Lecture 4: Variational AutoEncoder

Deep Generative Models

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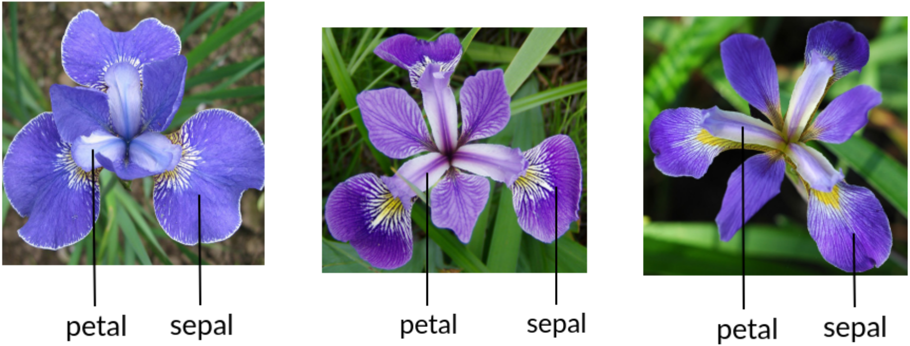
Contents

Section 1

Guassian Mixture Model

Example - Iris Flower



(a) Setosa (b) Versicolor (c) Virginica

Figure: Different types of Iris flower

Example - Iris Flower Data set

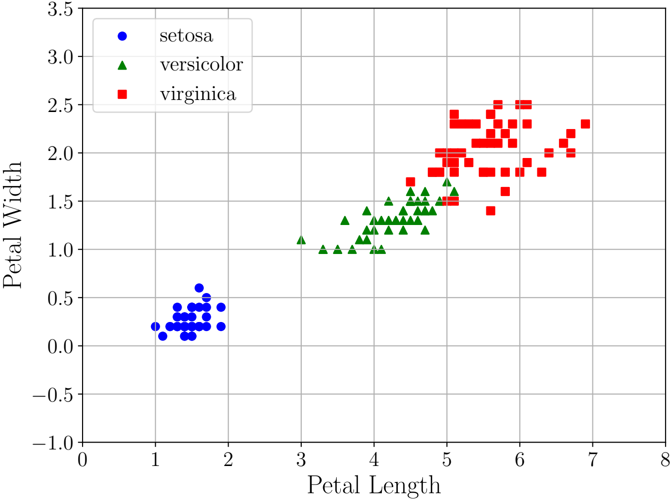


Figure: Labeled Iris dataset (in practive, you don't have the labels)

Example - Iris Flower Data set

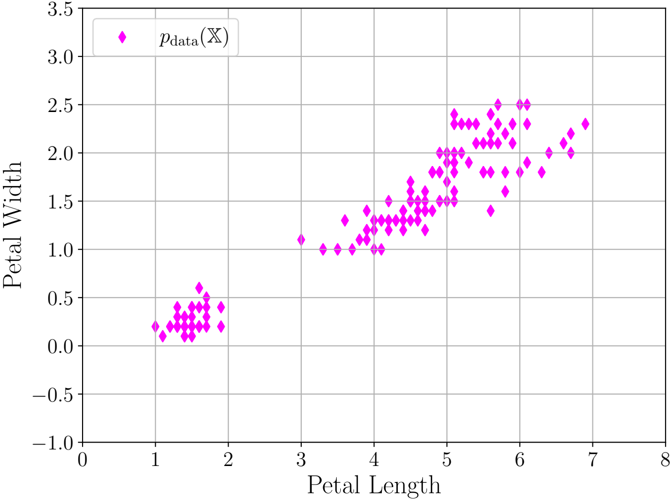


Figure: Iris dataset $\mathcal{D}$

Example - Iris Flower Data set

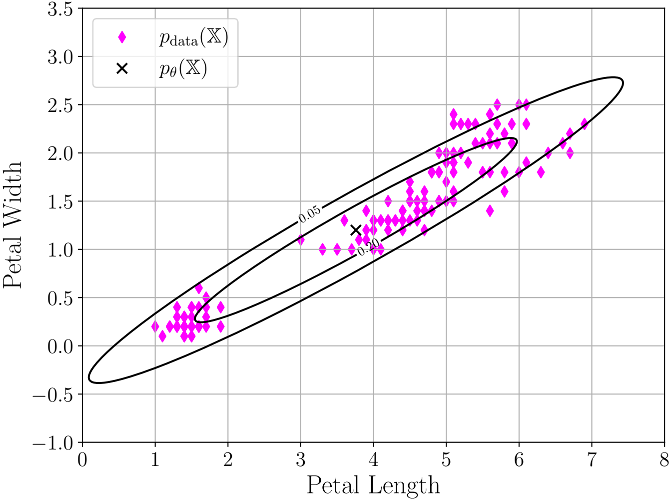


Figure: Modeling distribution using single Gaussian

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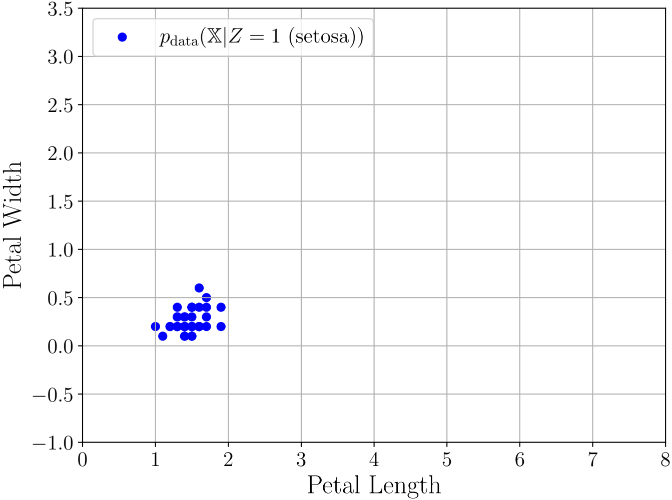

Figure: Data from $p_{\text{data}}(\mathbb{X}|Z = 1)$

Example - Iris Flower Data set

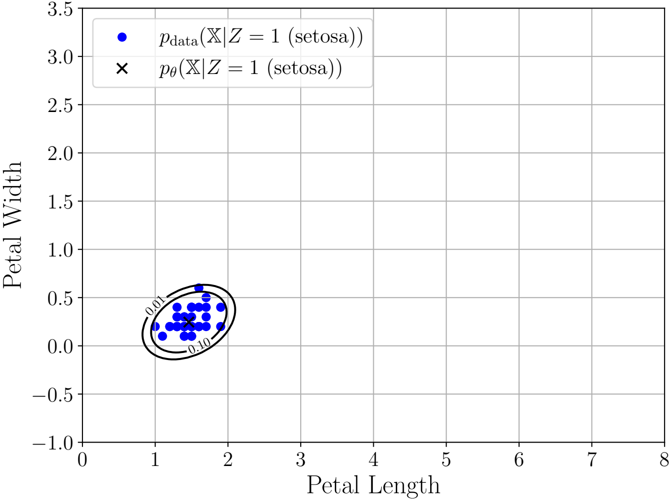

Figure: Modeling conditional distribution $p_{\text{data}}(\mathbb{X}|Z = 1)$ using signle Gaussian

Example - Iris Flower Data set

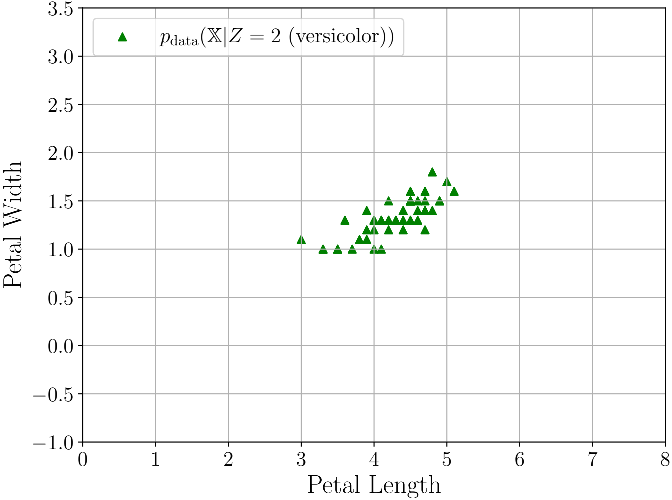

Figure: Data from $p_{\text{data}}(\mathbb{X}|Z = 2)$

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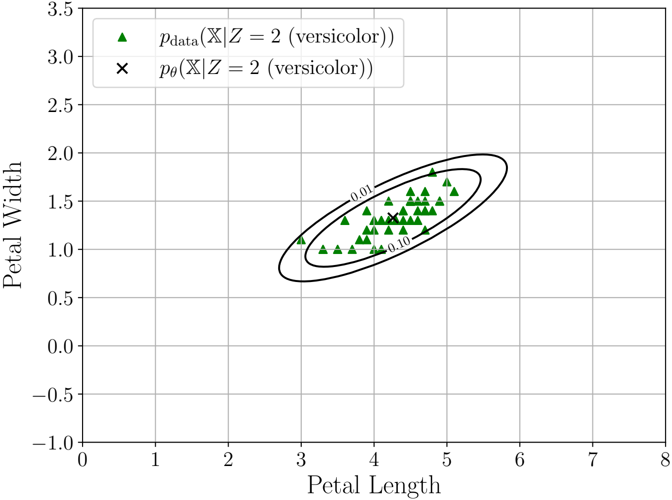

Figure: Modeling conditional distribution $p_{\text{data}}(\mathbb{X}|Z = 2)$ using signle Gaussian

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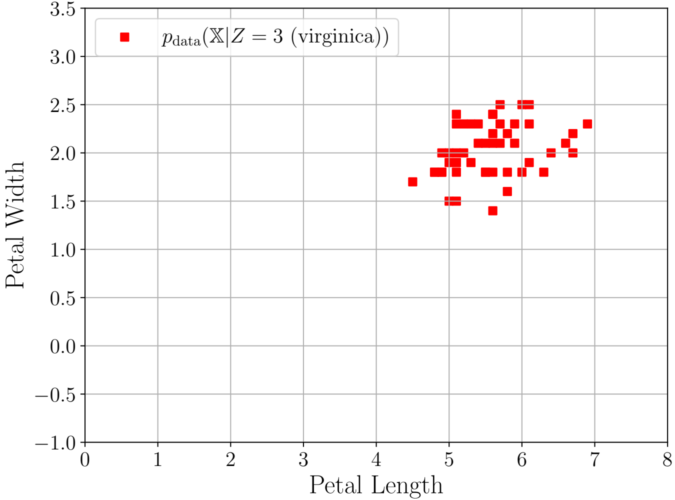

Figure: Data from $p_{\text{data}}(\mathbb{X}|Z3)$

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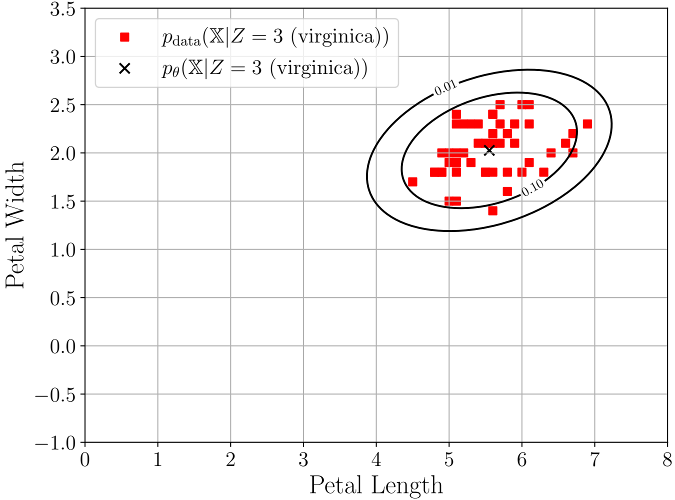

Figure: Modeling conditional distribution $p_{\text{data}}(\mathbb{X}|Z = 3)$ using signle Gaussian

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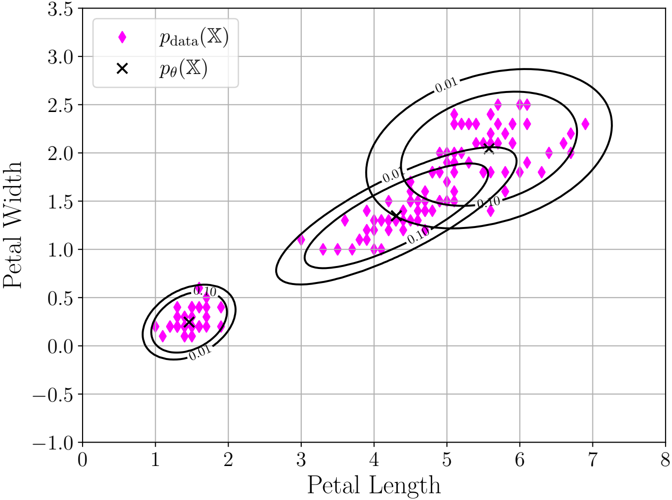

Figure: Modeling unconditional distribution using a Gaussian Mixture Model

Gaussian Mixture Model

Intuition

Intelligently combining simple distributions to create complex ones.

