VI & BNN (1)

Stochastic Variational Inference (SVI) and Variational Autoencoder (VAE)

Keywords: Variational Inference, Scalable Variational Inference, ELBO, Probabilistic Deep Learning, Variational Autoencoder

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Paper List (+ references)

- Practical variational inference for neural networks (2011)
- Stochastic variational inference (2013)
- Auto-Encoding Variational Bayes (2013)
- Variational Inference : A review for statisticians (2017)
- Advances in variational inference (2018)
- Deep Bayes (https://deepbayes.ru/)

1-1. MCMC vs Variational Inference

Two main approaches to find the (intractable) posterior in Bayesian Inference!

(1) MCMC: sampling from the unnormalized posterior

- (Pros) Unbiased
- (Cons) High computational cost

(2) Variational Inference: Approximating target distn with a simpler distn

- (Pros) Faster & Scalable
- (Cons) Biased

1-1. MCMC vs Variational Inference

Will be going to focus on Variational Inference

Before getting on...

- KL divergence

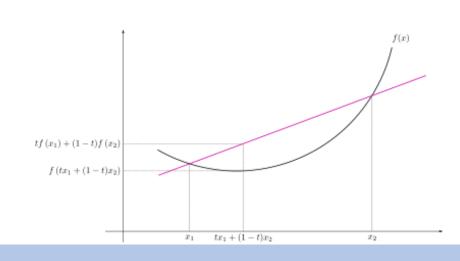
$$KL(q(\theta) || p(\theta | x)) = \int q(\theta) \log \frac{q(\theta)}{p(\theta | x)} d\theta$$

- $KL(q||p) \ge 0$
- $KL(q \parallel p) = 0 \Leftrightarrow q = p$
- $KL(q \parallel p) \neq KL(p \parallel q)$

- Jensen's Inequality

If g(x) is a convex function on R_X and E[g(X)] and g(E[X]) are finite,

$$E[g(X)] \ge g(E[X])$$



1-2. Evidence Lower Bound (ELBO)

$$\begin{split} \log p(x) &= \int q(\theta) \log p(x) d\theta = \int q(\theta) \log \frac{p(x,\theta)}{p(\theta\mid x)} d\theta = \\ &= \int q(\theta) \log \frac{p(x,\theta)q(\theta)}{p(\theta\mid x)q(\theta)} d\theta = \\ &= \int q(\theta) \log \frac{p(x,\theta)}{q(\theta)} d\theta + \int q(\theta) \log \frac{q(\theta)}{p(\theta\mid x)} d\theta = \\ &= \mathcal{L}(q(\theta)) + KL(q(\theta) || p(\theta\mid x))_{\text{(Non-negative)}} \end{split}$$

1-2. Evidence Lower Bound (ELBO)

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ELBO (Evidence Lower Bound)

Why called like that? Think of "Evidence" in Bayes rule!

$$\log p(x) \ge \mathcal{L}(q(\theta))$$

1-2. Evidence Lower Bound (ELBO)

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ELBO (Evidence Lower Bound)

Why called like that? Think of "Evidence" in Bayes rule!

$$\log p(x) \ge \mathcal{L}(q(\theta))$$

1-2. Evidence Lower Bound (ELBO)

Interpretation of ELBO

Rewrite ELBO as below

$$\mathcal{L}(q(\theta)) = \int q(\theta) \log \frac{p(x,\theta)}{q(\theta)} d\theta = \int q(\theta) \log \frac{p(x \mid \theta)p(\theta)}{q(\theta)} d\theta =$$

$$= \int q(\theta) \log p(x \mid \theta) d\theta + \int q(\theta) \log \frac{p(\theta)}{q(\theta)} d\theta =$$

$$= \mathbb{E}_{q(\theta)} \log p(x \mid \theta) - KL(q(\theta) \| p(\theta))$$

1-2. Evidence Lower Bound (ELBO)

Interpretation of ELBO

Rewrite ELBO as below

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$$= \mathbb{E}_{q(\theta)} \log p(x \mid \theta) - KL(q(\theta) || p(\theta))$$

