{KL}(q_{\phi}(z \mid x^i) \mid \mid p_{\theta}(z))$ doesn't require sample z, only require parameter of approximate dist.

AUTO ENCODING VARIATIONAL BAYES ALGORITHM(1)

Algorithm 1 Minibatch version of the Auto-Encoding VB (AEVB) algorithm. Either of the two SGVB estimators in section 2.3 can be used. We use settings M = 100 and L = 1 in experiments.

```
\begin{array}{l} \boldsymbol{\theta}, \boldsymbol{\phi} \leftarrow \text{Initialize parameters} \\ \textbf{repeat} \\ \textbf{X}^M \leftarrow \text{Random minibatch of } M \text{ datapoints (drawn from full dataset)} \\ \boldsymbol{\epsilon} \leftarrow \text{Random samples from noise distribution } p(\boldsymbol{\epsilon}) \\ \textbf{g} \leftarrow \nabla_{\boldsymbol{\theta}, \boldsymbol{\phi}} \widetilde{\mathcal{L}}^M(\boldsymbol{\theta}, \boldsymbol{\phi}; \mathbf{X}^M, \boldsymbol{\epsilon}) \text{ (Gradients of minibatch estimator (8))} \\ \boldsymbol{\theta}, \boldsymbol{\phi} \leftarrow \text{Update parameters using gradients } \textbf{g (e.g. SGD or Adagrad [DHS10])} \\ \textbf{until convergence of parameters } (\boldsymbol{\theta}, \boldsymbol{\phi}) \\ \textbf{return } \boldsymbol{\theta}, \boldsymbol{\phi} \end{array}
```





$$\begin{split} lnp_{\theta}(X,Z) &= \sum_{i} lnp_{\theta}(x^{i} \mid z^{i}) \\ lnq_{\phi}(Z) &= \sum_{i} lnq_{\phi}(z^{i}) \\ lnp_{\theta}(Z) &= \sum_{i} lnp_{\theta}(z^{i}) \end{split}$$

AUTO ENCODING VARIATIONAL BAYES ALGORITHM (2)

AEVB for SGVB estimator

$$\frac{1}{M} \sum_{i} \widetilde{L}^{A}(\theta, \phi; x^{i}) = \frac{1}{M} \sum_{i} \frac{1}{L} \sum_{l} log p_{\theta}(x^{i}, z^{i,l}) - log q_{\phi}(z^{i,l} | x^{i})$$

$$\frac{1}{M} \sum_{i} \widetilde{L}^{B}(\theta, \, \phi; x^{i}) = \frac{1}{M} \sum_{i} \frac{1}{L} \sum_{l} log p_{\theta} (x^{i} | z^{i,l}) - D_{KL}(q_{\phi}(z | x^{i}) | | p_{\theta}(z))$$

CHAPTER SUMMARY

SGVB Estimator

- This estimator was developed to use an approach of neural network for learning probabilistic latent variable model
- Reparameterization trick is the key point to derive SGVB estimator

AEVB algorithm

- It can train a neural network using gradient of loss function (SGVB estimator) w.r.t hyper-parameters in recognition and generative network at once.
- This gradient can be evaluated by back-propagation

VARIATIONAL AUTO ENCODER

FRAMEWORK
NETWORK ARCHITECTURE
FULL VARIATIONAL BAYES
MARGINAL LIKELIHOOD ESTIMATOR

FRAMEWORK (1)

Loss function (Bernoulli Case)

- $p(z) \sim N(0,I)$
- $p_{\theta}(x \mid z) \sim N(u_{\theta}(z), \sigma_{\theta}(z))$ or $Bern(p_{\theta}(z))$
- $q_{\phi}(z \mid x) \sim N(u_{\phi}(x), diag_{\phi}(x))$

