Theoretic Fundamentals of Machine and Deep Learning

Variational Inference, Autoencoder, Variational Autoencoder, Conditional Variational Autoencoder

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Content

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Variety of generative models

Main representatives of generative models:

- Mixture models (e.g., GMM)
- Hidden Markov Models (HMMs)
- Bayesian Network (and Autoregressive Models)
- Flow-based Models
- Energy-based Models (EBMs)
- Diffusion Models
- Variational Autoencoder (VAE)
- Generative Adversarial Networks (GANs)

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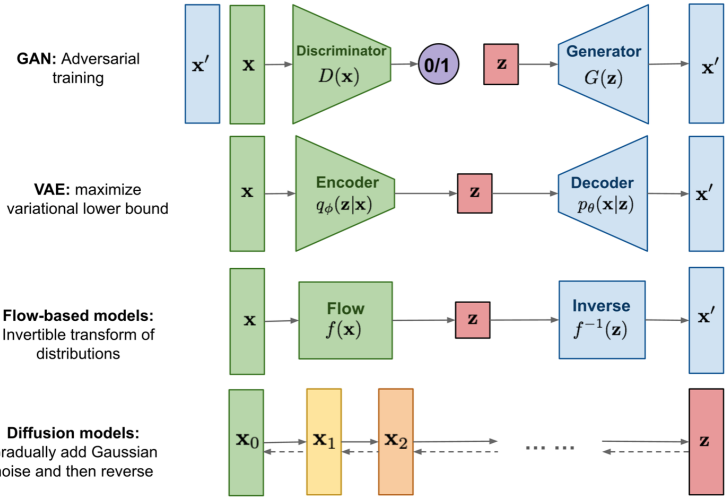
Variety of generative models: illustration[1]



[1] Lil'log blog

Main formulas

- Conditional probability: $p(x|y) = \frac{p(x,y)}{p(y)}$
- Law of total probability: $p(x) = \int_y p(x,y)dy$
- Expectation through integral: $E_{p(x)}f(x) = \int_x p(x)f(x)dx$
- Bayes' theorem: $p(x|y) = \frac{p(y|x)p(x)}{p(y)}$

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Bayesian inference: preliminaries

- Observed input data: x
- Unobserved parameters of the model z : $z \sim p(z)$ (prior distribution)
- A parametric model = joint distribution of latent variable z and observed x: $p(x, z)$
- Likelihood – distribution of the observed data conditioned on parameters $p(x|z)$
- Marginal likelihood: $p(x) = \int p(x, z)dz = \int p(x|z)p(z)dz$

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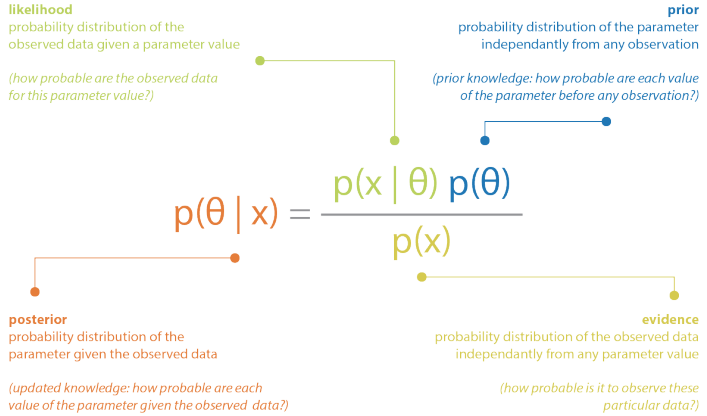
Bayesian inference terms illustration[2]



[2] Joseph Rocca's blog

Bayesian inference

- Inference = **posterior** probability (Bayes' rule):

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

- **Posterior predictive distribution** for the new input x': $p(x'|x) = \int p(x'|z)p(z|x)dz$
- **Prior predictive distribution** for the new input x': $p(x') = \int p(x'|z)p(z)dz$