Term 1) Encourage good fit! Term 2) Regularize! Encourage posterior to be close to prior

1-3. Mean Field Variational Inference (MFVI)

We have to optimize w.r.t ELBO, but how?

$$\mathcal{L}(q(\theta)) = \int q(\theta) \log \frac{p(x,\theta)}{q(\theta)} d\theta \to \max_{q(\theta) \in \mathcal{Q}}$$

Mean Field Assumption

(For simplicity, variational parameters are factorized as below, with an Independent Assumption)

$$q(\theta) = \prod_{j=1}^{m} q_j(\theta_j), \quad \theta = [\theta_1, \dots, \theta_m]$$

Due to the assumption, its flexibility is limited!

1-3. Mean Field Variational Inference (MFVI)

$$\mathcal{L}(q(\theta)) = \int q(\theta) \log \frac{p(x,\theta)}{q(\theta)} d\theta \to \max_{q(\theta) \in \mathcal{Q}}$$

$$\mathcal{L}(q(\theta)) = \int q(\theta) \log \frac{p(x,\theta)}{q(\theta)} d\theta \to \max_{q(\theta) = q_1(\theta_1) \cdot \dots \cdot q_m(\theta_m)}$$

1-3. Mean Field Variational Inference (MFVI)

$$\mathcal{L}(q(\theta)) = \int q(\theta) \log \frac{p(x,\theta)}{q(\theta)} d\theta \to \max_{q(\theta) \in \mathcal{Q}}$$

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Solution (proof on the next page)

$$q_j(\theta_j) = r_j(\theta_j) = \frac{1}{Z_j} \exp\left(\mathbb{E}_{q_{i\neq j}} \log p(x, \theta)\right)$$

Coordinate-ascent method

CAVI (Coordinate Ascent Variational Inference)

1-3. Mean Field Variational Inference (MFVI)

$$q_j(\theta_j) = r_j(\theta_j) = \frac{1}{Z_j} \exp\left(\mathbb{E}_{q_{i\neq j}} \log p(x, \theta)\right)$$

Proof)

$$\begin{split} \mathcal{L}(q(\theta)) &= \mathbb{E}_{q(\theta)} \log p(x,\theta) - \mathbb{E}_{q(\theta)} \log q(\theta) = \\ &= \mathbb{E}_{q(\theta)} \log p(x,\theta) - \sum_{k=1}^{m} \mathbb{E}_{q_k(\theta_k)} \log q_k(\theta_k) = \\ &= \mathbb{E}_{q_j(\theta_j)} \left[\mathbb{E}_{q_{i\neq j}} \log p(x,\theta) \right] - \mathbb{E}_{q_j(\theta_j)} \log q_j(\theta_j) + Const = \\ &= \left\{ r_j(\theta_j) = \frac{1}{Z_j} \exp \left(\mathbb{E}_{q_{i\neq j}} \log p(x,\theta) \right) \right\} = \\ &= \mathbb{E}_{q_j(\theta_j)} \log \frac{r_j(\theta_j)}{q_j(\theta_j)} + Const = -KL \left(q_j(\theta_j) \| r_j(\theta_j) \right) + Const \end{split}$$

1-3. Mean Field Variational Inference (MFVI)

Algorithm

Initialize
$$q(\theta) = \prod_{j=1}^{m} q_j(\theta_j)$$

Iterations:

• Update each factor q_1, \ldots, q_m :

$$q_j(\theta_j) = \frac{1}{Z_j} \exp\left(\mathbb{E}_{q_{i\neq j}} \log p(x, \theta)\right)$$

• Compute ELBO $\mathcal{L}(q(\theta))$

Repeat until convergence of ELBO

Stochastic Variational Inference (SVI)?

a stochastic optimization algorithm for mean-field variational inference,

that can handle massive dataset (scalability)

- Mean Field Variational Inference
- Stochastic Optimization



Mean Field Variational Inference

(This time, we will set hidden variables into 2 parts)

Factorize joint distribution

$$p(x,z,\beta \mid \alpha) = p(\beta \mid \alpha) \prod_{n=1}^{N} p(x_n,z_n \mid \beta)$$