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GMM

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In the above process, the distribution over $\mathbb{X}$ is:

$$p(\mathbb{X}) = \sum_z p(\mathbb{X}, Z = z) = \sum_z p(\mathbb{X}|z)p(z) = \sum_z \pi_z \mathcal{N}(\mathbb{X}|\boldsymbol{\mu}_z, \boldsymbol{\Sigma}_z)$$

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while the Gaussian distribution is unimodal, the above distribution is multi-modal.

GMM

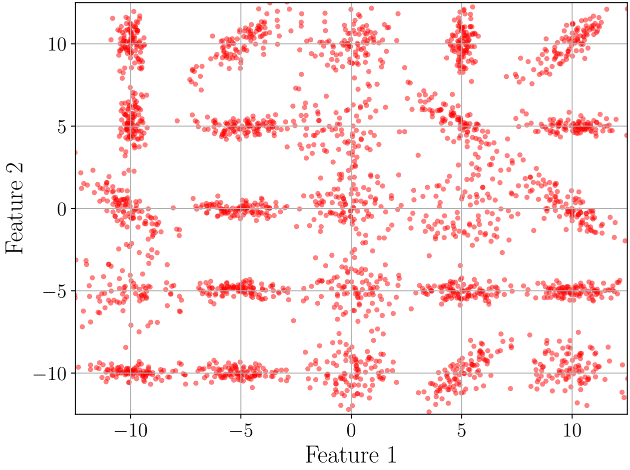

Figure: Synthesis dataset $\mathcal{D}$ samples

GMM

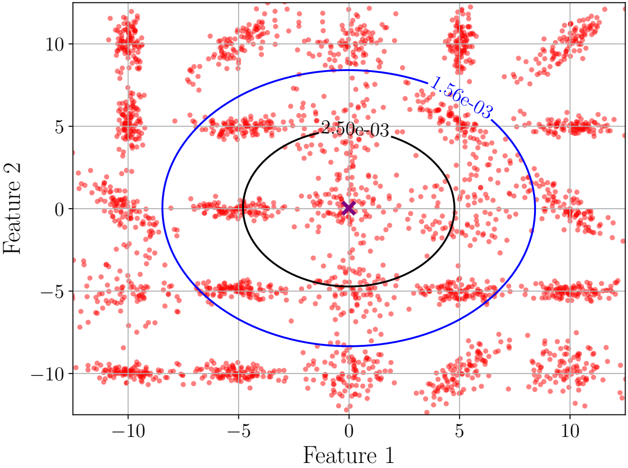

Figure: Gaussian distribution fitted to dataset $\mathcal{D}$ (the purple '×'symbol shows the mean location)

GMM

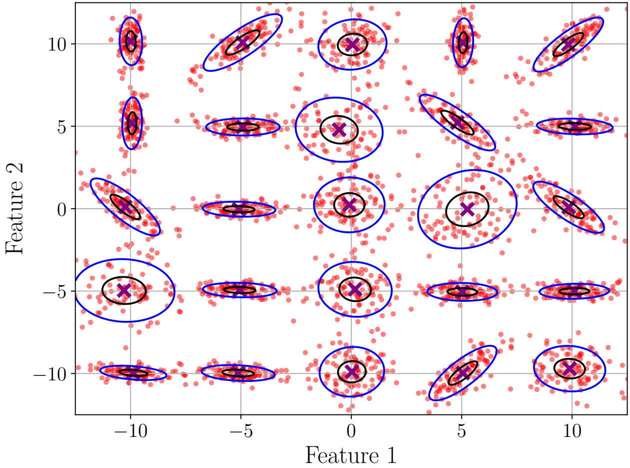

Figure: GMM distribution with four component fitted to dataset $\mathcal{D}$ with 25 components (the purple '$\times$'symbols shows each component mean location)

GMM

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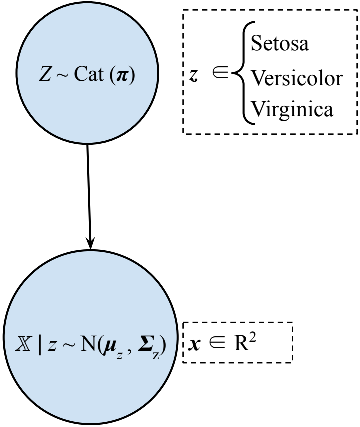
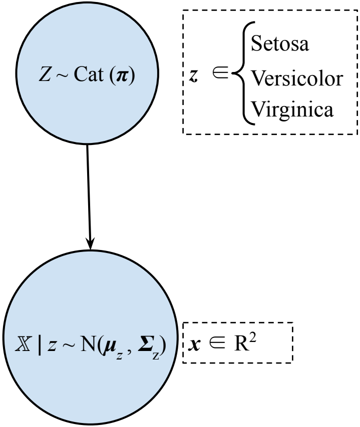
- Number of component

Extending GMM



(a) GMM Concept

Extending GMM



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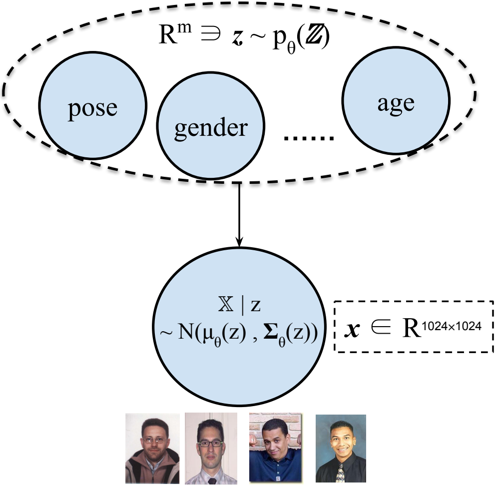

(b) VAE Concept (images sourse: [1])

Section 2

Model Specification

Sample Model

Model Specification

Assume we have the following simple distributions:

- Latent variable distribution:

$$p_\theta(\mathbb{Z}) = \mathcal{N}(\mathbb{Z}|\boldsymbol{\mu}_z, \sigma_z^2\boldsymbol{I}),\ \mathbb{Z} \in \mathbb{R}^m$$

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thus $\boldsymbol{\theta} = \{\boldsymbol{\mu}_z, \sigma_z^2, \boldsymbol{\alpha}, \boldsymbol{\beta}\}$.

Task 1: Generation

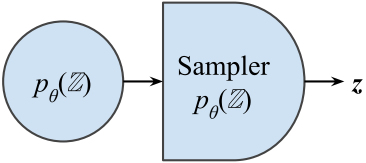

Figure: Sampling latent vector

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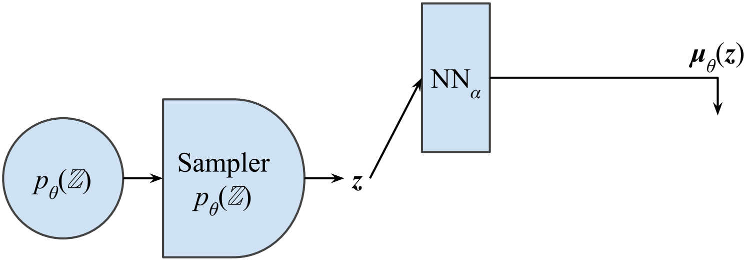

Figure: Calculating conditional distribution mean vector

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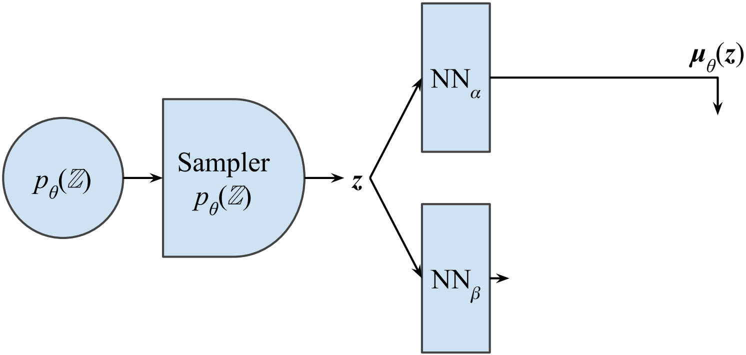

Figure: Calculating conditional distribution covariance matrix

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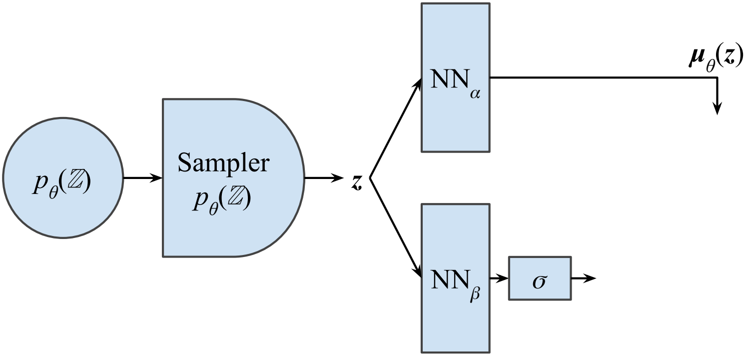

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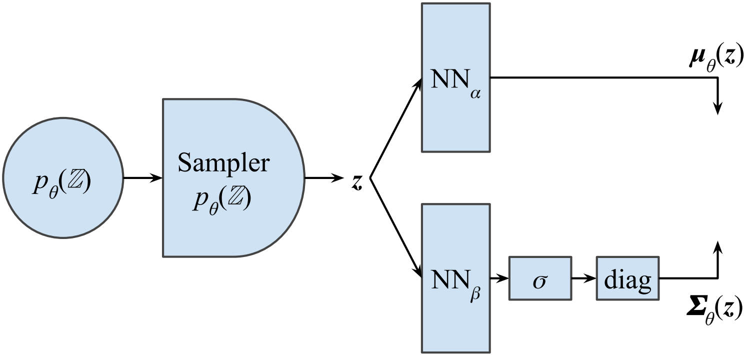

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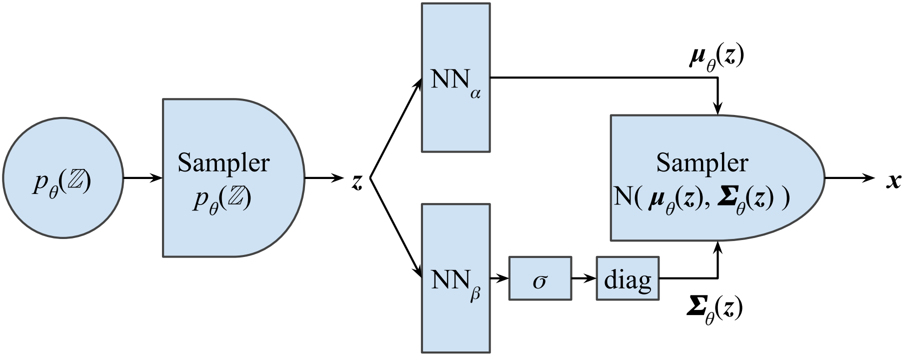

Figure: Sampling conditional distribution

Task 2: High-level Representation

High-level Representation

Remember the example of the Iris dataset. Accessing the latent random variable Z can reveal information about the type of flower. So Z can be considered as *High-level Representation*.

