Deep Generative Models

Lecture 3

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Recap of previous lecture

MLE problem for autoregressive model

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} p(\mathbf{X}|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \sum_{j=1}^{m} \log p(x_{ij}|\mathbf{x}_{i,1:j-1}\boldsymbol{\theta}).$$

Sampling

$$\hat{x}_1 \sim p(x_1|\boldsymbol{\theta}), \quad \hat{x}_2 \sim p(x_2|\hat{x}_1, \boldsymbol{\theta}), \dots, \quad \hat{x}_m \sim p(x_m|\hat{\mathbf{x}}_{1:m-1}, \boldsymbol{\theta})$$

New generated object is $\hat{\mathbf{x}} = (\hat{x}_1, \hat{x}_2, \dots, \hat{x}_m)$.

Masking helps to make neural network autoregressive.

- **MADE** - masked autoencoder (MLP).
- **WaveNet** - masked 1D convolutions.
- **PixelCNN** - masked 2D convolutions.

PixelCNN++ uses discretized mixture of logistic distribution to make the output distribution more natural.

Recap of previous lecture

Posterior distribution

$$p(\boldsymbol{\theta}|\mathbf{X}) = \frac{p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathbf{X})} = \frac{p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{\int p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}}$$

Bayesian inference

$$p(\mathbf{x}|\mathbf{X}) = \int p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathbf{X})d\boldsymbol{\theta}$$

Maximum a posteriori (MAP) estimation

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} p(\boldsymbol{\theta}|\mathbf{X}) = \arg\max_{\boldsymbol{\theta}} \big(\log p(\mathbf{X}|\boldsymbol{\theta}) + \log p(\boldsymbol{\theta})\big)$$

MAP inference

$$p(\mathbf{x}|\mathbf{X}) = \int p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathbf{X})d\boldsymbol{\theta} \approx p(\mathbf{x}|\boldsymbol{\theta}^*).$$

Latent variable models (LVM)

MLE problem

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} p(\mathbf{X}|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \prod_{i=1}^{n} p(\mathbf{x}_i|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p(\mathbf{x}_i|\boldsymbol{\theta}).$$

The distribution $p(\mathbf{x}|\boldsymbol{\theta})$ could be very complex and intractable (as well as real distribution $\pi(\mathbf{x})$).

Extended probabilistic model

Introduce latent variable $\mathbf{z}$ for each sample $\mathbf{x}$

$$p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) = p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})p(\mathbf{z}); \quad \log p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) = \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \log p(\mathbf{z}).$$

$$p(\mathbf{x}|\boldsymbol{\theta}) = \int p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} = \int p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})p(\mathbf{z}) d\mathbf{z}.$$

Motivation

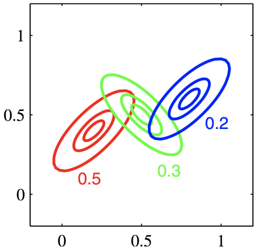
The distributions $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$ and $p(\mathbf{z})$ could be quite simple.

Latent variable models (LVM)

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log \int p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) p(\mathbf{z}) d\mathbf{z} \to \max_{\boldsymbol{\theta}}$$

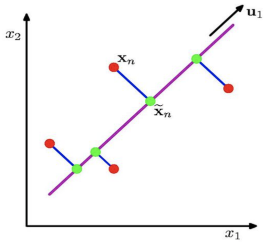
Examples

Mixture of gaussians



- $p(\mathbf{x}|z, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_z, \boldsymbol{\Sigma}_z)$
- $p(z) = \text{Categorical}(\boldsymbol{\pi})$

PCA model



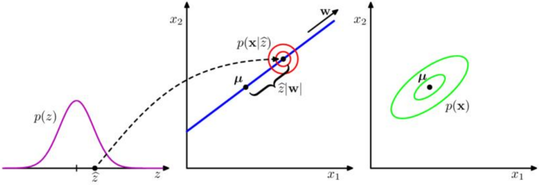
- $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}|\mathbf{W}\mathbf{z} + \boldsymbol{\mu}, \sigma^2 \mathbf{I})$
- $p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|0, \mathbf{I})$