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Posterior inference

- Inference = **posterior** probability: $p(z|x) = \frac{p(x,z)}{p(x)}$
- Due to unknown $p(x) = \int p(x|z)p(z)dz$, $p(z|x)$ is done via **approximate posterior inference**
  - We're going to work with posteriors known up to a normalization constant $p(x)$
- The most widely used ways to do it:
  - By Variational Inference
    - Bayes by Backprop (VAE)
    - Deep Ensembles / Monte Carlo Dropout
  - By Markov Chain Monte Carlo
    - Samplers (Gibbs, Metropolis)
    - Stochastic Gradient Langevin Dynamics

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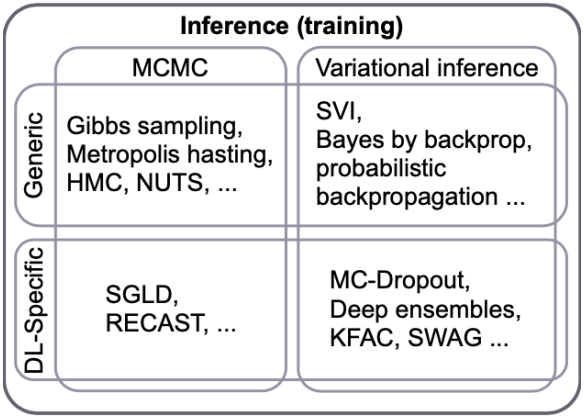
Posterior inference

Diagram[3] shows important means of Bayesian Inference:

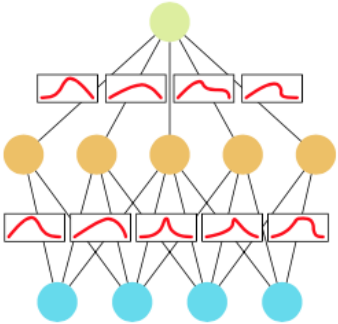


[3] Jospin, L. V., Laga, H., Boussaid, F., Buntine, W., and Bennamoun, M. Hands-on Bayesian neural networks — A tutorial for deep learning users. 2020.

Bayesian Neural Nets (BNN)

BNN

BNN = a *stochastic* neural network trained using Bayesian inference.
Stochastic neural network = NN with a probability distribution over weights.



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BNN: design choice

To design a BNN, one need to choose:

- A prior over weights $\theta \sim p(\theta)$
- Output distribution $p(y|x, \theta)$ (usually modeled as NN $y = \Phi_\theta(x)$ with finite $|Y| < \infty, y \in Y$ in case of classifiers)

Let's denote $D = (D_x, D_y)$ as the training set. In this case the posterior

$$p(\theta|D) = \frac{p(D_y|D_x, \theta)p(\theta)}{\int_\Theta p(D_y|D_x, \theta')p(\theta')d\theta'}$$

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BNN: inference

- BNN inference (posterior predictive distribution):

$$p(y|x, D) = \int_{\Theta} p(y|x, \theta')p(\theta'|D)d\theta'$$

- Is done through Monte Carlo and the output is $\frac{1}{|\Theta|}\sum_{\theta_i \in \Theta} \Phi_{\theta_i}(x)$

Algorithm 1 Inference procedure for a BNN.

Define $p(\boldsymbol{\theta}|D) = \dfrac{p(D_{\boldsymbol{y}}|D_{\boldsymbol{x}}, \boldsymbol{\theta})p(\boldsymbol{\theta})}{\int_{\boldsymbol{\theta}} p(D_{\boldsymbol{y}}|D_{\boldsymbol{x}}, \boldsymbol{\theta'})p(\boldsymbol{\theta'})d\boldsymbol{\theta'}}$;
for $i = 0$ **to** N **do**
  Draw $\boldsymbol{\theta}_i \sim p(\boldsymbol{\theta}|D)$;
  $\boldsymbol{y}_i = \Phi_{\boldsymbol{\theta}_i}(\boldsymbol{x})$;
end for
return $Y = \{\boldsymbol{y}_i | i \in [0, N)\}$, $\Theta = \{\boldsymbol{\theta}_i | i \in [0, N)\}$;

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BNN: online learning

BNN provide a natural way of **online learning**: *previous posteriors* can be *recycled* as *priors* when new data become available to avoid the so-called problem of catastrophic forgetting

Algorithm 3 Online learning loop with a BNN.