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Challenges

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- Estimating the parameters of conditional distribution $\mathcal{N}(\boldsymbol{\mu}_\theta(\boldsymbol{z}), \boldsymbol{\Sigma}_\theta(\boldsymbol{z}))$ with only one sample $\boldsymbol{x}$ has a high variance.

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- Assume you have access to both $\boldsymbol{\mu}_\theta(\boldsymbol{z})$ and $\boldsymbol{\Sigma}_\theta(\boldsymbol{z})$. Then calculating $\boldsymbol{z}$ is impossible because Deep Neural Networks are non-invertible.

Task 3: Density Estimation

Density Estimation

We have access to both $p_\theta(\mathbb{Z})$ and $p_\theta(\mathbb{X}|\mathbb{Z})$, thus:

$$p_\theta(\mathbb{X}, \mathbb{Z}) = p_\theta(\mathbb{X}|\mathbb{Z})p_\theta(\mathbb{Z})$$

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\end{aligned}$$

Challenge 1

Calculating the likelihood and thus training the model seems to be intractable.

Section 3

Casting Likelihood Calculation as Expectation

No Free Lunch: Challenges Start

Calculating the Likelihood for Sample $\boldsymbol{x}$

As we see before, we are interested in the following optimization:

$$\boldsymbol{\theta}^\star = \underset{\boldsymbol{\theta}}{\operatorname{argmin}} -\frac{1}{|\mathcal{D}|} \sum_{i=1}^{N} \log p_\theta(\boldsymbol{x}_i)$$

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$$p_\theta(\boldsymbol{x}) = \int_{\boldsymbol{z}} p_\theta(\boldsymbol{x}, \boldsymbol{z})\mathrm{d}\boldsymbol{z}$$

The above integral is hard to compute and in each update of the optimization problem, we want:

- Evaluate the integral as a function of $\boldsymbol{\theta}$
- Evaluate the gradient vector of the log-likelihood

Likelihood as Expectation

We can write the data likelihood as:

$$p_\theta(\boldsymbol{x}) = \int_{\boldsymbol{z}} p_\theta(\boldsymbol{x}, \boldsymbol{z}) \mathrm{d}\boldsymbol{z} = \int_{\boldsymbol{z}} p_\theta(\boldsymbol{z}) p_\theta(\boldsymbol{x}|\boldsymbol{z}) \mathrm{d}\boldsymbol{z} = \mathbb{E}_{\boldsymbol{z} \sim p_\theta(\mathbb{Z})} \left[p_\theta(\boldsymbol{x}|\boldsymbol{z}) \right]$$

Thus we have an expectation. How can we estimate it?

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Mante Carlo Extimate

We can estimate the expectation using the Monte Carlo estimate by k samples from the distribution as:

$$p_\theta(\boldsymbol{x}) \simeq \frac{1}{k}\sum_{i=1}^{k} p_\theta(\boldsymbol{x}|\boldsymbol{z}_i), \;\; \boldsymbol{z}_i \sim p_\theta(\mathbb{Z}) \text{ for } i = 1, \ldots, k$$

The above estimate, while unbiased, exhibits significant variance. Why?

High Variance Estimation - Toy Example

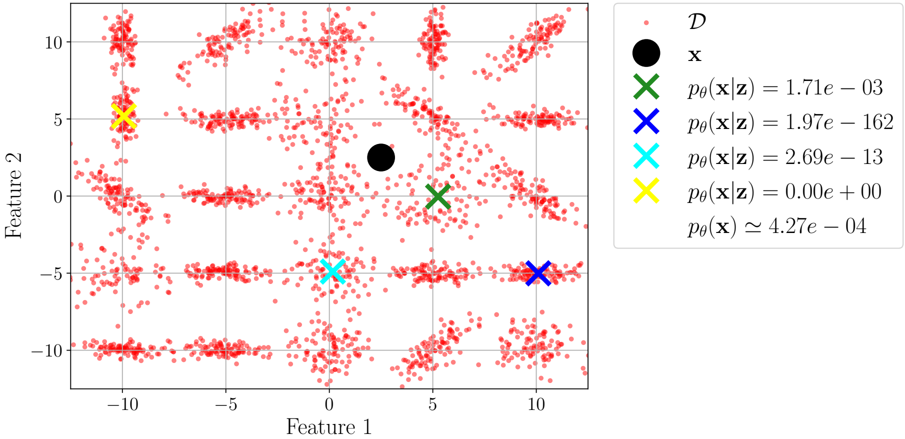

Figure: $[4.27 \times 10^{-4}]$

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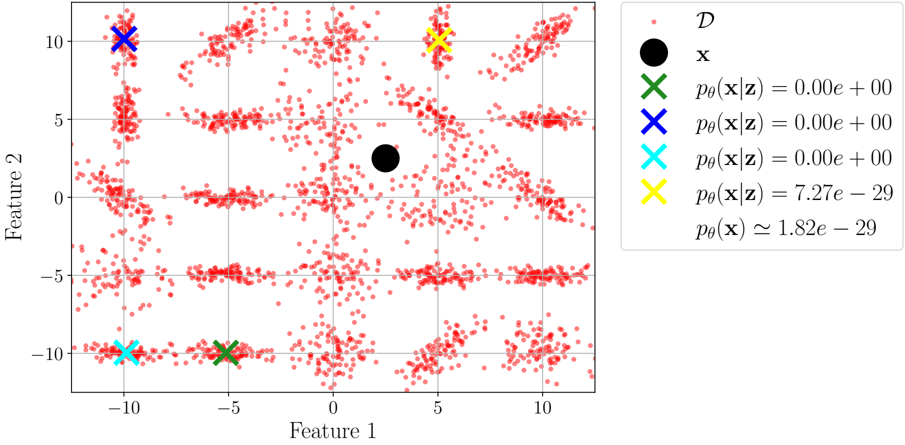

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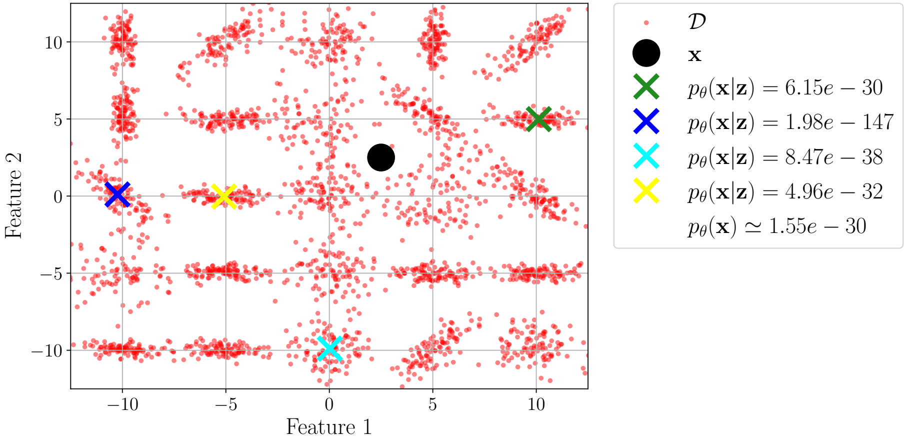

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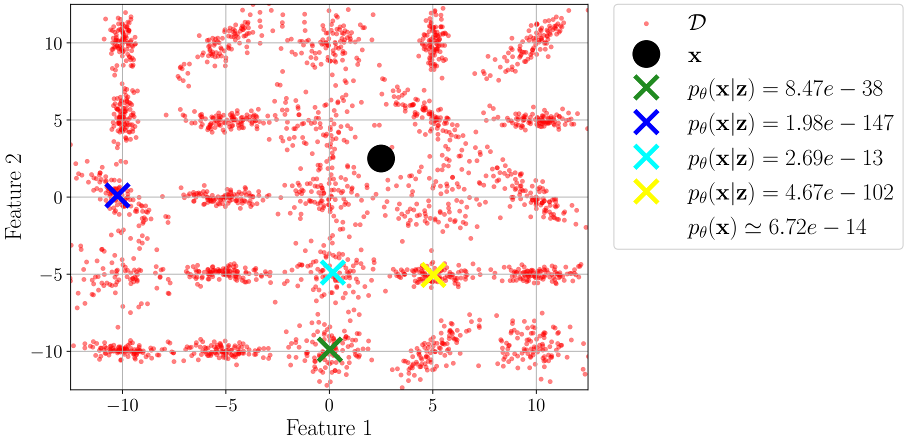

Figure: $[4.27 \times 10^{-4},\ 1.82 \times 10^{-29},\ 1.55 \times 10^{-30},\ 6.72 \times 10^{-14}]$

High Variance Estimate - Real World Example

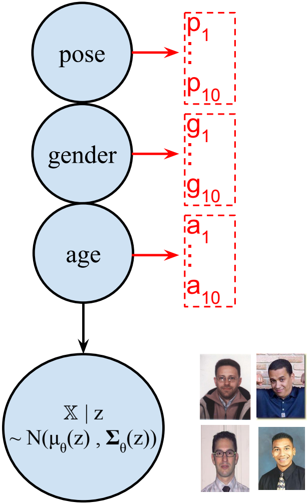

Figure: (images source: [1])

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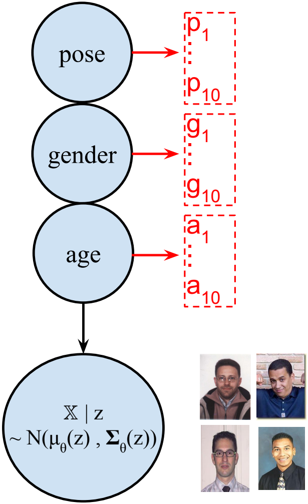

Figure: (images source: [1])

Scenario

As we can see $|\mathcal{Z}| = 10^3$. Assume we want to compute $p_\theta(\overline{\boldsymbol{x}})$, the true latent is $\overline{\boldsymbol{z}}$ and:

- $k = 10$
- $\mathcal{S}$ is the set of generated latent vectors

Then:

High Variance Estimate - Real World Example

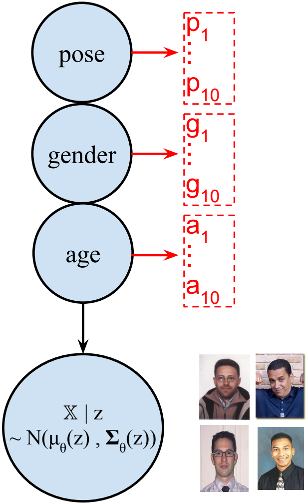

Figure: (images source: [1])

Scenario

As we can see $|\mathcal{Z}| = 10^3$. Assume we want to compute $p_\theta(\overline{\boldsymbol{x}})$, the true latent is $\overline{\boldsymbol{z}}$ and:

- $k = 10$
- $\mathcal{S}$ is the set of generated latent vectors

Then:

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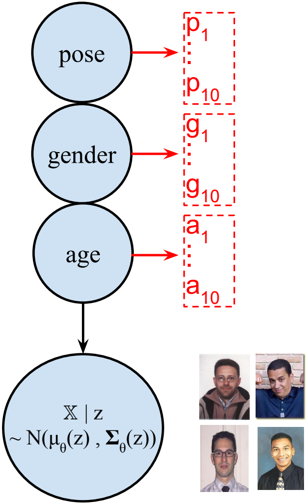

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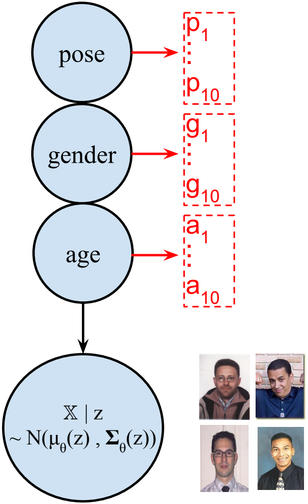

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while the estimation has a high variance and cannot be used in practice.