Bishop C. Pattern Recognition and Machine Learning, 2006

Latent variable models (LVM)

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log \int p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) p(\mathbf{z}) d\mathbf{z} \to \max_{\boldsymbol{\theta}}$$

PCA projects original data **X** onto a low dimensional latent space while maximizing the variance of the projected data.



$$\boldsymbol{x} = W\boldsymbol{z} + \boldsymbol{\mu} + \boldsymbol{\epsilon}$$

- $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}|\mathbf{Wz} + \boldsymbol{\mu}, \sigma^2\mathbf{I})$
- $p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|0, \mathbf{I})$
- $p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \mathbf{WW}^T + \sigma^2\mathbf{I})$
- $p(\mathbf{z}|\mathbf{x}) = \mathcal{N}\big(\mathbf{M}^{-1}\mathbf{W}^T(\mathbf{x} - \boldsymbol{\mu}), \sigma^2\mathbf{M}\big)$, where $\mathbf{M} = \mathbf{WW}^T + \sigma^2\mathbf{I}$

Maximum likelihood estimation for LVM

MLE for extended problem

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \prod_{i=1}^{n} p(\mathbf{x}_i, \mathbf{z}_i|\boldsymbol{\theta}) =$$

$$= \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p(\mathbf{x}_i, \mathbf{z}_i|\boldsymbol{\theta}).$$

However, $\mathbf{Z}$ is unknown.

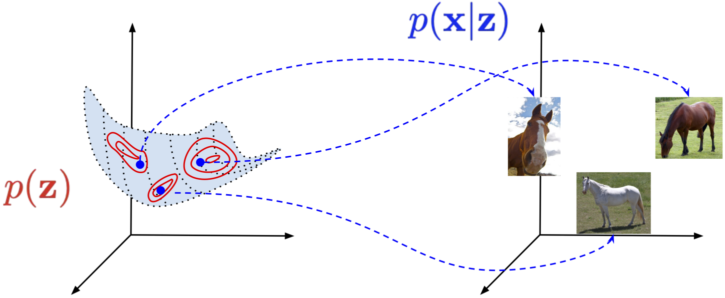
MLE for original problem

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} \log p(\mathbf{X}|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p(\mathbf{x}_i|\boldsymbol{\theta}) =$$

$$= \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log \int p(\mathbf{x}_i, \mathbf{z}_i|\boldsymbol{\theta}) d\mathbf{z}_i =$$

$$= \arg\max_{\boldsymbol{\theta}} \log \sum_{i=1}^{n} \int p(\mathbf{x}_i|\mathbf{z}_i, \boldsymbol{\theta}) p(\mathbf{z}_i) d\mathbf{z}_i.$$

Naive approach



Monte-Carlo estimation

$$p(\mathbf{x}|\boldsymbol{\theta}) = \int p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})p(\mathbf{z})d\mathbf{z} = \mathbb{E}_{p(\mathbf{z})}p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) \approx \frac{1}{K}\sum_{k=1}^{K} p(\mathbf{x}|\mathbf{z}_k, \boldsymbol{\theta})$$

Challenge: to cover the space properly, the number of samples grows exponentially with respect to dimensionality of $\mathbf{z}$.