Define $p(\boldsymbol{\theta}) = p(\boldsymbol{\theta})_0$;
while true do
  Define $p(\boldsymbol{\theta}|D_i) = \frac{p(D_{\boldsymbol{y},i}|D_{\boldsymbol{x},i}, \boldsymbol{\theta})p(\boldsymbol{\theta})_i}{\int_{\boldsymbol{\theta}} .p(D_{\boldsymbol{y},i}|D_{\boldsymbol{x},i}, \boldsymbol{\theta'})p(\boldsymbol{\theta'})_i d\boldsymbol{\theta'}}$;
  Define $p(\boldsymbol{\theta})_{i+1} = p(\boldsymbol{\theta}|D_i)$;
end while

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Deep ensembles

One of the Deep Learning (DL)-specific methods to simplify working with posterior $p(\theta|D)$ is **Deep ensembles**[4]

- Main idea is to train M neural nets $\Phi_{\theta_i}(x), i = 1 \dots M$
  - Different order of training samples, different initializations of weights
- When making a prediction, just average the outcomes: $\hat{y} = \frac{1}{M} \sum_{i=1}^{M} \Phi_{\theta_i}(x)$
- Can be understood as posterior approximation by distribution parameterized as multiple Dirac deltas, where $\sum_{\theta_i \in \phi} \alpha_{\theta_i} = 1, \alpha_{\theta_i} \geq 0$:

$$q_\phi(\theta) = \sum_{\theta_i \in \phi} \alpha_{\theta_i} \delta_{\theta_i}(\theta)$$

[4] Lakshminarayanan, B., Pritzel, A., and Blundell, C. "Simple and scalable predictive uncertainty estimation using deep ensembles." 2016

MC-dropout

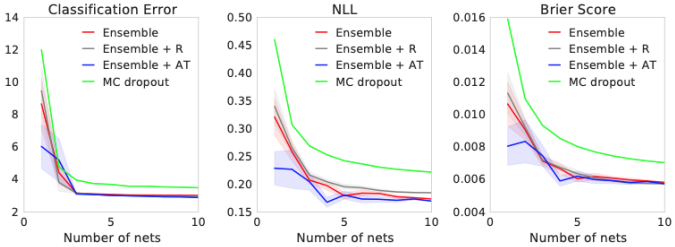
Another (DL)-specific methods to simplify working with posterior $p(\theta|D)$ is **Monte Carlo (MC)-dropout**[5]

- Suppose that layer i of MLP (for other types of NN the approach is quite similar) is a matrix $W_i, i = 1 \dots L$, of size $K_i \times K_{i-1}$
- In usual NN training dropout is applied only during training
- For MC-dropout it is applied during inference for distribution $q(\theta)$:
  - $z_{i,j} \sim Bernoulli(p_i), i = 1 \dots L, j = 1 \dots K_{i-1}$
  - $z_{i,j} = 0$ corresponds to unit j in layer $i-1$ being dropped out as an input to layer i
  - $\Theta_i = diag([z_{i,j}]_{j=1}^{K_i})$, $\theta = \{\Theta_i\}_{i=1}^{L}$
- Then we sample $\theta \sim q(\theta)$ and estimate posterior through Monte Carlo

[5] Gal, Y., and Ghahramani, Z. "Dropout as a bayesian approximation: Representing model uncertainty in deep learning." 2015

Deep ensembles vs MC-dropout

MC-dropout can be understood as Deep ensembles via single NN. But even having only one NN (this is pro) the performance is worse (con):



(b) SVHN using VGG-style convnet

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Variational Inference (VI)

VI

VI = a method of approximating a complex distribution with some family of parameterized distributions.