☞ So, what can we do?

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Section 4

Importance Sampling

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Challenge

What is a good option for $q(\mathbb{Z})$. Maybe we need optimization over q too!

Importance Sampling in Toy Example

Estimating Latent Posterior

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Let's use importance sampling technique to calculate $p_\theta(\boldsymbol{x})$ with $q(Z) = p_\theta(Z|\boldsymbol{x})$

GMM - Posterior

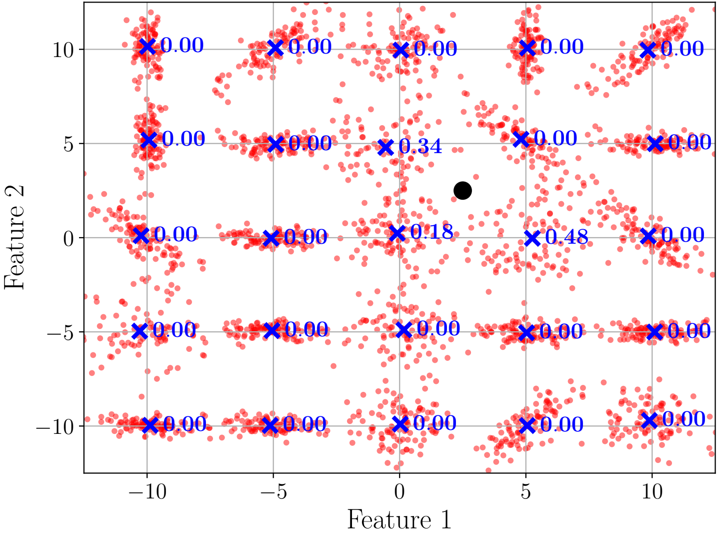

Figure: Posterior distribution $p(Z|\boldsymbol{x})$ (black circle represents $\boldsymbol{x}$)

High Variance Estimation - Toy Example

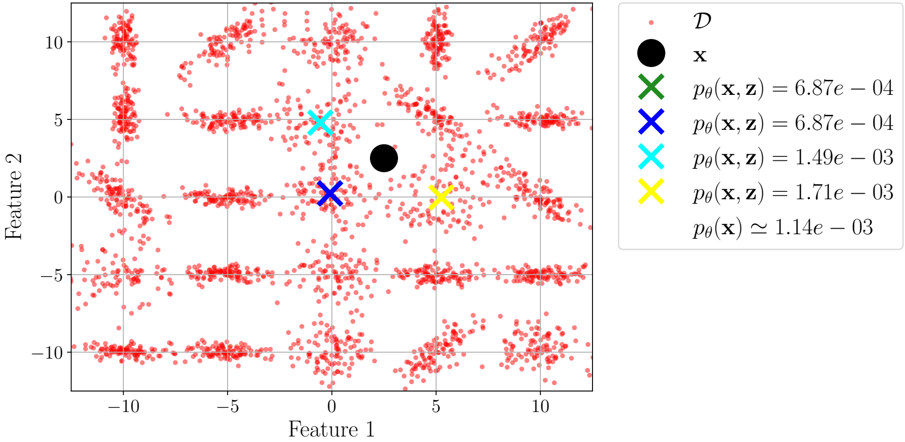

Figure: $[1.14 \times 10^{-3}]$

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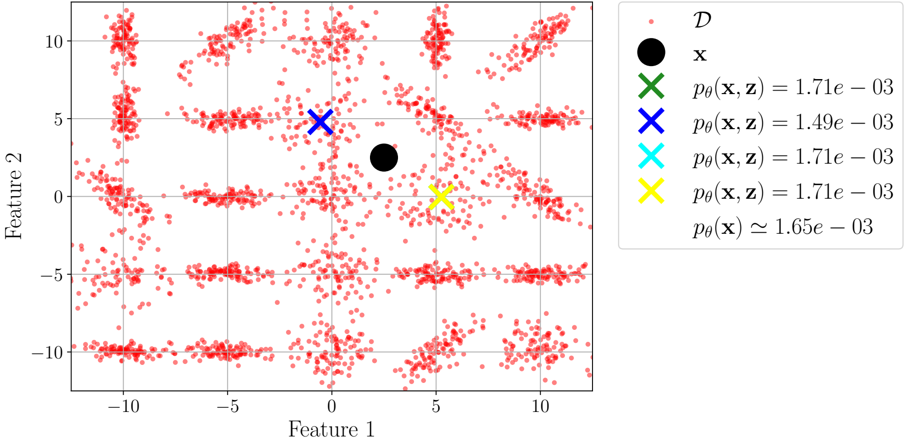

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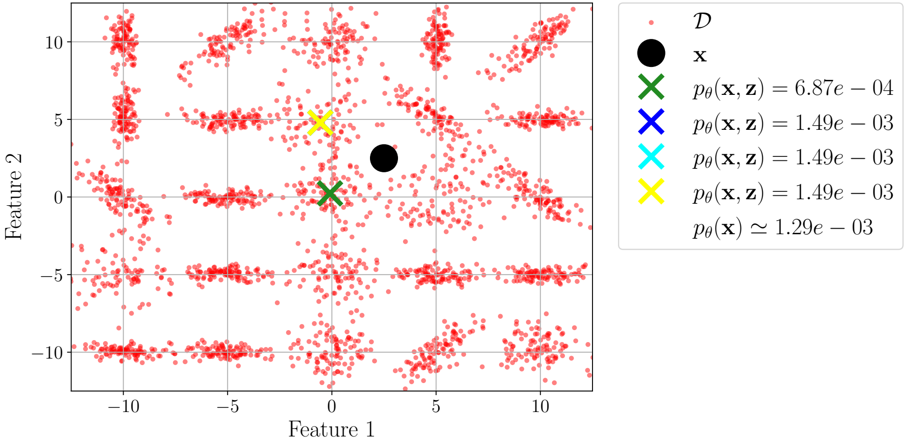

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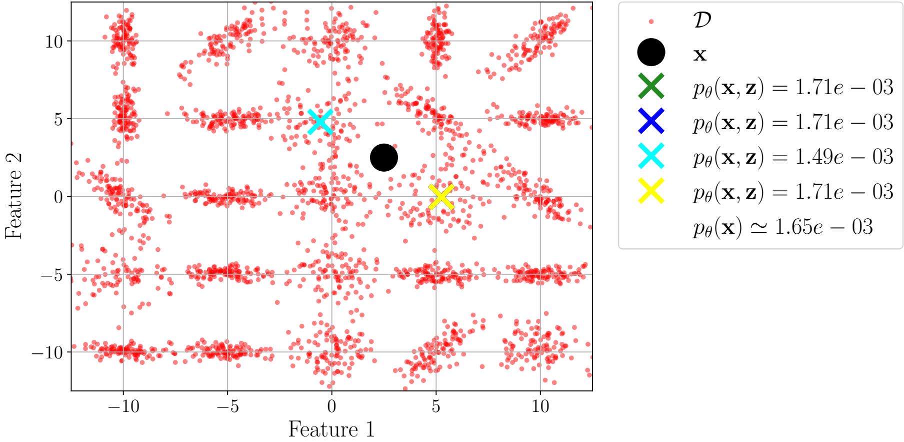

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Lowering Estimation Variance

Real-World Case

Although for the case of GMM latent variable posterior is tractable, in real-world application we have (assuming the latent prior is standard Gaussian):

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and we know that calculating $p_\theta(\boldsymbol{x})$ is challenging (indeed we are looking for it!). So you can't use $p_\theta(\mathbb{Z}|\boldsymbol{x})$ as $q(\mathbb{Z})$ in the importance sampling technique.

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Estimating the likelihood using prior distribution, while unbiased, represents high variance.

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Challenge 3

We have no formal derivation for the suitability of $p_\theta(\mathbb{Z}|\boldsymbol{x})$ to be used for importance sampling in the general real-world case (other than GMM). So we don't know how to select $q(\mathbb{Z})$

Section 5

Evidence Lower BOund

Working on Log Likelihood

Log Likelihood

In the previous section, we have seen that:

$$p_\theta(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{z}\sim q(\boldsymbol{z})}\left[\frac{p_\theta(\boldsymbol{x},\boldsymbol{z})}{q(\boldsymbol{z})}\right]$$

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For two important reasons (among others), we need to change the order of expectation and log on RHS.

Working on Log Likelihood

Reason 1: Disentangling Parameters

If we can change the order then on RHS we have:

$$\mathbb{E}_{\boldsymbol{z}\sim q(\mathbb{Z})}\left[\log \frac{p_\theta(\boldsymbol{x},\boldsymbol{z})}{q(\boldsymbol{z})}\right] = \mathbb{E}_{\boldsymbol{z}\sim q(\mathbb{Z})}\left[\log p_\theta(\boldsymbol{x},\boldsymbol{z})\right] - \mathbb{E}_{\boldsymbol{z}\sim q(\mathbb{Z})}\left[\log q(\boldsymbol{z})\right]$$

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- The optimization over model parameters $\boldsymbol{\theta}$ is done using the first term.
- The prospective optimization over q functions should still be done using both terms.

Working on Log Likelihood

Reason 2: Two Separate Learning Signals

For the log-likelihood, we have:

$$\log p_\theta(\boldsymbol{x}) = \log \mathbb{E}_{\boldsymbol{z}\sim q(\boldsymbol{z})}\left[\frac{p_\theta(\boldsymbol{x},\boldsymbol{z})}{q(\boldsymbol{z})}\right] \simeq \log\left[\frac{1}{k}\sum_k\left[\frac{p_\theta(\boldsymbol{x},\boldsymbol{z}_i)}{q(\boldsymbol{z}_i)}\right]\right],\ \ \boldsymbol{z}_i \sim q(\mathbb{Z})$$

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Because we are estimating the expectations with MCE, then in the second case, the learning signal from each of the terms is separated leading to a better approximation.

Working on Log Likelihood

Challenge

The challenge is to relate the following terms:

$$\text{We have} \Rightarrow \log \mathbb{E}_{\boldsymbol{z}\sim q(\boldsymbol{z})}\left[\frac{p_\theta(\boldsymbol{x},\boldsymbol{z})}{q(\boldsymbol{z})}\right] \boxed{\begin{matrix}\leq \\ = \\ \geq\end{matrix}} \mathbb{E}_{\boldsymbol{z}\sim q(\mathbb{Z})}\left[\log \frac{p_\theta(\boldsymbol{x},\boldsymbol{z})}{q(\boldsymbol{z})}\right] \Leftarrow \text{We want}$$

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Jensen's Inequality

Assume random vector $\mathbb{X}$ and concave function $\psi(\cdot)$. Then:

$$\psi\left(\mathbb{E}[\mathbb{X}]\right) \geq \mathbb{E}\left[\psi(X)\right]$$

Evidence Lower BOund (ELBO)

The Log function is concave. So using Jensen's inequality, we have:

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So by changing the order of log function and expectation, we get a lower bound for the log-likelihood known as *Evidence Lower BOund* or abbreviately ELBO.

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So by changing the order of log function and expectation, we get a lower bound for the log-likelihood known as *Evidence Lower BOund* or abbreviately ELBO.