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image credit: https://jmtomczak.github.io/blog/4/4_VAE.html

Variational lower bound

Derivation 1

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log \int p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} =$$

$$= \log \int \frac{q(\mathbf{z})}{q(\mathbf{z})} p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} = \log \mathbb{E}_q \left[\frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z})} \right] \geq$$

$$\geq \mathbb{E}_q \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z})} = \int q(\mathbf{z}) \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z})} d\mathbf{z} = \mathcal{L}(q, \boldsymbol{\theta})$$

Derivation 2

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \int q(\mathbf{z}) \log p(\mathbf{x}|\boldsymbol{\theta}) d\mathbf{z} =$$

$$= \int q(\mathbf{z}) \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})} d\mathbf{z} = \int q(\mathbf{z}) \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) q(\mathbf{z})}{p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}) q(\mathbf{z})} d\mathbf{z} =$$

$$= \int q(\mathbf{z}) \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z})} d\mathbf{z} + \int q(\mathbf{z}) \log \frac{q(\mathbf{z})}{p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})} d\mathbf{z} =$$

$$= \mathcal{L}(q, \boldsymbol{\theta}) + KL(q(\mathbf{z}) || p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})) \geq \mathcal{L}(q, \boldsymbol{\theta}).$$

Variational lower bound

Evidence Lower Bound (ELBO)

$$
\begin{aligned}
\mathcal{L}(q, \boldsymbol{\theta}) &= \int q(\mathbf{z}) \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z})} d\mathbf{z} = \\
&= \int q(\mathbf{z}) \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) d\mathbf{z} + \int q(\mathbf{z}) \log \frac{p(\mathbf{z})}{q(\mathbf{z})} d\mathbf{z} \\
&= \mathbb{E}_q \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - KL(q(\mathbf{z})||p(\mathbf{z}))
\end{aligned}
$$

Log-likelihood decomposition

$$
\log p(\mathbf{x}|\boldsymbol{\theta}) = \mathbb{E}_q \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - KL(q(\mathbf{z})||p(\mathbf{z})) + KL(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})).
$$

Instead of maximizing incomplete likelihood, maximize ELBO (equivalently minimize KL)

$$
\max_{\boldsymbol{\theta}} p(\mathbf{x}|\boldsymbol{\theta}) \quad \rightarrow \quad \max_{q, \boldsymbol{\theta}} \mathcal{L}(q, \boldsymbol{\theta}) \equiv \min_{q, \boldsymbol{\theta}} KL(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})).
$$

EM-algorithm

$$\mathcal{L}(q, \boldsymbol{\theta}) = \int q(\mathbf{z}) \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) d\mathbf{z} + \int q(\mathbf{z}) \log \frac{p(\mathbf{z})}{q(\mathbf{z})} d\mathbf{z}.$$

Block-coordinate optimization

- Initialize $\boldsymbol{\theta}^*$;
- E-step

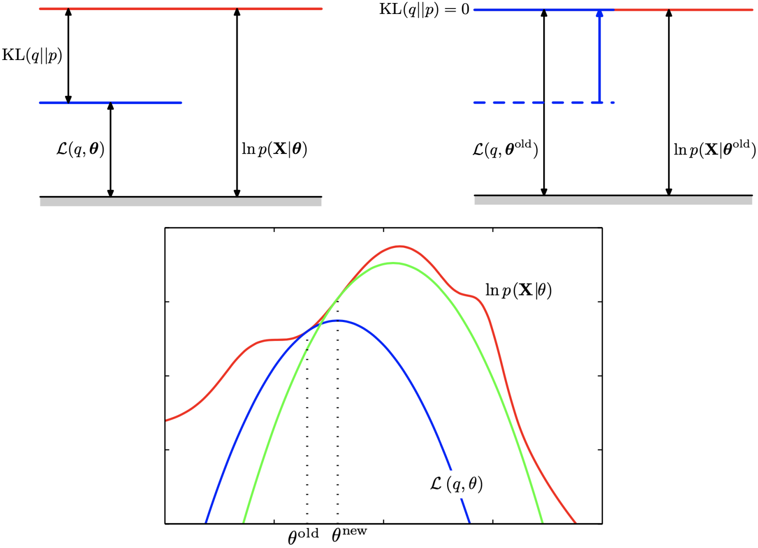
$$q^*(\mathbf{z}) = \arg\max_q \mathcal{L}(q, \boldsymbol{\theta}^*) =$$
$$= \arg\min_q KL(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}^*)) = p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}^*);$$

- M-step

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} \mathcal{L}(q^*, \boldsymbol{\theta});$$

- Repeat E-step and M-step until convergence.