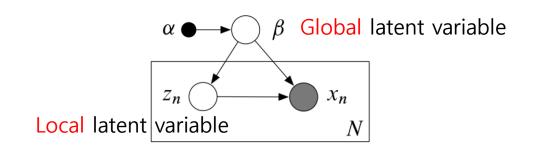


Figure 2: A graphical model with observations $x_{1:N}$, local hidden variables $z_{1:N}$ and global hidden variables β . The distribution of each observation x_n only depends on its corresponding local variable z_n and the global variables β . (Though not pictured, each hidden variable z_n , observation x_n , and global variable β may be a collection of multiple random variables.)

Approximate using MFVI

$$p(z,\beta|x) = \frac{p(x,z,\beta)}{\int p(x,z,\beta)dzd\beta}$$

Approximating distn:

$$q(z,\beta) = q(\beta | \lambda) \prod_{n=1}^{N} \prod_{j=1}^{J} q(z_{nj} | \phi_{nj})$$

Mean Field Variational Inference

$$q(z,\beta) = q(\beta | \lambda) \prod_{n=1}^{N} \prod_{j=1}^{J} q(z_{nj} | \phi_{nj})$$

Set $q(\beta \mid \lambda)$ and $q(z_{nj} \mid \phi_{nj})$ to be in the same exponential family

$$ullet q(eta \mid \lambda) = h(eta) \exp \left\{ \lambda^ op t(eta) - a_g(\lambda)
ight\}$$

$$ullet \ q\left(z_{nj}\mid\phi_{nj}
ight)=h\left(z_{nj}
ight)\exp\Bigl\{\phi_{nj}^{ op}t\left(z_{nj}
ight)-a_{\ell}\left(\phi_{nj}
ight)\Bigr\}$$

$$\nabla_{\lambda} \mathcal{L} = \nabla_{\lambda}^{2} a_{g}(\lambda) (\mathbb{E}_{q}[\eta_{g}(x, z, \alpha)] - \lambda) \qquad \longrightarrow \qquad \lambda = \mathbb{E}_{q}[\eta_{g}(x, z, \alpha)]$$