- VI treats posterior inference as optimization problem
- For this purpose a family of parameterized (by ϕ) distributions $q_\phi(z)$ is introduced
  - No any guarantee that $q_\phi(z)$ can cover (or even be very close) to the real posterior
  - Usually this family is simple Gaussian $q_\phi = N(\mu_\phi, \sigma^2_\phi)$
- Optimization objective:

$$D_{KL}(q_\phi(z)||p(z|x)) \to \min_\phi$$

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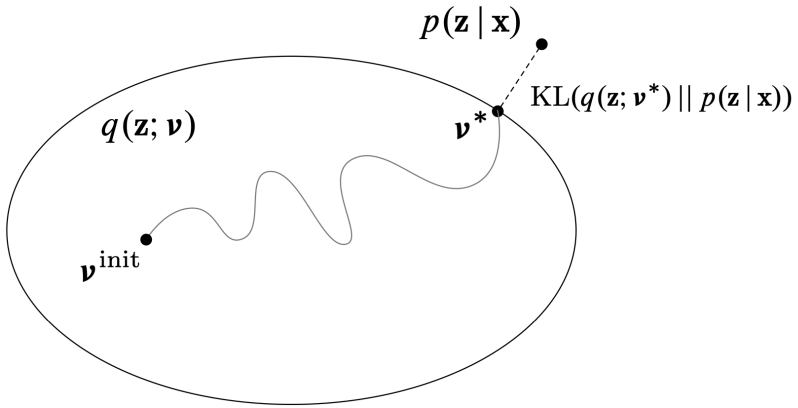
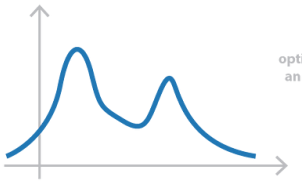
VI scheme

- Optimization process scheme: can never lead to a perfect solution[6]

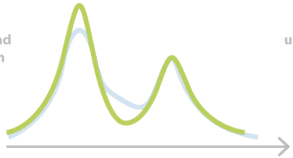


[6] David Blei, Rajesh Ranganath, Shakir Mohamed. Variational Inference: Foundations and Modern Methods

VI illustration[7]



optimisation to find an approximation



use of the approximate distribution

$$\int x.\pi(x)\,dx \approx \int x.f(x)\,dx$$

Unnormalised distribution (π)
whose normalisation factor computation is intractable

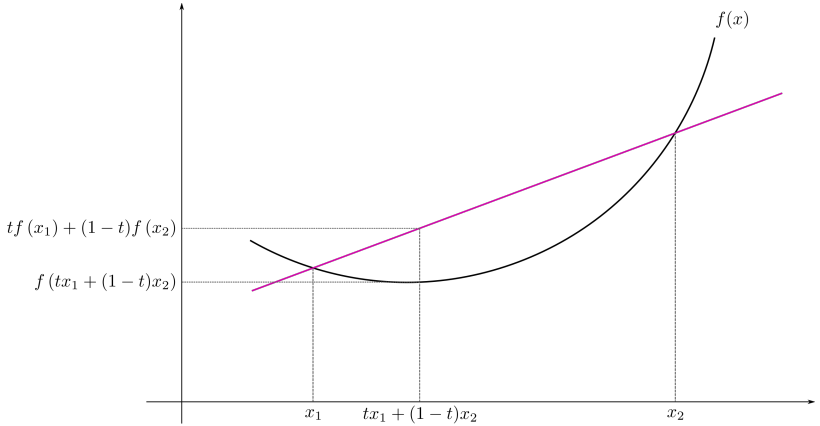
Best approximation (f)
among a parametrised family, obtained by optimising over the family parameters and without proceeding to the normalisation

Approximate computations
obtained by replacing the exact distribution by the approximate one

[7] Joseph Rocca's blog

Jensen's inequality

- Jensen's inequality for a convex function f can be written as a $f(E[x]) \leq E[f(x)]$ [8]
- For a concave function (e.g., log) we have the opposite: $f(E[x]) \geq E[f(x)]$



[8] Wiki: Jensen's inequality

Evidence Lower BOund (ELBO)

- Let's recall: $p(x)$ is called the **evidence**
- Then using the marginalization property and expectation through integral notation:

$$\log p(x) = \log \int_z p(x, z) = \log \int_z p(x, z) \frac{q_\phi(z)}{q_\phi(z)} = \log E_{q_\phi} \frac{p(x, z)}{q_\phi(z)}$$