Estimator (Loss function)

$$\widetilde{L}^{B}(\theta, \; \phi; x^{i}) = \frac{1}{L} \sum_{l} log p_{\theta}(x^{i} | z^{i,l}) - D_{KL}(q_{\phi}(z | x^{i}) | | p_{\theta}(z))$$

where
$$g_{\phi}(\epsilon, x^{i}) = u_{\theta}(x) + \epsilon \cdot \sigma_{\theta}(x)$$

$$\epsilon \sim N(0,I), l=1$$

• Since l = 1, neural network architecture can be similar to "auto-encoder"

FRAMEWORK (2)

Loss function

- $p_{\theta}(x \mid z) \sim Bern(p_{\theta}(z))$
- $\bullet \quad D_{KL}(q_{\phi}(z\,|\,x^i)\,|\,|\,p_{\theta}(z))$
 - $p(z) \sim N(0,I), \ q_{\phi}(z \mid x) \sim N(u_{\phi}(x), diag_{\phi}(x))$
 - $D_{KL}(q_{\phi}(z \mid x) \mid p_{\theta}(z)) =$

$$\frac{1}{2}\{\left(0-u_{\phi}(x)\right)I^{-1}\left(0-u_{\phi}(x)\right)+trace(I^{-1}diag_{\phi}(x)\right)-k+ln\frac{\mid I\mid}{\mid diag_{\phi}(x)\mid}$$

$$= \sum_{j} u_{\phi}(x)_{(j)}^{2} - 1 + \sigma_{\phi}^{2}(x)_{(j)} - \ln \sigma_{\phi}^{2}(x)_{(j)}$$

where $j = index \ of \ dimension \ of \ latent \ variable \ z$

FRAMEWORK (3)

Loss Function

$$\therefore \sum_{i} x_{i} log p(z_{i}) + (1 - x_{i}) log(1 - p_{\theta}(z_{i})) +$$

$$\sum_{i} \sum_{j} u_{\phi}(x_{i})_{(j)}^{2} - 1 + \sigma_{\phi}^{2}(x_{i})_{(j)} - \ln \sigma_{\phi}^{2}(x_{i})_{(j)}$$

STRUCTURE OF VAE(1)

Network Architecture

Recognition network (like density network)

$$u_{\phi}(x_i) = w_2 tanh(w_1 x_i + b_1) + b_2$$

$$\sigma_{\phi}(x_i) = w_4 tanh(w_3 x_i + b_3) + b_4$$

- Generative network
 - Bernoulli Case

$$\begin{aligned} \mathbf{p}_{\theta}(z_i) &= f_a\Big(w_2 \mathrm{tanh}\big(w_1 z_i + b_1\big) + b_2\Big) \\ where \ f_a(\,\cdot\,) &: element-wise \ sigmoid \ function \\ \theta &= \{w_1, b_1, w_2, b_2\} \end{aligned}$$

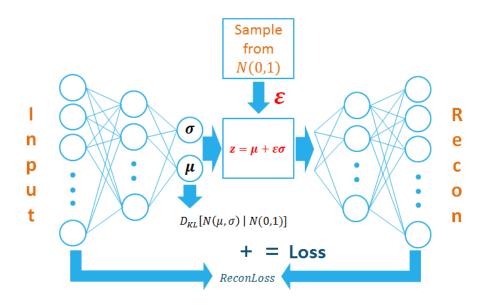
Gaussian Case

$$u_{\theta}(z_{i}) = w_{4}(tanh(w_{3}z + b_{3}) + b_{4})$$

$$\sigma_{\theta}(z_{i}) = w_{5}(tanh(w_{3}z + b_{3}) + b_{5})$$

$$\theta = \{w_{3}, w_{4}, w_{5}, b_{3}, b_{4}, b_{5}\}$$

VAE



Probabilistic modeling

- All data should be mapped to latent space defined by probability graph model
- Robust against some noises
 - Key difference between VAE and general AE

MARGINAL LIKELIHOOD ESTIMATOR (1)