$$\nabla_{\phi_{nj}} \mathcal{L} = \nabla_{\phi_{nj}}^2 a_{\ell}(\phi_{nj}) (\mathbb{E}_q[\eta_{\ell}(x_n, z_{n,-j}, \beta)] - \phi_{nj}) \quad \Longrightarrow \quad \phi_{nj} = \mathbb{E}_q[\eta_{\ell}(x_n, z_{n,-j}, \beta)]$$

```
1: Initialize \lambda^{(0)} randomly.

2: repeat

3: for each local variational parameter \phi_{nj} do

4: Update \phi_{nj}, \phi_{nj}^{(t)} = \mathbb{E}_{q^{(t-1)}}[\eta_{\ell,j}(x_n, z_{n,-j}, \beta)].

5: end for

6: Update the global variational parameters, \lambda^{(t)} = \mathbb{E}_{q^{(t)}}[\eta_g(z_{1:N}, x_{1:N})].

7: until the ELBO converges
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Figure 3: Coordinate ascent mean-field variational inference.

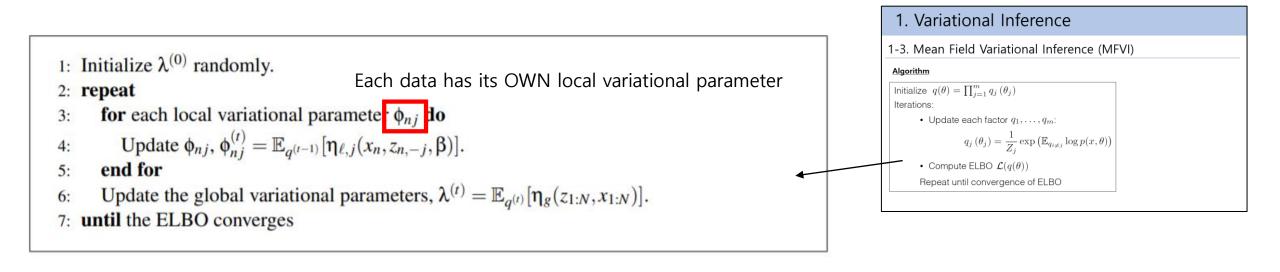


Figure 3: Coordinate ascent mean-field variational inference.

INEFFICIENT for large data sets!

(should optimize the local variational params for each data, before re-estimating the global variational params)

SVI uses "stochastic optimization" to fit global variational parameters.

Algorithm

- 1: Initialize $\lambda^{(0)}$ randomly.
- 2: Set the step-size schedule ρ_t appropriately.
- 3: repeat
- 4: Sample a data point x_i uniformly from the data set.
- 5: Compute its local variational parameter,

$$\phi = \mathbb{E}_{\lambda^{(t-1)}}[\eta_g(x_i^{(N)}, z_i^{(N)})].$$

6: Compute intermediate global parameters as though x_i is replicated N times,

$$\hat{\lambda} = \mathbb{E}_{\phi}[\eta_g(x_i^{(N)}, z_i^{(N)})].$$

7: Update the current estimate of the global variational parameters,

$$\lambda^{(t)} = (1 - \rho_t)\lambda^{(t-1)} + \rho_t \hat{\lambda}.$$

8: until forever

Simple! Just think it as

$$(1) SGD + (2) VI$$

$$\lambda^{(t)} = \lambda^{(t-1)} + \rho_t \left(\hat{\lambda}_t - \lambda^{(t-1)} \right)$$
$$= (1 - \rho_t) \lambda^{(t-1)} + \rho_t \hat{\lambda}_t.$$

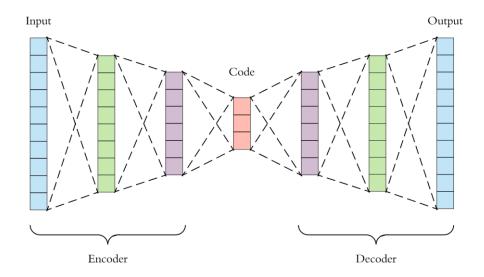
Figure 4: Stochastic variational inference.

3. Variational Auto Encoder (VAE)

3-1. Structure of VAE

Auto Encoder: "The aim of an autoencoder is to learn a representation (encoding) for a set of data "

What's the difference between AE & VAE?



Auto Encoder (AE)

3-1. Structure of VAE

- (1) Encoder
 - inference network
 - input : x, output : z
 - $\bullet \ q(z \mid x, \phi)$