- And using the Jensen's inequality for concave function:

$$\log p(x) \geq E_{q_\phi} \log \frac{p(x, z)}{q_\phi(z)}$$

- $E_{q_\phi} \log \frac{p(x,z)}{q_\phi(z)}$ is called Evidence Lower BOund (**ELBO**), as it is the lower bound for the evidence $\log p(x)$

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ELBO and KL-divergence

- Conditional probability property: $p(z|x) = \frac{p(x,z)}{p(x)}$
- Let's work on $D_{KL}(q_\phi(z)||p(z|x))$:

$$D_{KL}(q_\phi(z)||p(z|x)) = E_{q_\phi} \log \frac{q_\phi(z)}{p(z|x)} = E_{q_\phi} \log \frac{q_\phi(z)p(x)}{p(x,z)} = E_{q_\phi} \log \frac{q_\phi(z)}{p(x,z)} + E_{q_\phi} \log p(x)$$

- Replacing $E_{q_\phi} \log p(x) = \log p(x)$ and $E_{q_\phi} \log \frac{q_\phi(z)}{p(x,z)} = -E_{q_\phi} \log \frac{p(x,z)}{q_\phi(z)}$, we get:

$$D_{KL}(q_\phi(z)||p(z|x)) = \log p(x) - E_{q_\phi} \log \frac{p(x,z)}{q_\phi(z)} \tag{1}$$

- $q_\phi(z) \to p(z|x) \Rightarrow D_{KL}(q_\phi(z)||p(z|x)) \to 0 \Rightarrow E_{q_\phi} \log \frac{p(x,z)}{q_\phi(z)} \to \max_\phi$
- In other words, we need to **maximize** ELBO

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ELBO and normalization

- ELBO is equivalent to: $E_{q_\phi} \log \frac{p(x,z)}{q_\phi(z)} = E_{q_\phi} \log \frac{p(x|z)p(z)}{q_\phi(z)}$
- Suppose the unnormalized distribution $\hat{p}(x|z)$ (usually implemented as a Neural Net) is one that $p(x|z) = \frac{\hat{p}(x|z)}{C}$, where C is the normalization constant
- Then the ELBO becomes:

$$E_{q_\phi} \log \frac{p(x|z)p(z)}{q_\phi(z)} = E_{q_\phi} \log \frac{\hat{p}(x|z)p(z)}{q_\phi(z)} - E_{q_\phi} \log C = E_{q_\phi} \log \frac{\hat{p}(x|z)p(z)}{q_\phi(z)} - \log C$$

- And we can still work on maximization of ELBO using the unnormalized $\hat{p}(x|z)$ as $\log C$ being constant is not changing the optimization target

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Another optimization form

- Let's work on Eq. 1 in a different way: $0 \leq D_{KL}(q_\phi(z)||p(z|x)) =$

$$= \log p(x) - E_{q_\phi(z)} \log \frac{p(x,z)}{q_\phi(z)} = \log p(x) + E_{q_\phi(z)} \log \frac{q_\phi(z)}{p(x|z)p(z)} =$$

$$= \log p(x) + D_{KL}(q_\phi(z)||p(z)) - E_{q_\phi(z)} \log p(x|z) \Rightarrow$$

$$\log p(x) \geq E_{q_\phi(z)} p(x|z) - D_{KL}(q_\phi(z)||p(z))$$

- Maximization of ELBO $\Leftrightarrow$

$$L(x, z; \phi) = D_{KL}(q_\phi(z)||p(z)) - E_{q_\phi(z)} \log p(x|z) \rightarrow \min_\phi \tag{2}$$