Derivation

- Marginal Likelihood : $p_{\theta}(x)$
- Marginal likelihood estimator

$$\frac{1}{p_{\theta}(x_i)} = \int \frac{q(z)}{p_{\theta}(x_i)} dz = \frac{\int q(z) \cdot \frac{p_{\theta}(x_i, z)}{p_{\theta}(x_i, z)} dz}{p_{\theta}(x_i)} = \int \frac{p_{\theta}(x_i, z)}{p_{\theta}(x_i)} \cdot \frac{q(z)}{p_{\theta}(x_i, z)} dz$$

$$= \int p_{\theta}(z \mid x_i) \frac{q(z)}{p_{\theta}(x_i, z)} dz \approx \frac{1}{L} \sum_{l} \frac{q_{\phi}(z^{(l)})}{p_{\theta}(z) p_{\theta}(x_i \mid z^{(l)})}$$

- In VAE, marginal likelihood estimator cannot be evaluated because it requires l > 1
- If it was forced to evaluate the marginal likelihood in VAE, the result is almost same as loss function, it doesn't give any special meaning.

MARGINAL LIKELIHOOD ESTIMATOR (2)

Gradient MCMC

 Max Welling and published "Bayesian learning via stochastic gradient langevin dynamics (2011), ICML2011"

$$\Delta \theta_{t} = \frac{\epsilon_{t}}{2} (\nabla log p(\theta_{t}) + \frac{N}{n} \sum_{i=1}^{n} \nabla log p(x_{i} | \theta_{t})) + \eta_{t}$$

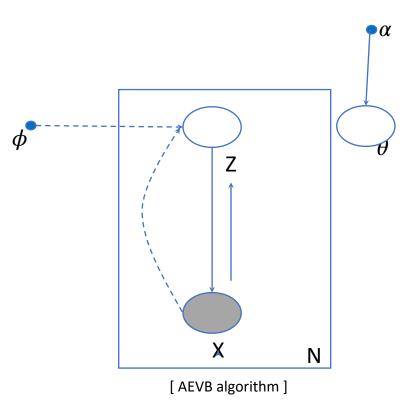
$$where \ \eta_{t} \sim N(0, \epsilon_{t})$$

Update (stochastic gradient descent)

$$\theta = \theta_t + \epsilon_t' \cdot \Delta \theta_t$$

- In this paper, $\nabla \log p(z_t)$, $\nabla \log p(x_i | z_t)$ can be evaluated.
- Under this method, marginal likelihood estimator is established.

FULL VARIATIONAL BAYES



Framework

- $p_{\theta}(z) \sim N(0,I)$, where $z \in R^{J}$, $I \in R^{J \times J}$
- $p_{\alpha}(\theta) \sim N(0,I)$, where $\theta \in \mathbb{R}^{M}$, $I \in \mathbb{R}^{M \times M}$
- $p_{\theta}(x \mid z) \sim N(u_{\theta}(z), \sigma_{\theta}(z))$ or $Bern(p_{\theta}(z))$
- $q_{\phi}(z|x) \sim N(u_{\phi}(x), diag_{\phi}(x))$

FULL VARIATIONAL BAYES

Variational Bound

$$\begin{split} &lnp_{\theta}(X) \approx \int \left(lnP_{\alpha}(X \mid \theta) + lnP_{\alpha}(\theta) - lnq_{\phi}(\theta) \right) \cdot q_{\theta}(\theta) d\theta \\ &= \frac{1}{L} \sum_{l=1}^{L} E \left[lnP_{\alpha}(X \mid \theta) \right] + \frac{1}{2} \sum_{M=1}^{M} \left\{ 1 + ln\sigma_{\theta_{m}}^{2(l)} - \mu_{\theta_{m}}^{2(l)} - \sigma_{\theta_{m}}^{2(l)} \right\} \end{split}$$