EM illustration



Bishop C. Pattern Recognition and Machine Learning, 2006

Amortized variational inference

E-step

$$q(\mathbf{z}) = \arg\max_q \mathcal{L}(q, \boldsymbol{\theta}^*) = \arg\min_q KL(q||p) = p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}^*).$$

- $p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}^*)$ could be **intractable**;
- $q(\mathbf{z})$ is different for each object $\mathbf{x}$.

Idea

Restrict a family of all possible distributions $q(\mathbf{z})$ to a parametric class $q(\mathbf{z}|\mathbf{x}, \phi)$ conditioned on samples $\mathbf{x}$ with parameters ϕ.

Variational Bayes

- E-step
$$\boldsymbol{\phi}_k = \boldsymbol{\phi}_{k-1} + \eta \nabla_{\boldsymbol{\phi}} \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}_{k-1})|_{\boldsymbol{\phi}=\boldsymbol{\phi}_{k-1}}$$
- M-step
$$\boldsymbol{\theta}_k = \boldsymbol{\theta}_{k-1} + \eta \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\phi}_k, \boldsymbol{\theta})|_{\boldsymbol{\theta}=\boldsymbol{\theta}_{k-1}}$$

Variational EM-algorithm

ELBO

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \mathcal{L}(\phi, \boldsymbol{\theta}) + KL(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})) \geq \mathcal{L}(\phi, \boldsymbol{\theta}).$$

- E-step

$$\boldsymbol{\phi}_k = \boldsymbol{\phi}_{k-1} + \eta \nabla_{\boldsymbol{\phi}} \mathcal{L}(\phi, \boldsymbol{\theta}_{k-1})\big|_{\boldsymbol{\phi}=\boldsymbol{\phi}_{k-1}},$$

  where ϕ – parameters of variational distribution $q(\mathbf{z}|\mathbf{x}, \phi)$.
- M-step

$$\boldsymbol{\theta}_k = \boldsymbol{\theta}_{k-1} + \eta \nabla_{\boldsymbol{\theta}} \mathcal{L}(\phi_k, \boldsymbol{\theta})\big|_{\boldsymbol{\theta}=\boldsymbol{\theta}_{k-1}},$$

  where $\boldsymbol{\theta}$ – parameters of the generative distribution $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$.

Now all we have to do is to obtain two gradients $\nabla_{\boldsymbol{\phi}} \mathcal{L}(\phi, \boldsymbol{\theta})$, $\nabla_{\boldsymbol{\theta}} \mathcal{L}(\phi, \boldsymbol{\theta})$.
Challenge: Number of samples n could be huge (we heed to derive unbiased stochastic gradients).

ELBO gradients

$$\mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}) = \mathbb{E}_q \left[\log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \log \frac{p(\mathbf{z})}{q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})} \right] \rightarrow \max_{\boldsymbol{\phi}, \boldsymbol{\theta}}.$$

M-step: $\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta})$

$$\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}) = \int q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi}) \nabla_{\boldsymbol{\theta}} \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) d\mathbf{z} \approx$$

$$\approx \nabla_{\boldsymbol{\theta}} \log p(\mathbf{x}|\mathbf{z}^*, \boldsymbol{\theta}), \quad \mathbf{z}^* \sim q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi}).$$

E-step: $\nabla_{\boldsymbol{\phi}} \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta})$

Difference from M-step: density function $q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})$ depends on the parameters $\boldsymbol{\phi}$, it is impossible to use the Monte-Carlo estimation:

$$\nabla_{\boldsymbol{\phi}} \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}) = \nabla_{\boldsymbol{\phi}} \int q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi}) \left[\log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \log \frac{p(\mathbf{z})}{q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})} \right] d\mathbf{z}$$

$$\neq \int q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi}) \nabla_{\boldsymbol{\phi}} \left[\log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \log \frac{p(\mathbf{z})}{q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})} \right] d\mathbf{z}$$