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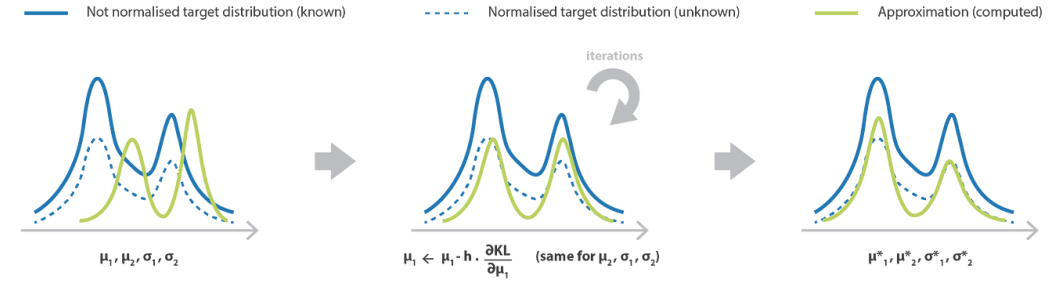
BNN training: Bayes by backprop[9]

- Now we have everything to train the whole BNN
- Let's treat z as a vector of all NN weights
- To train efficiently, we need to apply the reparameterization trick: $\phi = (\mu, \sigma)$, $z = \mu + \sigma \cdot \epsilon$, where $\epsilon \sim N(0, 1) \Rightarrow z \sim_\phi N(\mu, \sigma^2)$
- Prior $z \sim_p N(0, 1)$, and point-wise NN output is $p(x|z)$
- Eq. 2 can be rewritten as $E_{q_\phi(z)}[\log q_\phi(z) - \log p(z) - \log p(x|z)]$ Let $f(z, \phi) = \log q_\phi(z) - \log p(z)p(x|z)$
- Calculate gradient w.r.t. (μ, σ): $\nabla_\mu f(z, \phi) = \frac{\partial f(z,\phi)}{\partial z}\frac{\partial z}{\partial \mu} + \frac{\partial f(z,\phi)}{\partial \mu}$ (and the same for σ)
- And finally, apply SGD! $\phi = \phi - \eta \nabla_\phi f(z)$

[9] Blundell, Charles, et al. "Weight uncertainty in neural network." 2015.

VI optimization process illustration[10]



Initialisation of the family parameters and computation of KL divergence between corresponding approximation and raw target

Iteratively compute derivative of KL divergence with respect to parameters to update and make a step in the opposite direction for these parameters

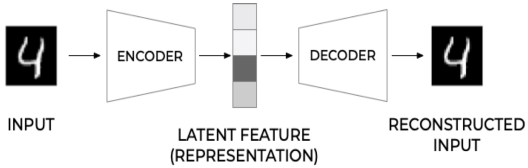
The best approximation among the chosen family is then obtained (up to the efficiency of the optimisation process and local minima)

[10] Joseph Rocca's blog

Auto Encoder (AE)

- Suppose that the data dimensionality is large: $x \in \mathbb{R}^N$
- To extract the lower-dimensional semantic representation of the data the so called **Auto Encoders** (**AE**) are used[11]
- For this purpose, two neural nets – **Encoder** $f : \mathbb{R}^N \to \mathbb{R}^K$, where usually $K \ll N$, and **Decoder**[12] $g : \mathbb{R}^K \to \mathbb{R}^N$ – are trained to minimize the Reconstruction Error:

$$\min_{f,g} \Delta(x, g \circ f(x)) = \min_{f,g} \Delta(x, g(f(x)))$$

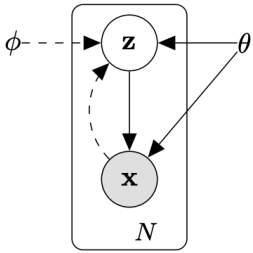


[11] Rumelhart, David E., Geoffrey E. Hinton, and Ronald J. Williams. Learning internal representations by error propagation. 1985.

[12] Michelucci, Umberto. "An Introduction to Autoencoders." 2022.