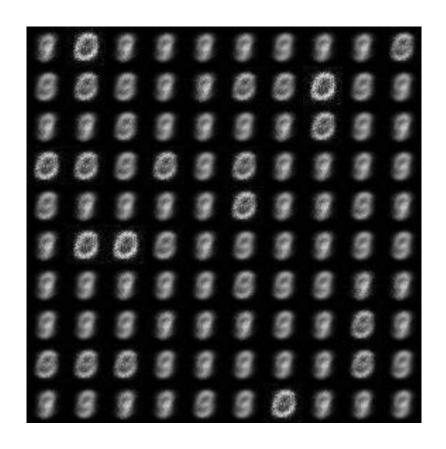
$$\begin{split} \ln P_{\alpha}(X \, \Big| \, \theta) &= \int \log \frac{p(x,z)}{q(z)} \cdot q(z) dz \, - \int \log \frac{q(z)}{p(z \, | \, x)} \cdot q(z) dz \\ &\approx \frac{1}{K} \sum_{i=1}^{N} \big(\sum_{k=1}^{K} \ln p_{\theta} \Big(x_{i} \, \Big| \, z_{i,j} \Big) + \frac{1}{2} \sum_{j=1}^{K} \big\{ 1 + \ln \sigma_{z_{i,j}}^{2(k)} - \mu_{z_{i,j}}^{2(k)} - \sigma_{z_{i,j}}^{2(k)} \big\} \big) \end{split}$$

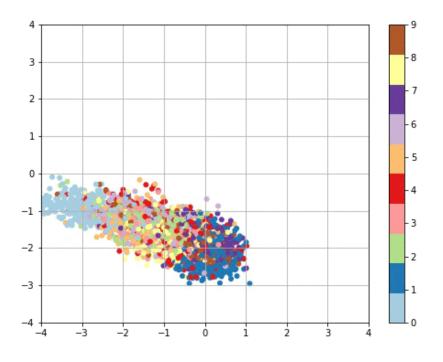
. In this paper, L=K=1 and $\ln p_{\theta}\Big(x_i\,\Big|\,z_{i,j}\Big)=\ln p_{\theta}(x\,|\,z), \forall x_i$

$$\therefore N \cdot lnp(x \mid z) + \frac{N}{2} \cdot \sum_{j=1}^{J} \left\{ 1 + ln\sigma_{z_{i,j}}^{2'} - \mu_{z_{i,j}}^{2'} - \sigma_{z_{i},j}^{2'} \right\} + \frac{1}{2} \sum_{M=1}^{M} \left\{ 1 + ln\sigma_{\theta_{m}}^{2(l)} - \mu_{\theta_{m}}^{2(l)} - \sigma_{\theta_{m}}^{2(l)} \right\}$$

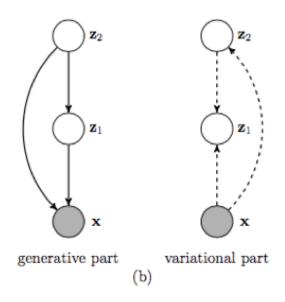
EXPERIMENTAL RESULT

STANDARD VAE





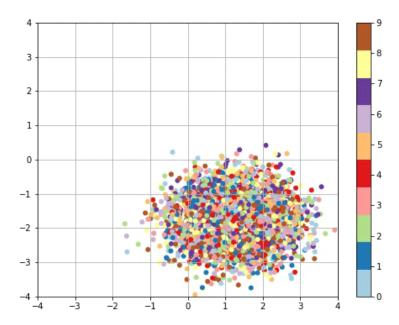
HIERARCHICAL VAE



$$p_{\lambda}(\mathbf{z}_{1}|\mathbf{z}_{2}) = \mathcal{N}(\mathbf{z}_{1}|\mu_{\lambda}(\mathbf{z}_{2}), \operatorname{diag}(\sigma_{\lambda}^{2}(\mathbf{z}_{2}))),$$

$$q_{\phi}(\mathbf{z}_{1}|\mathbf{x}, \mathbf{z}_{2}) = \mathcal{N}(\mathbf{z}_{1}|\mu_{\phi}(\mathbf{x}, \mathbf{z}_{2}), \operatorname{diag}(\sigma_{\phi}^{2}(\mathbf{x}, \mathbf{z}_{2}), \mathbf{z}_{2}),$$

$$q_{\psi}(\mathbf{z}_{2}|\mathbf{x}) = \mathcal{N}(\mathbf{z}_{2}|\mu_{\psi}(\mathbf{x}), \operatorname{diag}(\sigma_{\psi}^{2}(\mathbf{x})))$$