Reparametrization trick

Law of the unconscious statistician (LOTUS)

Let X be a random variable and let $Y = g(X)$. Then

$$\mathbb{E}_{p_Y} Y = \mathbb{E}_{p_X} g(X) = \int g(\mathbf{x}) p(\mathbf{x}) d\mathbf{x}.$$

Examples

- $r(x) = \mathcal{N}(x|0,1)$, $y = \sigma \cdot x + \mu$, $p_Y(y|\theta) = \mathcal{N}(y|\mu, \sigma^2)$, $\theta = [\mu, \sigma]$.
- $\boldsymbol{\epsilon}^* \sim r(\boldsymbol{\epsilon}), \quad \mathbf{z} = g(\mathbf{x}, \boldsymbol{\epsilon}, \boldsymbol{\phi}), \quad \mathbf{z} \sim q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})$

$$\begin{aligned}\nabla_{\boldsymbol{\phi}} \int q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi}) f(\mathbf{z}) d\mathbf{z} &= \nabla_{\boldsymbol{\phi}} \int r(\boldsymbol{\epsilon}) f(\mathbf{z}) d\boldsymbol{\epsilon} \\ &= \int r(\boldsymbol{\epsilon}) \nabla_{\boldsymbol{\phi}} f(g(\mathbf{x}, \boldsymbol{\epsilon}, \boldsymbol{\phi})) d\boldsymbol{\epsilon} \approx \nabla_{\boldsymbol{\phi}} f(g(\mathbf{x}, \boldsymbol{\epsilon}^*, \boldsymbol{\phi}))\end{aligned}$$

ELBO gradient (E-step, $\nabla_\phi \mathcal{L}(\phi, \boldsymbol{\theta})$)

$$\nabla_\phi \mathcal{L}(\phi, \boldsymbol{\theta}) = \nabla_\phi \int q(\mathbf{z}|\mathbf{x}, \phi) \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) d\mathbf{z} - \nabla_\phi \mathrm{KL}(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z}))$$

$$= \int r(\boldsymbol{\epsilon}) \nabla_\phi \log p(\mathbf{x}|g(\mathbf{x}, \boldsymbol{\epsilon}, \phi), \boldsymbol{\theta}) d\boldsymbol{\epsilon} - \nabla_\phi \mathrm{KL}(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z}))$$

$$\approx \nabla_\phi \log p(\mathbf{x}|g(\mathbf{x}, \boldsymbol{\epsilon}^*, \phi), \boldsymbol{\theta}) - \nabla_\phi \mathrm{KL}(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z}))$$

Variational assumption

$$r(\boldsymbol{\epsilon}) = \mathcal{N}(0, \mathbf{I}); \quad q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\boldsymbol{\mu}_\phi(\mathbf{x}), \boldsymbol{\sigma}^2_\phi(\mathbf{x})).$$

$$\mathbf{z} = g(\mathbf{x}, \boldsymbol{\epsilon}, \phi) = \boldsymbol{\sigma}_\phi(\mathbf{x}) \cdot \boldsymbol{\epsilon} + \boldsymbol{\mu}_\phi(\mathbf{x}).$$

Here $\boldsymbol{\mu}_\phi(\cdot), \boldsymbol{\sigma}_\phi(\cdot)$ are parameterized functions (outputs of neural network).

- $p(\mathbf{z})$ – prior distribution on latent variables $\mathbf{z}$. We could specify any distribution that we want. Let say $p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I})$.
- $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$ - generative distibution. Since it is a parameterized function let it be neural network with parameters $\boldsymbol{\theta}$.