Variational Auto Encoder (VAE)

- Suppose that the we would like to sample from the real data distribution $p(x), x \in \mathbb{R}^N$
- We could do it from the lower dimension $K \ll N$ with the help of the Decoder g
- But we need to know the distribution of the latent $z \in \mathbb{R}^K$ to apply $g(z)$
- It can be done by **Variational Auto Encoder (VAE)**[13]
  - Using the generative model $p_\theta(x, z) = p_\theta(x|z)p_\theta(z)$, we would like to approximate the posterior $p_\theta(z|x)$ by $q_\phi(z|x)$, as working solely on unconditional $q_\phi(z)$ is very hard



[13] Kingma, Diederik P., and Max Welling. "Auto-encoding variational bayes." 2013.

VAE objective

- Let's work on $q_\phi(z|x)$ instead of $q_\phi(z)$ in Eq. 2
- And use $p_\theta(z)$, $p_\theta(z|x)$ instead of $p(z)$, $p(z|x)$:

$$\log p(x) \geq E_{q_\phi(z|x)} p_\theta(x|z) - D_{KL}(q_\phi(z|x)||p_\theta(z))$$

- Maximization of ELBO $\Leftrightarrow$

$$L(x, z; \phi, \theta) = D_{KL}(q_\phi(z|x)||p_\theta(z)) - E_{q_\phi(z|x)} \log p_\theta(x|z) \to \min_{\phi,\theta} \tag{3}$$

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VAE loss

- Common design choices:
  - $p_\theta(z) = N(0, 1)$
  - $q_\phi(z|x) = N(\mu_\phi(x), \sigma^2_\phi(x))$
  - $p_\theta(x|z) = N(g(z), c^2 I)$
- Then
  - $E_{q_\phi(z|x)} \log p_\theta(x|z) = -E_{q_\phi(z|x)} \frac{(x-g(z))^2}{2c^2}$ (upto some constant)
  - $D_{KL}(q_\phi(z|x)||p_\theta(z)) = \frac{1}{2} \sum_{j=1}^{K} \left(\mu_{j,\phi}(x)^2 + \sigma^2_{j,\phi}(x) - 1 - \log \sigma^2_{j,\phi}(x) \right)$
- And the final loss $L(x, z; \phi, \theta) = D_{KL}(q_\phi(z|x)||p_\theta(z)) - E_{q_\phi(z|x)} \log p_\theta(x|z) =$

$$= \frac{1}{2} \sum_{j=1}^{K} \left(\mu_{j,\phi}(x)^2 + \sigma^2_{j,\phi}(x) - 1 - \log \sigma^2_{j,\phi}(x) \right) + E_{q_\phi(z|x)} \frac{(x - g(z))^2}{2c^2}$$

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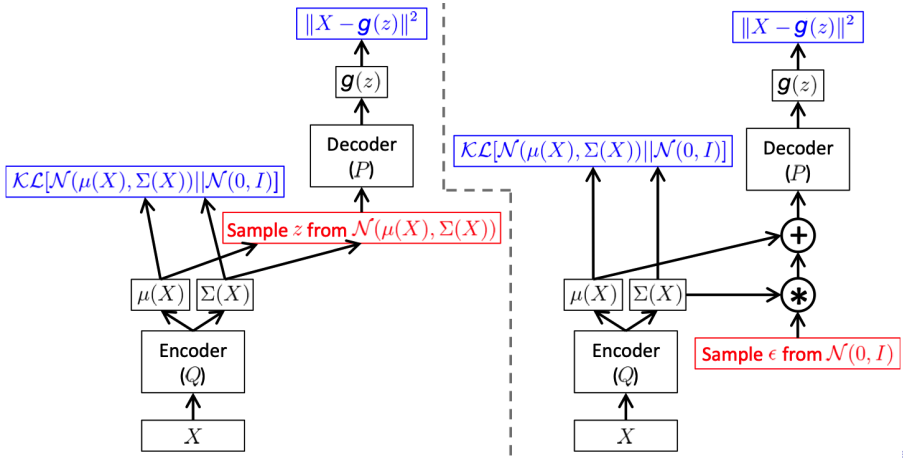
VAE as a Neural Net — training

When implementing VAE as Neural Net, we need to apply Reparametrization Trick in order to have backpropagation of gradients through Decoder **and** Encoder (left – w/o, right – w/ this trick; no backprop; loss):