EXPERIMENTAL RESULTS

Table

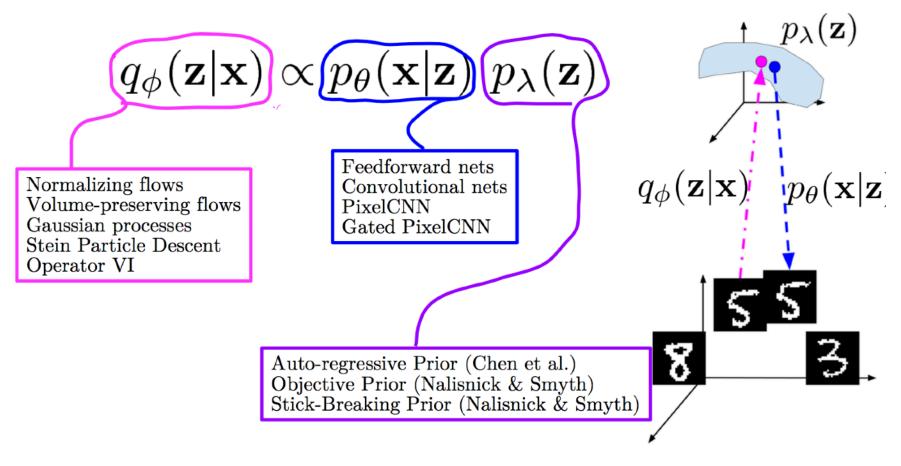
	V	AE	Hierarchical VAE			
Epoch	Variational Bound	Log Marginal Likelihood	Variational Bound	Log Marginal Likelihood		
1	212.87	-210.73	214.06	-214.11		
50	152.83	-151.75	152.75	-152.85		
100	154.24	-153.59	149.95	-150.15		
150	152.32	-152.15	139.21	-139.29		
200	138.41	-137.42	132.70	-132.82		

WHAT'S NEXT?

CURRENT RESEARCH

RESEARCH SUMMARY

DGM: Variational Auto-Encoder

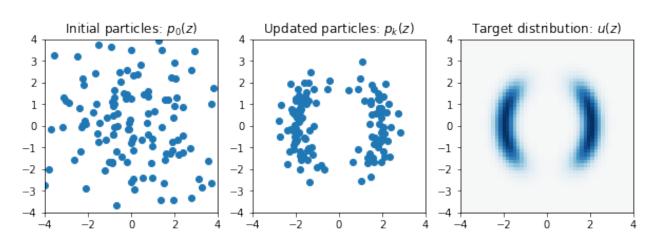


J. Tomczak (2018) VAM with a Vamp Prior at MPI Tubingen presentation

NORMALIZING FLOW / STEIN METHOD

- Iterative update : $z_i \sim q_{\phi}(z_i | x_i)$
 - Based on change of variable
 - Objective : minimizing KLD(q | | p)
 - Normalizing flow: using tractable determinant of Jacobian
 - Stein method : using the RKHS kernel to describe direction for minimizing KLD $T_l^*(x) = x + \epsilon_l \phi_{q_l,p}^*(x)$.

$$q_0 \stackrel{\boldsymbol{T}_0^*}{\rightarrow} q_1 \stackrel{\boldsymbol{T}_1^*}{\rightarrow} q_2 \stackrel{\boldsymbol{T}_2^*}{\rightarrow} \cdots \rightarrow q_{\infty} = p(\boldsymbol{\phi}_{q_1,p}^* = 0)$$