- (2) Decoder
 - generative network
 - input : z, output : as closely as x
 - $p(x \mid z, \theta)$

 $q_{\phi}(\cdot)$

Variational Autoencoder Latent Vector Encoder Decoder

 $p_{\theta}(\cdot)$

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3-1. Structure of VAE

Variational Inference: approximate with variational distribution!

$$p(z_i \mid x_i, \theta) \approx q(z_i \mid x_i, \phi) = \prod_{i=1}^d N(z_{ij} \mid \underline{\mu_j(x_i)}, \underline{\sigma_j^2(x_i)})$$

(use Neural Network! Flexible!)

Objective Function (ELBO)

- Minimize KL-divergence $q(Z \mid X, \phi) = \arg\min_{\phi} KL(q(Z \mid X, \phi) || p(Z \mid X, \theta))$

= Maximize ELBO
$$\mathcal{L}(\phi, \theta) = \int q(Z \mid X, \phi) \log \frac{p(X|Z, \theta)p(Z)}{q(Z|X, \phi)} dZ \to \max_{\phi, \theta}$$

3-1. Structure of VAE

Update the parameters of **Encoder & Decoder**.

Due to flexible & complex model (Neural Network), it seems hard to solve...

But using some techniques (+ tricks), we can solve it!

Stochastic Optimization

- 1) Mini-batch
- 2) Monte Carlo Estimation

Tricks

- 1) Log-derivative trick
- 2) Reparameterization trick

3-2. Update Decoder (parameter : θ)

Not that hard to solve!

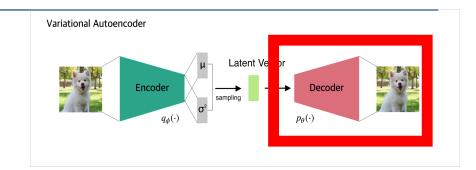
(1) Mini-batch
$$\nabla_{\theta} \mathcal{L}(\phi, \theta) = \nabla_{\theta} \sum_{i=1}^{n} \int q(z_{i} \mid x_{i}, \phi) \log \frac{p(x_{i} \mid z_{i}, \theta) p(z_{i})}{q(z_{i} \mid x_{i}, \phi)} dz_{i}$$

$$= \sum_{i=1}^{n} \int q(z_{i} \mid x_{i}, \phi) \nabla_{\theta} \log p(x_{i} \mid z_{i}, \theta) dz_{i}$$

$$\approx n \int q(z_{i} \mid x_{i}, \phi) \nabla_{\theta} \log p(x_{i} \mid z_{i}, \theta) dz_{i}, \quad i \sim \mathcal{U}\{1, \dots, n\}$$

(2) Monte-Carlo estimation

$$n \int q(z_i \mid x_i, \phi) \nabla_{\theta} \log p(x_i \mid z_i, \theta) dz_i \approx n \nabla_{\theta} \log p(x_i \mid z_i^*, \theta), \quad z_i^* \sim q(z_i \mid x_i, \phi)$$

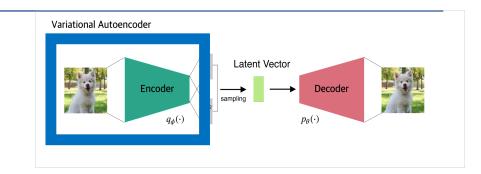


3-3. Update Encoder (parameter : ϕ)

A bit trickier than updating Encoder... 🕾

$$egin{aligned}
abla_{\phi} \mathcal{L}(\phi, heta) &=
abla_{\phi} \sum_{i=1}^{n} \int q\left(z_{i} \mid x_{i}, \phi
ight) \log rac{p\left(x_{i} \mid z_{i}, heta
ight) p\left(z_{i}
ight)}{q\left(z_{i} \mid x_{i}, \phi