Notation

ELBO is defined for one sample $\boldsymbol{x}$, while the model parameters $\boldsymbol{\theta}$ and q distributions can be changed. Thus we use the following notation:

$$\mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},q) = \mathbb{E}_{\boldsymbol{z}\sim q(\mathbb{Z})}\left[\log\left(\frac{p_\theta(\boldsymbol{x},\boldsymbol{z})}{q(\boldsymbol{z})}\right)\right]$$

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We can work on ELBO as:

$$\log p_\theta(\boldsymbol{x}) \geq \mathrm{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, q)$$

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\log p_\theta(\boldsymbol{x}) \geq & \operatorname{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, q) \\
= & \mathbb{E}_{\boldsymbol{z} \sim q(\mathbb{Z})} \left[\log \left(\frac{p_\theta(\boldsymbol{x}, \boldsymbol{z})}{q(\boldsymbol{z})} \right) \right] \\
= & \mathbb{E}_{\boldsymbol{z} \sim q(\mathbb{Z})} \left[\log p_\theta(\boldsymbol{x}, \boldsymbol{z}) \right] - \mathbb{E}_{\boldsymbol{z} \sim q(\mathbb{Z})} \left[\log q(\boldsymbol{z}) \right] \\
= & \mathbb{E}_{\boldsymbol{z} \sim q(\mathbb{Z})} \left[\log p_\theta(\boldsymbol{x}, \boldsymbol{z}) \right] + \mathbb{H}(q)
\end{aligned}$$

ELBO

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$$

where $\mathbb{H}(q)$, called *distribution entropy*, is a well-known quantity in information theory.

ELBO Instead of Data Log-likelihood

Replacing Data Log-likelihood with ELBO

To train a model, we need to solve the following optimization:

$$\boldsymbol{\theta}^\star = \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \log p_\theta(\boldsymbol{x})$$

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$$\boldsymbol{\theta}^{\star} = \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \, \mathrm{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, q)$$

Tightness Matters

As we are replacing $\log p_{\theta}(\boldsymbol{x})$ with $\mathrm{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, q)$, the tightness of the lower bound becomes important.

ELBO Tightness

Reframing ELBO

Based on KL divergence, we have:

$$\mathrm{KL}(q(\mathbb{Z}) \| p_\theta(\mathbb{Z}|\boldsymbol{x})) = \int_{\boldsymbol{z}} q(\boldsymbol{z}) \log \frac{q(\boldsymbol{z})}{p_\theta(\boldsymbol{z}|\boldsymbol{x})} \mathrm{d}\boldsymbol{z}$$

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ELBO Tightness

Tightest ELBO

So we have the following interesting equality:

$$\mathrm{KL}(q(\mathbb{Z}) \| p_\theta(\mathbb{Z}|\boldsymbol{x})) = \log p_\theta(\boldsymbol{x}) - \mathrm{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, q)$$

Thus the gap is $\mathrm{KL}(q(\mathbb{Z}) \| p_\theta(\mathbb{Z}|\boldsymbol{x}))$.

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So for $q(\mathbb{Z}) = p_\theta(\mathbb{Z}|\boldsymbol{x})$, we have:

$$\mathrm{KL}(q(\mathbb{Z})\|p_\theta(\mathbb{Z}|\boldsymbol{x})) = 0 \Rightarrow \log p_\theta(\boldsymbol{x}) = \mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},q)$$

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Consequently, we have found the $q(\mathbb{Z})$ distribution resulting in the tightest ELBO.

Update on our Challenges

Challenge 3

We have no formal derivation for the suitability of $p_\theta(\mathbb{Z}|\boldsymbol{x})$ to be used for importance sampling in the general real-world case (other than GMM). So we don't know how to select $q(\mathbb{Z})$

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Challenge 4

Calculating $p_\theta(\mathbb{Z}|\boldsymbol{x})$ needs the data likelihood which is intractable as we observe in Slide 28. On the other hand, we need to decrease $\mathrm{KL}(q(\mathbb{Z})\|p_\theta(\mathbb{Z}|\boldsymbol{x}))$ to tighten the ELBO.

Section 6

ELBO Tightening

ELBO Tightening

Parameterizing q

To have control over distribution $q(\mathbb{Z})$, we should parameterize this distribution. An example can be:

- $q_\lambda(\mathbb{Z}) = \mathcal{N}(\mathbb{Z}|\boldsymbol{\mu}, \sigma^2\boldsymbol{I})$ and $\boldsymbol{\lambda} = \{\boldsymbol{\mu}, \sigma^2\}$

ELBO Tightening

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Note that we are currently focused on the likelihood of one sample point $\boldsymbol{x}$ and thus $\boldsymbol{\lambda}$ is the parameter of the distribution corresponding to $\boldsymbol{x}$.

ELBO Tightening

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Notation Update

By parameterizing q, instead of $\text{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, q)$ we use:

$$\text{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, \boldsymbol{\lambda}) = \mathbb{E}_{\boldsymbol{z} \sim q_\lambda(\mathbb{Z})} \left[\log \left(\frac{p_\theta(\boldsymbol{x}, \boldsymbol{z})}{q_\lambda(\boldsymbol{z})} \right) \right]$$

ELBO Tightening

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And again pay attention that everything is just about one data point $\boldsymbol{x}$.

ELBO Tightening

Optimization Problem

For ELBO tightening in a model with parameter $\boldsymbol{\theta}$, we need to solve the following optimization problem:

$$\boldsymbol{\lambda}^\star(\boldsymbol{\theta}) = \underset{\boldsymbol{\lambda}}{\operatorname{argmin}} \, \mathrm{KL}(q_\lambda(\mathbb{Z}) \,\|\, p_\theta(\mathbb{Z}|\boldsymbol{x}))$$

But pay attention to the following note:

ELBO Tightening

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But pay attention to the following note:

- If you can find $\boldsymbol{\lambda}^{\star}(\boldsymbol{\theta})$, then it is a function of $\boldsymbol{\theta}$. Thus by changing the model parameter $\boldsymbol{\theta}$, $\boldsymbol{\lambda}^{\star}$ is not optimum anymore and you should update it.

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Challenge 4

Solving the above optimization seems intractable as calculating $p_{\theta}(\mathbb{Z}|\boldsymbol{x})$ is intractable in general.

ELBO Tightening

Intuition

Pay attention to the following equality:

$$\log p_\theta(\boldsymbol{x}) = \text{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, \boldsymbol{\lambda}) + \text{KL}(q_\lambda(\mathbb{Z}) \| p_\theta(\mathbb{Z}|\boldsymbol{x}))$$

Two important points:

ELBO Tightening

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- LHS is independent of $\boldsymbol{\lambda}$.

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Two important points:

- LHS is independent of $\boldsymbol{\lambda}$.
- Both terms on the RHS are functions of $\boldsymbol{\lambda}$.

☞ How can we decrese the KL divergence between $q_\lambda(\mathbb{Z})$ and $p_\theta(\mathbb{Z}|\boldsymbol{x})$?

ELBO Tightening

Tightening Solution

We know:

$$\log p_\theta(\boldsymbol{x}) = \mathrm{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, \boldsymbol{\lambda}) + \mathrm{KL}(q_\lambda(\mathbb{Z}) \| p_\theta(\mathbb{Z}|\boldsymbol{x}))$$

Thus:

ELBO Tightening

Tightening Solution

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Thus:

$$\text{Because } \log p_\theta(\boldsymbol{x}) \text{ is independent of } \boldsymbol{\lambda} \Rightarrow \begin{cases} \text{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, \boldsymbol{\lambda}) \ \uparrow \\ \\ \text{KL}(q_\lambda(\mathbb{Z}) \| p_\theta(\mathbb{Z}|\boldsymbol{x})) \ \downarrow \end{cases}$$

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In other words for a fixed model $\boldsymbol{\theta}$:

$$\underset{\boldsymbol{\lambda}}{\operatorname{argmax}} \ \mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\lambda}) \equiv \underset{\boldsymbol{\lambda}}{\operatorname{argmin}} \ \mathrm{KL}(q_\lambda(\mathbb{Z}) \| p_\theta(\mathbb{Z}|\boldsymbol{x}))$$

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Thus we can tighten the ELBO by maximizing it with respect to $\boldsymbol{\lambda}$.

ELBO Tightening

ELBO Tightening

Assume the case of simple GMM with two components as:

$$p_\theta(\boldsymbol{x}) = \sum_{z\in\{0,1\}} p_\theta(Z=z)p_\theta(\boldsymbol{x}|Z=z), \quad \begin{cases} p_\theta(Z=z) = \pi_Z \\ p_\theta(\boldsymbol{x}|Z=z) = \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_z, \boldsymbol{\Sigma}_z) \end{cases}$$

So the model parameters are $\boldsymbol{\theta} = \{\pi_0, \pi_1 . \boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0, \mu_1, \boldsymbol{\Sigma}_1\}$ and given.

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So the model parameters are $\boldsymbol{\theta} = \{\pi_0, \pi_1.\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0, \mu_1, \boldsymbol{\Sigma}_1\}$ and given.
In this example, we want to show the following problems are equivalent:

$$\underset{\lambda}{\operatorname{argmax}} \;\; \text{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, \lambda) \equiv \underset{\lambda}{\operatorname{argmin}} \;\; \text{KL}(q_\lambda(Z) \| p_\theta(Z|\boldsymbol{x}))$$

We will follow by solving each optimization problem separately.

ELBO Tightening

RHS Optimization

We are interested in the following optimization:

$$\underset{\lambda}{\operatorname{argmin}} \;\; \mathrm{KL}(q_\lambda(Z) \| p_\theta(Z|\boldsymbol{x}))$$

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- Because Z is binary thus:
    - $q_\lambda(Z) = \mathrm{Ber}(Z|\lambda)$

ELBO Tightening

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- Because Z is binary thus:
  - $q_\lambda(Z) = \mathrm{Ber}(Z|\lambda)$
  - $p_\theta(Z|\boldsymbol{x}) = \mathrm{Ber}(Z|\beta(\boldsymbol{\theta}))$ (we write $\beta(\boldsymbol{\theta})$ to emphasize that $p_\theta(Z|\boldsymbol{x})$ has no new parameter and its parameter is a function of $\boldsymbol{\theta}$)

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- The optimum λ based on RHS is:

$$\lambda^\star = \beta(\boldsymbol{\theta})$$

ELBO Tightening

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$$\lambda^\star = \beta(\boldsymbol{\theta})$$

So we need to find $\beta(\boldsymbol{\theta}) = p_\theta(Z = 1|\boldsymbol{x})$

ELBO Tightening

RHS Optimization

$$\beta(\boldsymbol{\theta}) = p_\theta(Z = 1|\boldsymbol{x})$$

ELBO Tightening

RHS Optimization

$$\beta(\boldsymbol{\theta}) = p_\theta(Z = 1|\boldsymbol{x})$$

$$= \frac{p_\theta(\boldsymbol{x}, Z = 1)}{p_\theta(\boldsymbol{x})} \qquad \text{\#Bayes Rule}$$

ELBO Tightening

RHS Optimization

$$\beta(\boldsymbol{\theta}) = p_\theta(Z = 1|\boldsymbol{x})$$

$$= \frac{p_\theta(\boldsymbol{x}, Z = 1)}{p_\theta(\boldsymbol{x})} \quad \text{\#Bayes Rule}$$

$$= \frac{p_\theta(\boldsymbol{x}, Z = 1)}{\sum_{z \in \{0,1\}} p_\theta(\boldsymbol{x}, Z = z)} \quad \text{\#Marginalization}$$

RHS Optimization

$$
\begin{aligned}
\beta(\boldsymbol{\theta}) &= p_\theta(Z=1|\boldsymbol{x}) \\
&= \frac{p_\theta(\boldsymbol{x}, Z=1)}{p_\theta(\boldsymbol{x})} && \text{\#Bayes Rule} \\
&= \frac{p_\theta(\boldsymbol{x}, Z=1)}{\sum_{z\in\{0,1\}} p_\theta(\boldsymbol{x}, Z=z)} && \text{\#Marginalization} \\
&= \frac{p_\theta(\boldsymbol{x}|Z=1)p_\theta(Z=1)}{\sum_{z\in\{0,1\}} p_\theta(\boldsymbol{x}|Z=z)p_\theta(Z=z)} && \text{\#Conditioning}
\end{aligned}
$$

ELBO Tightening

RHS Optimization

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$$= \frac{p_\theta(\boldsymbol{x}, Z = 1)}{p_\theta(\boldsymbol{x})} \qquad \text{\#Bayes Rule}$$