VAE WITH VAMPPRIOR

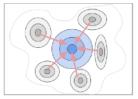
Main Idea

-. Prior Distribution = Aggregate Posterior Distribution

$$P_{\lambda}(\mathbf{z}) = \frac{1}{K} \sum_{k=1}^{K} q(\mathbf{z}|\mathbf{x})$$

- -. Pseudo inputs
 - . Users should select learnable pseudo inputs.
 - . If pseudo inputs are randomly chosen, we couldn't expect better performance.
- -. Expectation for this approach





Standard prior is too strong and overregularizes the encoder.

What is the "optimal" prior?

VAE WITH VAMPPRIOR

Variational Bound

$$\mathbb{E}_{\mathbf{x} \sim q(\mathbf{x})} \left[\ln p(\mathbf{x}) \right] \geq \mathbb{E}_{\mathbf{x} \sim q(\mathbf{x})} \left[\mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x})} \left[\ln p_{\theta}(\mathbf{x}|\mathbf{z}) \right] \right] + \\ + \mathbb{E}_{\mathbf{x} \sim q(\mathbf{x})} \left[\mathbb{H} \left[q_{\phi}(\mathbf{z}|\mathbf{x}) \right] \right] + \\ - \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z})} \left[- \ln p_{\lambda}(\mathbf{z}) \right]$$

$$\max_{p_{\lambda}(\mathbf{z})} - \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z})}[-\ln p_{\lambda}(\mathbf{z})] + \beta \left(\int p_{\lambda}(\mathbf{z}) d\mathbf{z} - 1 \right)$$



$$p_{\lambda}^{*}(\mathbf{z}) = \frac{1}{N} \sum_{n=1}^{N} q_{\phi}(\mathbf{z}|\mathbf{x}_{n})$$

VAE WITH VAMPPRIOR

Experimental Result

	VAE $(L=1)$		HVAE $(L=2)$		CONVHVAE $(L=2)$		PIXELHVAE $(L=2)$	
Dataset	standard	VampPrior	standard	VampPrior	standard	VampPrior	standard	VampPrior
staticMNIST	-88.56	-85.57	-86.05	-83.19	-82.41	-81.09	-80.58	-79.78
${\rm dynamic MNIST}$	-84.50	-82.38	-82.42	-81.24	-80.40	-79.75	-79.70	-78.45
Omniglot	-108.50	-104.75	-103.52	-101.18	-97.65	-97.56	-90.11	-89.76
Caltech 101	-123.43	-114.55	-112.08	-108.28	-106.35	-104.22	-85.51	-86.22
Frey Faces	4.63	4.57	4.61	4.51	4.49	4.45	4.43	4.38
Histopathology	6.07	6.04	5.82	5.75	5.59	5.58	4.84	4.82

Table 2: Test LL for static MNIST.

Model	LL
VAE (L = 1) + NF 32	-85.10
VAE $(L=2)$ 6	-87.86
IWAE $(L=2)$ 6	-85.32
HVAE (L = 2) + SG	-85.89
HVAE (L = 2) + MoG	-85.07
HVAE $(L=2)$ + VampPrior $data$	-85.71
HVAE $(L=2)$ + VampPrior	-83.19
AVB + AC (L = 1) 28	-80.20
VLAE 7	-79.03
VAE + IAF 18	-79.88
CONVHVAE $(L=2)$ + VampPrior	-81.09
PIXELHVAE ($L=2$) + VampPrior	-79.78

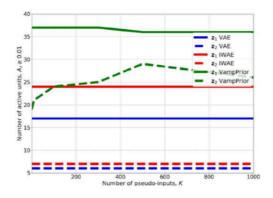


Figure 3: A comparison between two-level VAE and IWAE with the standard normal prior and theirs Vamp-Prior counterpart in terms of number of active units for varying number of pseudo-inputs on static MNIST.

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ANY QUESTIONS?