ight)} dz_{i} \end{aligned} \
otag \
ota$$

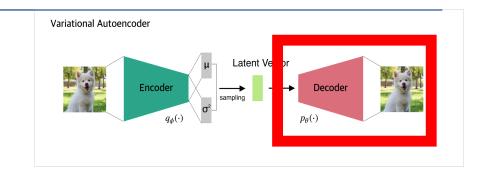
We need some tricks to solve this!



3-3. Update Encoder (parameter : ϕ)

a. Log Derivate Trick

$$\frac{\partial}{\partial x}p(y\mid x) = p(y\mid x)\frac{\partial}{\partial x}\log p(y\mid x)$$



For question like solving $E_{y|x}h(x,y)$

$$\frac{\partial}{\partial x} \int p(y \mid x) h(x, y) dy = \int \frac{\partial}{\partial x} (p(y \mid x) h(x, y)) dy$$

$$= \int \left(h(x, y) \frac{\partial}{\partial x} p(y \mid x) + p(y \mid x) \frac{\partial}{\partial x} h(x, y) \right) dy$$

$$= \int p(y \mid x) \frac{\partial}{\partial x} h(x, y) dy + \int h(x, y) \frac{\partial}{\partial x} p(y \mid x) dy$$

3-3. Update Encoder (parameter : ϕ)

a. Log Derivate Trick

$$\frac{\partial}{\partial x} \int p(y \mid x) h(x, y) dy = \int \frac{\partial}{\partial x} (p(y \mid x) h(x, y)) dy$$

$$= \int \left(h(x, y) \frac{\partial}{\partial x} p(y \mid x) + p(y \mid x) \frac{\partial}{\partial x} h(x, y) \right) dy$$

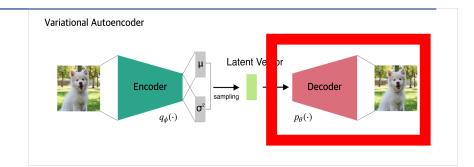
$$= \int p(y \mid x) \frac{\partial}{\partial x} h(x, y) dy + \int h(x, y) \frac{\partial}{\partial x} p(y \mid x) dy$$

First term

- $\int p(y \mid x) \frac{\partial}{\partial x} h(x, y) dy$ - easy to solve (using Monte Carlo estimation)

Second term

- $\int h(x,y) \frac{\partial}{\partial x} p(y \mid x) dy$ - hard to solve - but can be solved using "Log-derivative trick"



3-3. Update Encoder (parameter : ϕ)

a. Log Derivate Trick

$$\frac{\partial}{\partial \phi} \mathcal{L}(\phi, \theta) = \frac{\partial}{\partial \phi} \int q(Z \mid X, \phi) \log p(X \mid Z, \theta) dZ$$

$$\approx n \log p(x_i \mid z_i^*, \theta) \frac{\partial}{\partial \phi} \log q(z_i^* \mid x_i, \phi)$$

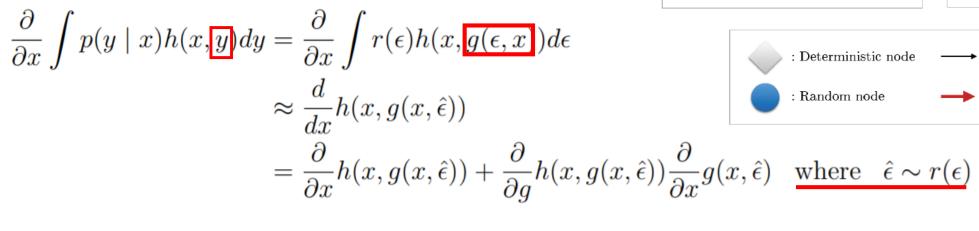


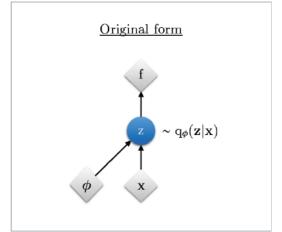
- 1. Mini batching
- 2. Log-derivative Trick

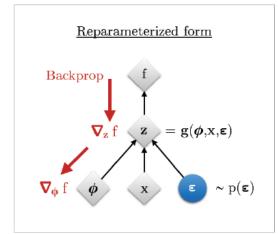
3-3. Update Encoder (parameter : ϕ)

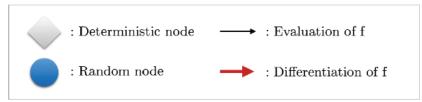
b. Reparameterization Trick

We can not backpropagate through "random" variable! It should be deterministic!









$$\frac{\partial}{\partial x}g(x,\hat{\epsilon})$$
 where $\hat{\epsilon} \sim r(\epsilon)$

3-3. Update Encoder (parameter : ϕ)

b. Reparameterization Trick