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$$= \frac{p_\theta(\boldsymbol{x}|Z = 1)p_\theta(Z = 1)}{\sum_{z\in\{0,1\}} p_\theta(\boldsymbol{x}|Z = z)p_\theta(Z = z)} \qquad \text{\#Conditioning}$$

$$= \frac{\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)\pi_1}{\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)\pi_0 + \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)\pi_1} = \lambda^\star$$

ELBO Tightening

RHS Optimization

Assume the model parameters are:

$$\boldsymbol{\theta} = \left\{ \begin{array}{lll} \pi_1 = 0.33 & \mu_1 = \begin{bmatrix} 4.04 \\ 3.83 \end{bmatrix} & \boldsymbol{\Sigma}_1 = \begin{bmatrix} 1.79 & -0.10 \\ -0.10 & 2.00 \end{bmatrix} \\ & & \\ \pi_0 = 0.67 & \mu_0 = \begin{bmatrix} 1.10 \\ 0.86 \end{bmatrix} & \boldsymbol{\Sigma}_0 = \begin{bmatrix} 1.20 & -0.97 \\ -0.97 & 1.15 \end{bmatrix} \end{array} \right\} \lambda^\star = \beta(\boldsymbol{\theta}) = 0.76$$

ELBO Tightening

RHS Optimization

Assume the model parameters are:

$$\boldsymbol{\theta} = \left\{ \begin{array}{ll} \pi_1 = 0.33 \quad \mu_1 = \begin{bmatrix} 4.04 \\ 3.83 \end{bmatrix} \boldsymbol{\Sigma}_1 = \begin{bmatrix} 1.79 & -0.10 \\ -0.10 & 2.00 \end{bmatrix} \\ \\ \pi_0 = 0.67 \quad \mu_0 = \begin{bmatrix} 1.10 \\ 0.86 \end{bmatrix} \boldsymbol{\Sigma}_0 = \begin{bmatrix} 1.20 & -0.97 \\ -0.97 & 1.15 \end{bmatrix} \end{array} \right\} \lambda^\star = \beta(\boldsymbol{\theta}) = 0.76$$

then using the equation in Slide 48 we have:

ELBO Tightening

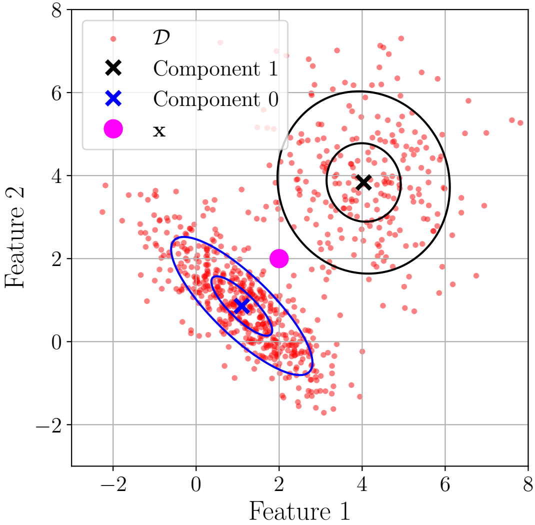

Figure: Dataset, GMM components and query point $\boldsymbol{x}$

ELBO Tightening

LHS Optimization

Assume distribution $q_\lambda(Z) = \mathrm{Ber}(Z|\lambda)$, then:

$$\mathrm{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, \lambda) = \mathbb{E}_{z \sim q_\lambda(Z)} \log \left[\frac{p_\theta(\boldsymbol{x}, z)}{q_\lambda(z)} \right]$$

ELBO Tightening

LHS Optimization

Assume distribution $q_\lambda(Z) = \mathrm{Ber}(Z|\lambda)$, then:

$$\begin{aligned}
\mathrm{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, \lambda) =& \mathbb{E}_{z \sim q_\lambda(Z)} \log \left[\frac{p_\theta(\boldsymbol{x}, z)}{q_\lambda(z)} \right] \\
=& q_\lambda(1) \log \left[\frac{p_\theta(\boldsymbol{x}, 1)}{q_\lambda(1)} \right] + q_\lambda(0) \log \left[\frac{p_\theta(\boldsymbol{x}, 0)}{q_\lambda(0)} \right]
\end{aligned}$$

ELBO Tightening

LHS Optimization

Assume distribution $q_\lambda(Z) = \text{Ber}(Z|\lambda)$, then:

$$
\begin{aligned}
\text{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\lambda) =& \mathbb{E}_{z\sim q_\lambda(Z)} \log\left[\frac{p_\theta(\boldsymbol{x},z)}{q_\lambda(z)}\right] \\
=& q_\lambda(1)\log\left[\frac{p_\theta(\boldsymbol{x},1)}{q_\lambda(1)}\right] + q_\lambda(0)\log\left[\frac{p_\theta(\boldsymbol{x},0)}{q_\lambda(0)}\right] \\
=& \lambda\log\left[\frac{\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_1,\boldsymbol{\Sigma}_1)\pi_1}{\lambda}\right] + (1-\lambda)\log\left[\frac{\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_0,\boldsymbol{\Sigma}_0)\pi_0}{1-\lambda}\right]
\end{aligned}
$$

ELBO Tightening

LHS Optimization

Assume distribution $q_\lambda(Z) = \text{Ber}(Z|\lambda)$, then:

$$\begin{aligned}
\text{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, \lambda) =& \mathbb{E}_{z\sim q_\lambda(Z)} \log \left[\frac{p_\theta(\boldsymbol{x}, z)}{q_\lambda(z)}\right] \\
=& q_\lambda(1) \log \left[\frac{p_\theta(\boldsymbol{x}, 1)}{q_\lambda(1)}\right] + q_\lambda(0) \log \left[\frac{p_\theta(\boldsymbol{x}, 0)}{q_\lambda(0)}\right] \\
=& \lambda \log \left[\frac{\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)\pi_1}{\lambda}\right] + (1-\lambda) \log \left[\frac{\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)\pi_0}{1-\lambda}\right]
\end{aligned}$$

Assuming fixed model parameter $\boldsymbol{\theta}$, we can plot $\text{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, \lambda)$ as a function of λ.

ELBO Tightening

LHS Optimization

We know $p_\theta(Z|\boldsymbol{x}) = \mathrm{Ber}(Z|0.76)$ and $q_\lambda(Z) = \mathrm{Ber}(Z|\lambda)$, so:

ELBO Tightening

LHS Optimization

We know $p_\theta(Z|\boldsymbol{x}) = \mathrm{Ber}(Z|0.76)$ and $q_\lambda(Z) = \mathrm{Ber}(Z|\lambda)$, so:

$$\mathrm{KL}(q_\lambda(Z) \| p_\theta(Z|\boldsymbol{x})) = \mathbb{E}_{z\sim q_\lambda(Z)} \log \frac{q_\lambda(z)}{p_\theta(z|\boldsymbol{x})}$$

ELBO Tightening

LHS Optimization

We know $p_\theta(Z|\boldsymbol{x}) = \mathrm{Ber}(Z|0.76)$ and $q_\lambda(Z) = \mathrm{Ber}(Z|\lambda)$, so:

$$\begin{aligned}\mathrm{KL}(q_\lambda(Z)\|p_\theta(Z|\boldsymbol{x})) =& \mathbb{E}_{z\sim q_\lambda(Z)} \log \frac{q_\lambda(z)}{p_\theta(z|\boldsymbol{x})} \\ =& q_\lambda(1)\log\frac{q_\lambda(1)}{p_\theta(1|\boldsymbol{x})} + q_\lambda(0)\log\frac{q_\lambda(0)}{p_\theta(0|\boldsymbol{x})}\end{aligned}$$

ELBO Tightening

LHS Optimization

We know $p_\theta(Z|\boldsymbol{x}) = \text{Ber}(Z|0.76)$ and $q_\lambda(Z) = \text{Ber}(Z|\lambda)$, so:

$$\begin{aligned}
\text{KL}(q_\lambda(Z)\|p_\theta(Z|\boldsymbol{x})) =& \mathbb{E}_{z\sim q_\lambda(Z)} \log \frac{q_\lambda(z)}{p_\theta(z|\boldsymbol{x})} \\
=& q_\lambda(1) \log \frac{q_\lambda(1)}{p_\theta(1|\boldsymbol{x})} + q_\lambda(0) \log \frac{q_\lambda(0)}{p_\theta(0|\boldsymbol{x})} \\
=& \lambda \log \frac{\lambda}{0.76} + (1-\lambda) \log \frac{1-\lambda}{(1-0.76)}
\end{aligned}$$

ELBO Tightening

LHS Optimization

We know $p_\theta(Z|\boldsymbol{x}) = \text{Ber}(Z|0.76)$ and $q_\lambda(Z) = \text{Ber}(Z|\lambda)$, so:

$$\begin{aligned}
\text{KL}(q_\lambda(Z)\|p_\theta(Z|\boldsymbol{x})) =& \mathbb{E}_{z\sim q_\lambda(Z)} \log \frac{q_\lambda(z)}{p_\theta(z|\boldsymbol{x})} \\
=& q_\lambda(1) \log \frac{q_\lambda(1)}{p_\theta(1|\boldsymbol{x})} + q_\lambda(0) \log \frac{q_\lambda(0)}{p_\theta(0|\boldsymbol{x})} \\
=& \lambda \log \frac{\lambda}{0.76} + (1-\lambda) \log \frac{1-\lambda}{(1-0.76)}
\end{aligned}$$

In Slide 48, we have also calculate $p_\theta(\boldsymbol{x})$.

ELBO Tightening

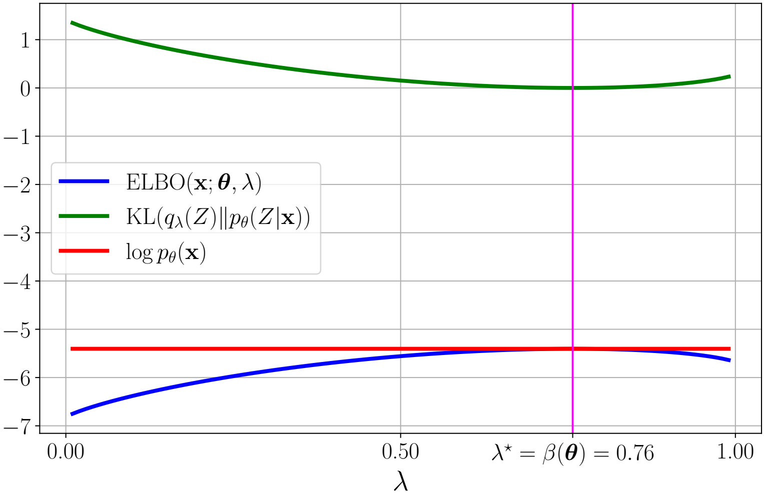

Figure: $\text{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, \lambda)$, $\text{KL}(q_\lambda(Z) \| p_\theta(Z|\boldsymbol{x}))$ and $\log p_\theta(\boldsymbol{x})$ as a function of λ

Altogether

Challenge 1 $\Rightarrow$ $$p_\theta(\boldsymbol{x}) = \int_{\boldsymbol{z}} \mathcal{N}\big(\boldsymbol{x}|\boldsymbol{\mu}_\theta(\boldsymbol{z}), \boldsymbol{\Sigma}_\theta(\boldsymbol{z})\big)\, p_\theta(\boldsymbol{z})\mathrm{d}\boldsymbol{z}$$

Altogether

Challenge 1

$$p_\theta(\boldsymbol{x}) = \int_{\boldsymbol{z}} \mathcal{N}\left(\boldsymbol{x}|\boldsymbol{\mu}_\theta(\boldsymbol{z}), \boldsymbol{\Sigma}_\theta(\boldsymbol{z})\right) p_\theta(\boldsymbol{z}) \mathrm{d}\boldsymbol{z}$$