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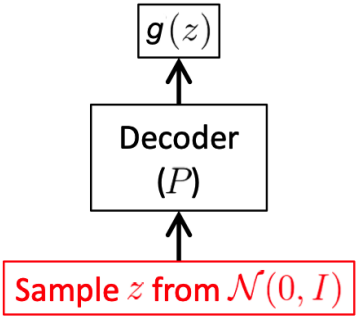
VAE as a Neural Net — inference

For inference[14], we just sample $z \sim N(0, 1)$ and apply the learned Decoder $g(z)$:



[14] Doersch, C. "Tutorial on variational autoencoders." 2016

Conditional VAE (cVAE)

- With VAE we cannot guide the sampling process: if data has multiple classes, we don't know in advance which class we are sampling with prior $z \sim p_\theta(z)$
- To add this ability, we need to sample based on some guidance signal (e.g., class label) y
- This leads to so called **Conditional** VAE (**cVAE**)[15]
- ELBO for cVAE can be done by conditioning all the distribution terms inside $L(x, z; \phi, \theta)$ on y
  - Usually $p_\varphi(x|z, y)$ is modeled by another Neural Net with parameters φ
- Final objective is obtained in the similar manner as Eq. 3:

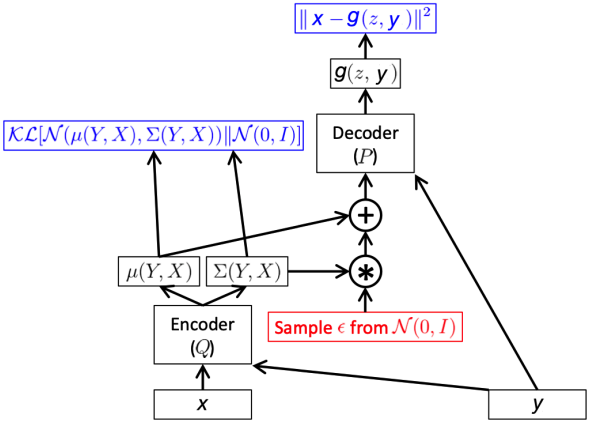
$$L(x, y, z; \phi, \varphi, \theta) = D_{KL}(q_\phi(z|x, y)||p_\theta(z|y)) - E_{q_\phi(z|x,y)} \log p_\varphi(x|z, y) \to \min_{\phi,\varphi,\theta}$$

[15] Sohn, K., Lee, H., and Yan, X. "Learning structured output representation using deep conditional generative models." 2015

cVAE — training

Common design choices:

- Sometimes (not always!) conditioning on y for sampling of z in prior is omitted: $p_\theta(z|y) = N(0, 1)$
- $q_\phi(z|x, y) = N(\mu_\phi(x, y), \sigma^2_\phi(x, y))$
- $p_\varphi(x|z, y) = N(g(z, y), c^2 I)$



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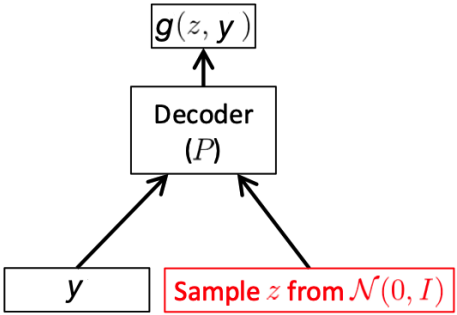
cVAE — inference

For inference, we just sample $z \sim N(0, 1)$ and apply the learned Decoder $g(z, y)$:



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Takeaway notes

- Bayesian Neural Nets: weights are distributions
- Variational Inference is just an approximating of one distribution by another parameterized distribution
- Posterior usually contains intractable constant $\Rightarrow$ VI to the rescue
- VI is sample-efficient during inference because we sample from the converged distribution (that we learned)
- VI can provide the low-variance (see above item) but probably highly biased solution (because it is hard to provide a good family of distributions to cover the original one)
- ELBO is a good bound because there is no need in normalization
- VAE is a classical example of VI
- cVAE (as well as cGAN) is much more widely used in practice

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Thank you!