Variational autoencoder (VAE)

Final algorithm

- pick $i \sim U[1, n]$;
- compute a stochastic gradient w.r.t. $\boldsymbol{\phi}$

$$\nabla_{\boldsymbol{\phi}} \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}) \approx\approx \nabla_{\boldsymbol{\phi}} \log p(\mathbf{x}|g(\mathbf{x}, \boldsymbol{\epsilon}^*, \boldsymbol{\phi}), \boldsymbol{\theta}) \\ - \nabla_{\boldsymbol{\phi}} \mathrm{KL}(q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi}) || p(\mathbf{z})), \quad \boldsymbol{\epsilon}^* \sim r(\boldsymbol{\epsilon});$$

- compute a stochastic gradient w.r.t. $\boldsymbol{\theta}$

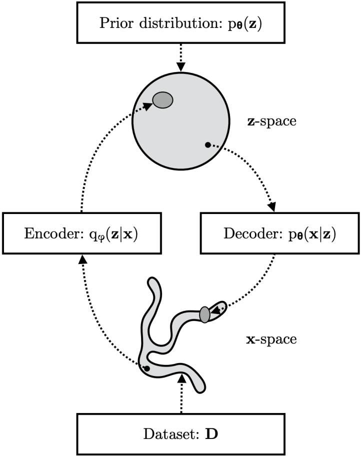
$$\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}) \approx \nabla_{\boldsymbol{\theta}} \log p(\mathbf{x}|\mathbf{z}^*, \boldsymbol{\theta}), \quad \mathbf{z}^* \sim q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi});$$

- update $\boldsymbol{\theta}, \boldsymbol{\phi}$ according to the selected optimization method (SGD, Adam, RMSProp):

$$\boldsymbol{\phi} := \boldsymbol{\phi} + \eta \nabla_{\boldsymbol{\phi}} \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}),$$
$$\boldsymbol{\theta} := \boldsymbol{\theta} + \eta \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}).$$

Variational autoencoder (VAE)

- VAE learns stochastic mapping between $\mathbf{x}$-space, from complicated distribution $\pi(\mathbf{x})$, and a latent $\mathbf{z}$-space, with simple distribution.
- The generative model learns a joint distribution $p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) = p(\mathbf{z})p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$, with a prior distribution $p(\mathbf{z})$, and a stochastic decoder $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$.
- The stochastic encoder $q(\mathbf{z}|\mathbf{x}, \phi)$ (inference model), approximates the true but intractable posterior $p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})$ of the generative model.



Kingma D. P., Welling M. An introduction to variational autoencoders, 2019

Variational Autoencoder

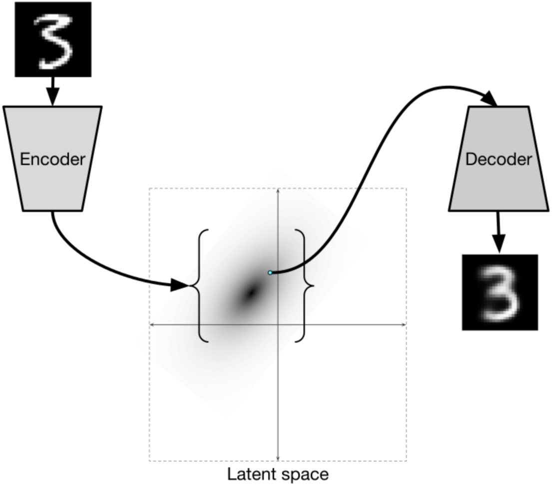


image credit: *http://ijdykeman.github.io/ml/2016/12/21/cvae.html*

Variational autoencoder (VAE)

- Encoder $q(\mathbf{z}|\mathbf{x}, \phi) = \mathrm{NN}_e(\mathbf{x}, \phi)$ outputs $\boldsymbol{\mu}_\phi(\mathbf{x})$ and $\boldsymbol{\sigma}_\phi(\mathbf{x})$.
- Decoder $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathrm{NN}_d(\mathbf{z}, \boldsymbol{\theta})$ outputs parameters of the sample distribution.