Solution 1

$$p_\theta(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{z}\sim p_\theta(\mathbb{Z})}\left[p_\theta(\boldsymbol{x}|\boldsymbol{z})\right]$$

Altogether

Challenge 1 $\rightarrow$ $p_\theta(\boldsymbol{x}) = \int_{\boldsymbol{z}} \mathcal{N}\big(\boldsymbol{x}|\boldsymbol{\mu}_\theta(\boldsymbol{z}), \boldsymbol{\Sigma}_\theta(\boldsymbol{z})\big)\, p_\theta(\boldsymbol{z})\mathrm{d}\boldsymbol{z}$

$p_\theta(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{z}\sim p_\theta(\mathbb{Z})}\left[p_\theta(\boldsymbol{x}|\boldsymbol{z})\right]$ $\leftarrow$ Solution 1

Challenge 2 $\rightarrow$ High Variance in Estimation with MCE

Altogether

Challenge 1

$$p_\theta(\boldsymbol{x}) = \int_{\boldsymbol{z}} \mathcal{N}\left(\boldsymbol{x} | \boldsymbol{\mu}_\theta(\boldsymbol{z}), \boldsymbol{\Sigma}_\theta(\boldsymbol{z})\right) p_\theta(\boldsymbol{z}) \mathrm{d}\boldsymbol{z}$$

Solution 1

$$p_\theta(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{z} \sim p_\theta(\mathbb{Z})}\left[p_\theta(\boldsymbol{x}|\boldsymbol{z})\right]$$

Challenge 2

High Variance in Estimation with MCE

Solution 2

$$p_\theta(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{z} \sim q(\mathbb{Z})}\left[\frac{p_\theta(\boldsymbol{x}, \boldsymbol{z})}{q(\boldsymbol{z})}\right]$$

Altogether

Challenge 1 → $p_\theta(\boldsymbol{x}) = \int_{\boldsymbol{z}} \mathcal{N}\left(\boldsymbol{x}|\boldsymbol{\mu}_\theta(\boldsymbol{z}), \boldsymbol{\Sigma}_\theta(\boldsymbol{z})\right) p_\theta(\boldsymbol{z})\mathrm{d}\boldsymbol{z}$

$p_\theta(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{z}\sim p_\theta(\mathbb{Z})}\left[p_\theta(\boldsymbol{x}|\boldsymbol{z})\right]$ ← Solution 1

Challenge 2 → High Variance in Estimation with MCE

$p_\theta(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{z}\sim q(\mathbb{Z})}\left[\frac{p_\theta(\boldsymbol{x},\boldsymbol{z})}{q(\boldsymbol{z})}\right]$ ← Solution 2

Challenge 3 → Selecting $q(\mathbb{Z})$

Altogether

Challenge 1 → $p_\theta(\boldsymbol{x}) = \int_{\boldsymbol{z}} \mathcal{N}\left(\boldsymbol{x}|\boldsymbol{\mu}_\theta(\boldsymbol{z}), \boldsymbol{\Sigma}_\theta(\boldsymbol{z})\right) p_\theta(\boldsymbol{z}) \mathrm{d}\boldsymbol{z}$

$p_\theta(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{z}\sim p_\theta(\mathbb{Z})}\left[p_\theta(\boldsymbol{x}|\boldsymbol{z})\right]$ ← Solution 1

Challenge 2 → High Variance in Estimation with MCE

$p_\theta(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{z}\sim q(\mathbb{Z})}\left[\frac{p_\theta(\boldsymbol{x},\boldsymbol{z})}{q(\boldsymbol{z})}\right]$ ← Solution 2

Challenge 3 → Selecting $q(\mathbb{Z})$

$\mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},q)$ ← Solution 3

Altogether

Challenge 1 $\rightarrow$ $p_\theta(\boldsymbol{x}) = \int_{\boldsymbol{z}} \mathcal{N}\left(\boldsymbol{x}|\boldsymbol{\mu}_\theta(\boldsymbol{z}), \boldsymbol{\Sigma}_\theta(\boldsymbol{z})\right) p_\theta(\boldsymbol{z}) \mathrm{d}\boldsymbol{z}$

$p_\theta(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{z} \sim p_\theta(\mathbb{Z})}\left[p_\theta(\boldsymbol{x}|\boldsymbol{z})\right]$ $\leftarrow$ Solution 1

Challenge 2 $\rightarrow$ High Variance in Estimation with MCE

$p_\theta(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{z} \sim q(\mathbb{Z})}\left[\frac{p_\theta(\boldsymbol{x}, \boldsymbol{z})}{q(\boldsymbol{z})}\right]$ $\leftarrow$ Solution 2

Challenge 3 $\rightarrow$ Selecting $q(\mathbb{Z})$

$\mathrm{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, q)$

$q(\mathbb{Z}) = p_\theta(\mathbb{Z}|\boldsymbol{x})$ $\leftarrow$ Solution 3

Altogether

Challenge 1 $p_\theta(\boldsymbol{x}) = \int_{\boldsymbol{z}} \mathcal{N}\left(\boldsymbol{x}|\boldsymbol{\mu}_\theta(\boldsymbol{z}), \boldsymbol{\Sigma}_\theta(\boldsymbol{z})\right) p_\theta(\boldsymbol{z}) \mathrm{d}\boldsymbol{z}$

$p_\theta(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{z}\sim p_\theta(\mathbb{Z})}\left[p_\theta(\boldsymbol{x}|\boldsymbol{z})\right]$ Solution 1

Challenge 2 High Variance in Estimation with MCE

$p_\theta(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{z}\sim q(\mathbb{Z})}\left[\frac{p_\theta(\boldsymbol{x},\boldsymbol{z})}{q(\boldsymbol{z})}\right]$ Solution 2

Challenge 3 Selecting $q(\mathbb{Z})$

$\mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},q)$

$q(\mathbb{Z}) = p_\theta(\mathbb{Z}|\boldsymbol{x})$ Solution 3

Challenge 4 Calulating $p_\theta(\mathbb{Z}|\boldsymbol{x})$

Altogether

Challenge 1 $\rightarrow$ $p_\theta(\boldsymbol{x}) = \int_{\boldsymbol{z}} \mathcal{N}\left(\boldsymbol{x}|\boldsymbol{\mu}_\theta(\boldsymbol{z}), \boldsymbol{\Sigma}_\theta(\boldsymbol{z})\right) p_\theta(\boldsymbol{z})\mathrm{d}\boldsymbol{z}$

$p_\theta(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{z}\sim p_\theta(\mathbb{Z})}\left[p_\theta(\boldsymbol{x}|\boldsymbol{z})\right]$ $\leftarrow$ Solution 1

Challenge 2 $\rightarrow$ High Variance in Estimation with MCE

$p_\theta(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{z}\sim q(\mathbb{Z})}\left[\frac{p_\theta(\boldsymbol{x},\boldsymbol{z})}{q(\boldsymbol{z})}\right]$ $\leftarrow$ Solution 2

Challenge 3 $\rightarrow$ Selecting $q(\mathbb{Z})$

$\mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},q)$

$q(\mathbb{Z}) = p_\theta(\mathbb{Z}|\boldsymbol{x})$ $\leftarrow$ Solution 3

Challenge 4 $\rightarrow$ Calulating $p_\theta(\mathbb{Z}|\boldsymbol{x})$

$\min_\lambda \mathrm{KL}(q_\lambda(\mathbb{Z})\|p_\theta(\mathbb{Z}|\boldsymbol{x}))$ $\leftarrow$ Solution 4

Altogether

Challenge 1 → $p_\theta(\boldsymbol{x}) = \int_{\boldsymbol{z}} \mathcal{N}\left(\boldsymbol{x}|\boldsymbol{\mu}_\theta(\boldsymbol{z}), \boldsymbol{\Sigma}_\theta(\boldsymbol{z})\right) p_\theta(\boldsymbol{z})\mathrm{d}\boldsymbol{z}$

$p_\theta(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{z}\sim p_\theta(\mathbb{Z})}\left[p_\theta(\boldsymbol{x}|\boldsymbol{z})\right]$ ← Solution 1

Challenge 2 → High Variance in Estimation with MCE

$p_\theta(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{z}\sim q(\mathbb{Z})}\left[\frac{p_\theta(\boldsymbol{x},\boldsymbol{z})}{q(\boldsymbol{z})}\right]$ ← Solution 2

Challenge 3 → Selecting $q(\mathbb{Z})$

$\mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},q)$

$q(\mathbb{Z}) = p_\theta(\mathbb{Z}|\boldsymbol{x})$ ← Solution 3

Challenge 4 → Calulating $p_\theta(\mathbb{Z}|\boldsymbol{x})$

$$\min_\lambda \mathrm{KL}(q_\lambda(\mathbb{Z})\|p_\theta(\mathbb{Z}|\boldsymbol{x})) \equiv \max_\lambda \mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\lambda})$$ ← Solution 4

Altogether

Challenge 1 → $p_\theta(\boldsymbol{x}) = \int_{\boldsymbol{z}} \mathcal{N}\left(\boldsymbol{x}|\boldsymbol{\mu}_\theta(\boldsymbol{z}), \boldsymbol{\Sigma}_\theta(\boldsymbol{z})\right) p_\theta(\boldsymbol{z}) \mathrm{d}\boldsymbol{z}$

Solution 1 → $p_\theta(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{z}\sim p_\theta(\mathbb{Z})}\left[p_\theta(\boldsymbol{x}|\boldsymbol{z})\right]$

Challenge 2 → High Variance in Estimation with MCE

Solution 2 → $p_\theta(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{z}\sim q(\mathbb{Z})}\left[\frac{p_\theta(\boldsymbol{x},\boldsymbol{z})}{q(\boldsymbol{z})}\right]$

Challenge 3 → Selecting $q(\mathbb{Z})$

Solution 3 → $\mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},q)$

$q(\mathbb{Z}) = p_\theta(\mathbb{Z}|\boldsymbol{x})$

Challenge 4 → Calulating $p_\theta(\mathbb{Z}|\boldsymbol{x})$

Solution 4 → $\min_\lambda \mathrm{KL}(q_\lambda(\mathbb{Z}) \| p_\theta(\mathbb{Z}|\boldsymbol{x}))$

$\equiv$

$\max_\lambda \mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\lambda})$

$$\boxed{\boxed{\max_{\boldsymbol{\lambda}}}\ \mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\lambda})}$$

Update on our Challenges

Challenge 4

Calculating $p_\theta(\mathbb{Z}|\boldsymbol{x})$ needs the data likelihood which is intractable as we observe in Slide 28. On the other hand, we need to decrease $\mathrm{KL}(q(\mathbb{Z})\|p_\theta(\mathbb{Z}|\boldsymbol{x}))$ to tighten the ELBO.

Update on our Challenges

Challenge 4

Calculating $p_\theta(\mathbb{Z}|\boldsymbol{x})$ needs the data likelihood which is intractable as we observe in Slide 28. On the other hand, we need to decrease $\mathrm{KL}(q(\mathbb{Z})\|p_\theta(\mathbb{Z}|\boldsymbol{x}))$ to tighten the ELBO.

- ☞ We can tighten the ELBO using the following optimization problem:

$$\max_{\boldsymbol{\lambda}} \ \mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\lambda})$$

Update on our Challenges

Challenge 4

Calculating $p_\theta(\mathbb{Z}|\boldsymbol{x})$ needs the data likelihood which is intractable as we observe in Slide 28. On the other hand, we need to decrease $\mathrm{KL}(q(\mathbb{Z})\|p_\theta(\mathbb{Z}|\boldsymbol{x}))$ to tighten the ELBO.