Apply it to our derivative of ELBO!

$$n rac{\partial}{\partial \phi} \int q\left(z_{i} \mid x_{i}, \phi
ight) \log p\left(x_{i} \mid z_{i}, heta
ight) = n rac{\partial}{\partial \phi} \int r(\epsilon) \log p\left(x_{i} \mid g\left(\epsilon, x_{i}, \phi
ight), heta
ight) d\epsilon \ pprox n rac{\partial}{\partial \phi} \log p\left(x_{i} \mid g\left(\hat{\epsilon}, x_{i}, \phi
ight), heta
ight), \quad ext{where } \hat{\epsilon} \sim r(\epsilon)$$

(simple example)

$$q_{\phi}\left(\mathbf{z}_{i}|\mathbf{x}_{i}\right)=\mathrm{N}\left(\mu_{i},\sigma_{i}^{2}\mathbf{I}\right)$$

$$ightharpoonup$$
 $\mathbf{z}_i = \boldsymbol{\mu}_i + \boldsymbol{\sigma}_i^2 \odot \boldsymbol{\epsilon}_i$ where $\boldsymbol{\epsilon}_i \sim \mathrm{N}\left(\mathbf{0}, \mathbf{I}\right)$

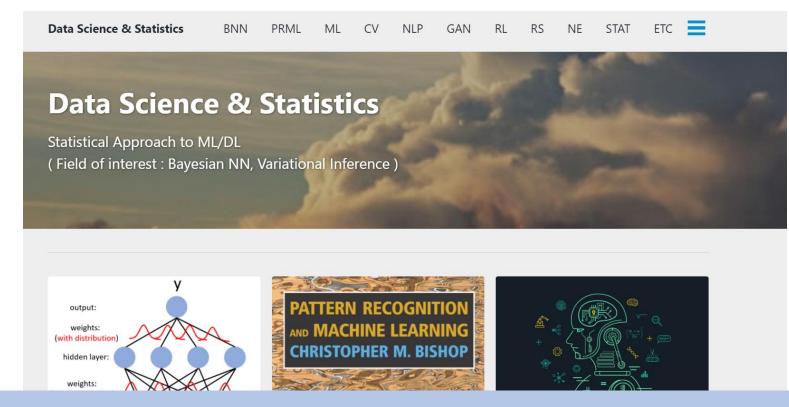
Summary of VAE

- step 1) sample $i \sim \mathcal{U}\{1, \ldots, n\}$
- step 2) compute stochastic gradient of ELBO (w.r.t θ and ϕ)
 - Update θ (decoder parameter)
 stoch. grad_{θ} $\mathcal{L}(\phi, \theta) = n \frac{\partial}{\partial \theta} \log p (x_i \mid z_i^*, \theta)$ where $z_i^* \sim q(z_i \mid x_i, \phi)$
 - Update ϕ (encoder parameter)

 stoch.grad $_{\phi}\mathcal{L}(\phi,\theta) = n\frac{\partial}{\partial\phi}\log p\left(x_{i} \mid g\left(\hat{\epsilon},x_{i},\phi\right),\theta\right) \frac{\partial}{\partial\phi}KL\left(q\left(z_{i} \mid x_{i},\phi\right) \parallel p\left(z_{i}\right)\right)$ where $\hat{\epsilon} \sim r(\epsilon)$
- Update until stopping criterion reaches

3-4. Implementation using Pytorch

https://seunghan96.github.io/stat/gan/bnn/code-6.Variational-Auto-Encoder/



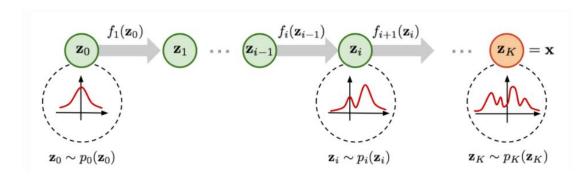
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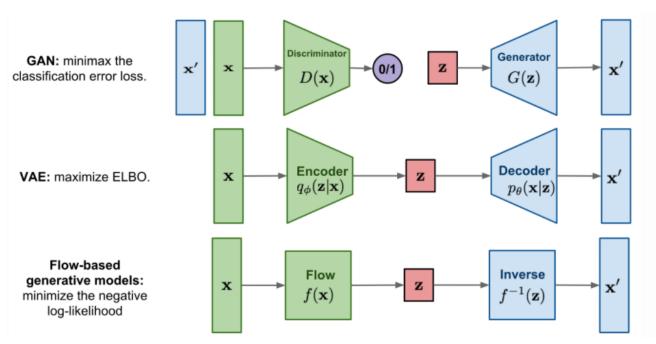
Summary

Have dealt with basic concepts to know before reading papers about

various variational inference methods, Bayesian NN.

Next Presentation: Normalizing Flow





Thank you!

```
Review of Papers regarding VI/BNN

( + some Statistical Models / Machine Learning / Deep Learning )

can be found in my github blog below :)
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https://seunghan96.github.io/

(for more about VI/BNN https://seunghan96.github.io/categories/bnn/)