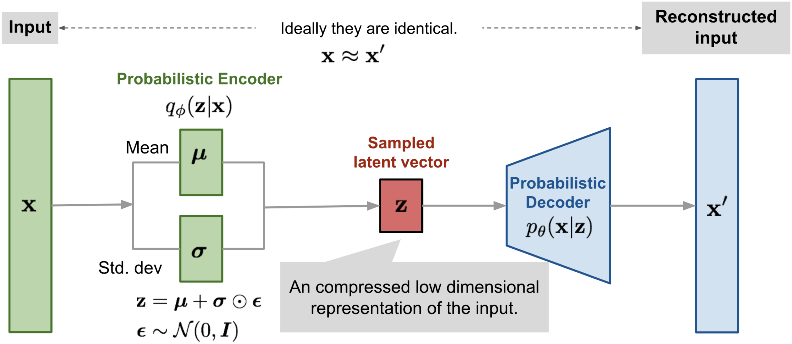


image credit: https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html

Bayesian framework

Posterior distribution

$$p(\boldsymbol{\theta}|\mathbf{X}) = \frac{p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathbf{X})} = \frac{p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{\int p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}}$$

Bayesian inference

$$p(\mathbf{x}|\mathbf{X}) = \int p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathbf{X})d\boldsymbol{\theta}$$

Maximum a posteriori (MAP) estimation

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} \log p(\boldsymbol{\theta}|\mathbf{X}) = \arg\max_{\boldsymbol{\theta}} \big(\log p(\mathbf{X}|\boldsymbol{\theta}) + \log p(\boldsymbol{\theta})\big)$$

MAP inference

$$p(\mathbf{x}|\mathbf{X}) = \int p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathbf{X})d\boldsymbol{\theta} = \int p(\mathbf{x}|\boldsymbol{\theta})\delta(\boldsymbol{\theta} - \boldsymbol{\theta}^*)d\boldsymbol{\theta} \approx p(\mathbf{x}|\boldsymbol{\theta}^*).$$

VAE as Bayesian model

Posterior distribution

$$p(\boldsymbol{\theta}|\mathbf{X}) = \frac{p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathbf{X})}$$

ELBO

$$\begin{aligned}\log p(\boldsymbol{\theta}|\mathbf{X}) &= \log p(\mathbf{X}|\boldsymbol{\theta}) + \log p(\boldsymbol{\theta}) - \log p(\mathbf{X}) \\ &= \mathcal{L}(q, \boldsymbol{\theta}) + KL(q||p) + \log p(\boldsymbol{\theta}) - \log p(\mathbf{X}) \\ &\geq [\mathcal{L}(q, \boldsymbol{\theta}) + \log p(\boldsymbol{\theta})] - \log p(\mathbf{X}).\end{aligned}$$

EM-algorithm

- E-step

$$q(\mathbf{z}) = \arg\max_q \mathcal{L}(q, \boldsymbol{\theta}^*) = \arg\min_q KL(q||p) = p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}^*);$$

- M-step

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} \left[\mathcal{L}(q, \boldsymbol{\theta}) + \log p(\boldsymbol{\theta})\right].$$

Summary

- LVM introduces latent representation of observed samples to make model more interpretable.
- LVM maximizes variational evidence lower bound (ELBO) to find MLE of model parameters.
- The general variational EM algorithm maximizes ELBO objective.
- Amortized inference allows to efficiently compute stochastic gradients for ELBO using Monte-Carlo estimation.
- The reparametrization trick gets unbiased gradients w.r.t to a variational posterior distribution.
- The VAE model is an LVM with two neural network: for stochastic encoder $q(\mathbf{z}|\mathbf{x}, \phi)$ and for stochastic decoder $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$.
- VAE is not a "true" bayesian model since parameters $\boldsymbol{\theta}$ do not have a prior distribution.