☞ We can tighten the ELBO using the following optimization problem:

$$\max_{\boldsymbol{\lambda}} \ \mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\lambda})$$

Challenge 5

We need to maximize ELBO with respect to both $\boldsymbol{\theta}$ and $\boldsymbol{\lambda}$. Thus we need the following gradient vectors:

- $\nabla_\theta \,\mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\lambda})$
- $\nabla_\lambda \,\mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\lambda})$

Section 7

ELBO Optimization

ELBO Gradients

With Respect to $\boldsymbol{\theta}$

For the gradient w.r.t to $\boldsymbol{\theta}$, we have:

$$\nabla_\theta \operatorname{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\lambda}) = \nabla_\theta \left(\mathbb{E}_{\boldsymbol{z}\sim q_\lambda(\mathbb{Z})}\left[\log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \log q_{\boldsymbol{\lambda}}(\boldsymbol{z})\right]\right)$$

ELBO Gradients

With Respect to $\boldsymbol{\theta}$

For the gradient w.r.t to $\boldsymbol{\theta}$, we have:

$$\begin{aligned}
\nabla_\theta \operatorname{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\lambda}) =& \nabla_\theta \left(\mathbb{E}_{\boldsymbol{z}\sim q_\lambda(\mathbb{Z})}\left[\log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \log q_{\boldsymbol{\lambda}}(\boldsymbol{z})\right]\right) \\
\overset{a}{=}& \mathbb{E}_{\boldsymbol{z}\sim q_\lambda(\mathbb{Z})}\left[\nabla_\theta \left(\log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \log q_{\boldsymbol{\lambda}}(\boldsymbol{z})\right)\right]
\end{aligned}$$

ELBO Gradients

With Respect to $\boldsymbol{\theta}$

For the gradient w.r.t to $\boldsymbol{\theta}$, we have:

$$\begin{aligned}
\nabla_\theta \operatorname{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\lambda}) =& \nabla_\theta \left(\mathbb{E}_{\boldsymbol{z}\sim q_\lambda(\mathbb{Z})}\left[\log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \log q_{\boldsymbol{\lambda}}(\boldsymbol{z})\right]\right) \\
\overset{a}{=}& \mathbb{E}_{\boldsymbol{z}\sim q_\lambda(\mathbb{Z})}\left[\nabla_\theta \left(\log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \log q_{\boldsymbol{\lambda}}(\boldsymbol{z})\right)\right] \\
\overset{b}{=}& \mathbb{E}_{\boldsymbol{z}\sim q_\lambda(\mathbb{Z})}\left[\nabla_\theta \log p_\theta(\boldsymbol{x},\boldsymbol{z})\right]
\end{aligned}$$

ELBO Gradients

With Respect to $\boldsymbol{\theta}$

For the gradient w.r.t to $\boldsymbol{\theta}$, we have:

$$
\begin{aligned}
\nabla_\theta \operatorname{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\lambda}) =& \nabla_\theta \left(\mathbb{E}_{\boldsymbol{z}\sim q_\lambda(\mathbb{Z})}\left[\log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \log q_{\boldsymbol{\lambda}}(\boldsymbol{z})\right]\right) \\
\overset{a}{=}& \mathbb{E}_{\boldsymbol{z}\sim q_\lambda(\mathbb{Z})}\left[\nabla_\theta \left(\log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \log q_{\boldsymbol{\lambda}}(\boldsymbol{z})\right)\right] \\
\overset{b}{=}& \mathbb{E}_{\boldsymbol{z}\sim q_\lambda(\mathbb{Z})}\left[\nabla_\theta \log p_\theta(\boldsymbol{x},\boldsymbol{z})\right] \\
\overset{c}{\simeq}& \frac{1}{K}\sum_{k=1}^{K} \nabla_\theta \log p_\theta(\boldsymbol{x},\boldsymbol{z}_k)
\end{aligned}
$$

ELBO Gradients

With Respect to $\boldsymbol{\theta}$

For the gradient w.r.t to $\boldsymbol{\theta}$, we have:

$$\begin{aligned}
\nabla_\theta \, \mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\lambda}) =& \nabla_\theta \left(\mathbb{E}_{\boldsymbol{z}\sim q_\lambda(\mathbb{Z})}\left[\log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \log q_{\boldsymbol{\lambda}}(\boldsymbol{z})\right]\right) \\
\stackrel{a}{=}& \mathbb{E}_{\boldsymbol{z}\sim q_\lambda(\mathbb{Z})}\left[\nabla_\theta \left(\log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \log q_{\boldsymbol{\lambda}}(\boldsymbol{z})\right)\right] \\
\stackrel{b}{=}& \mathbb{E}_{\boldsymbol{z}\sim q_\lambda(\mathbb{Z})}\left[\nabla_\theta \log p_\theta(\boldsymbol{x},\boldsymbol{z})\right] \\
\stackrel{c}{\simeq}& \frac{1}{K}\sum_{k=1}^{K} \nabla_\theta \log p_\theta(\boldsymbol{x},\boldsymbol{z}_k)
\end{aligned}$$

where:

- $a \Rightarrow$ Expectation is with respect to a distribution independent of $\boldsymbol{\theta}$
- $b \Rightarrow q_\lambda(\boldsymbol{z})$ is independent of $\boldsymbol{\theta}$
- $c \Rightarrow$ Monte-Carlo estimation

ELBO Gradients

With Respect to $\boldsymbol{\lambda}$

For the gradient w.r.t to $\boldsymbol{\lambda}$, we have:

$$\nabla_\lambda \, \mathrm{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, \boldsymbol{\lambda}) = \nabla_\lambda \left(\mathbb{E}_{q_\lambda(Z)} \left[\log p_\theta(\boldsymbol{x}, \boldsymbol{z}) - \log q_\lambda(\boldsymbol{z}) \right] \right)$$

ELBO Gradients

With Respect to $\boldsymbol{\lambda}$

For the gradient w.r.t to $\boldsymbol{\lambda}$, we have:

$$\nabla_\lambda \operatorname{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\lambda}) = \nabla_\lambda \left(\mathbb{E}_{q_\lambda(Z)}\left[\log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \log q_\lambda(\boldsymbol{z})\right]\right)$$

Note that here we can not change the order of gradient and expectation as the distribution of expectation is a function of $\boldsymbol{\lambda}$.

Update on our Challenges

Challenge 5

Calculating $p_\theta(\mathbb{Z}|\boldsymbol{x})$ needs the data likelihood which is intractable as we observe in Slide 28. On the other hand, we need to decrease $\mathrm{KL}(q(\mathbb{Z})\|p_\theta(\mathbb{Z}|\boldsymbol{x}))$ to tighten the ELBO.

Update on our Challenges

Challenge 5

Calculating $p_\theta(\mathbb{Z}|\boldsymbol{x})$ needs the data likelihood which is intractable as we observe in Slide 28. On the other hand, we need to decrease $\mathrm{KL}(q(\mathbb{Z})\|p_\theta(\mathbb{Z}|\boldsymbol{x}))$ to tighten the ELBO.

- ☞ We can tighten the ELBO using the following optimization problem:

$$\max_{\boldsymbol{\lambda}} \ \mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\lambda})$$

Update on our Challenges

Challenge 5

Calculating $p_\theta(\mathbb{Z}|\boldsymbol{x})$ needs the data likelihood which is intractable as we observe in Slide 28. On the other hand, we need to decrease $\mathrm{KL}(q(\mathbb{Z})\|p_\theta(\mathbb{Z}|\boldsymbol{x}))$ to tighten the ELBO.

☞ We can tighten the ELBO using the following optimization problem:

$$\max_{\boldsymbol{\lambda}} \ \mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\lambda})$$

Challenge 6

We need to maximize ELBO with respect to $\boldsymbol{\lambda}$. Thus we need the following gradient vector:

- $\nabla_\lambda \mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\lambda})$

Section 8

Reparameterization Trick

Reparameterization Trick

Reparameterization Trick

Again pay attention to the following gradient.

$$\nabla_\lambda \,\mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\lambda}) = \nabla_\lambda \left(\mathbb{E}_{q_\lambda(Z)}\left[\log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \log q_\lambda(\boldsymbol{z})\right]\right)$$

Reparameterization Trick

Again pay attention to the following gradient.

$$\nabla_\lambda \operatorname{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\lambda}) = \nabla_\lambda \left(\mathbb{E}_{q_\lambda(Z)}\left[\log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \log q_\lambda(\boldsymbol{z})\right]\right)$$

To handle the above challenge we use the following steps:

Reparameterization Trick

Again pay attention to the following gradient.

$$\nabla_\lambda \, \text{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, \boldsymbol{\lambda}) = \nabla_\lambda \left(\mathbb{E}_{q_\lambda(Z)} \left[\log p_\theta(\boldsymbol{x}, \boldsymbol{z}) - \log q_\lambda(\boldsymbol{z}) \right] \right)$$

To handle the above challenge we use the following steps:

- Limit the $q_\lambda(\mathbb{Z})$ to Gaussian distribtuion as:

$$q_\lambda(\mathbb{Z}) = \mathcal{N}(\mathbb{Z} | \boldsymbol{\mu}, \sigma^2 \boldsymbol{I}) \Rightarrow \boldsymbol{\lambda} = \{\boldsymbol{\mu}, \sigma^2\}$$

Reparameterization Trick

Reparameterization Trick

Again pay attention to the following gradient.

$$\nabla_\lambda \, \mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\lambda}) = \nabla_\lambda \left(\mathbb{E}_{q_\lambda(Z)}\left[\log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \log q_\lambda(\boldsymbol{z})\right]\right)$$

To handle the above challenge we use the following steps:

- Limit the $q_\lambda(\mathbb{Z})$ to Gaussian distribtuion as:

$$q_\lambda(\mathbb{Z}) = \mathcal{N}(\mathbb{Z}|\boldsymbol{\mu},\sigma^2\boldsymbol{I}) \Rightarrow \boldsymbol{\lambda} = \{\boldsymbol{\mu},\sigma^2\}$$

- Reparameterize the random vector as:

$$\boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{0},\boldsymbol{I}) \Rightarrow \boldsymbol{z} = \boldsymbol{\mu} + \sigma\boldsymbol{\epsilon} = g(\boldsymbol{\epsilon};\boldsymbol{\lambda}) \sim \mathcal{N}(\mathbb{Z}\boldsymbol{\mu},\sigma^2\boldsymbol{I}) = q_\lambda(\mathbb{Z})$$

ELBO Gradients

With Respect to $\boldsymbol{\lambda}$

For the gradient w.r.t to $\boldsymbol{\lambda}$, we have:

$$\nabla_\lambda \, \mathrm{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, \boldsymbol{\lambda}) = \nabla_\lambda \left(\mathbb{E}_{\boldsymbol{z} \sim q_\lambda(\mathbb{Z})} \left[\log p_\theta(\boldsymbol{x}, \boldsymbol{z}) - \log q_{\boldsymbol{\lambda}}(\boldsymbol{z}) \right] \right)$$

ELBO Gradients

With Respect to $\boldsymbol{\lambda}$

For the gradient w.r.t to $\boldsymbol{\lambda}$, we have:

$$\begin{aligned}\nabla_\lambda \, \mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\lambda}) =& \nabla_\lambda \left(\mathbb{E}_{\boldsymbol{z}\sim q_\lambda(\mathbb{Z})}\left[\log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \log q_{\boldsymbol{\lambda}}(\boldsymbol{z})\right]\right)\\ \overset{a}{=}& \nabla_\lambda \left(\mathbb{E}_{\boldsymbol{\epsilon}\sim\mathcal{N}(\mathbf{0},\boldsymbol{I})}\left[\log p_\theta(\boldsymbol{x},g(\boldsymbol{\epsilon};\boldsymbol{\lambda})) - \log q_{\boldsymbol{\lambda}}(g(\boldsymbol{\epsilon};\boldsymbol{\lambda}))\right]\right)\end{aligned}$$

ELBO Gradients

With Respect to $\boldsymbol{\lambda}$

For the gradient w.r.t to $\boldsymbol{\lambda}$, we have:

$$\begin{aligned}
\nabla_\lambda \operatorname{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\lambda}) =& \nabla_\lambda \left(\mathbb{E}_{\boldsymbol{z}\sim q_\lambda(\mathbb{Z})}\left[\log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \log q_{\boldsymbol{\lambda}}(\boldsymbol{z})\right]\right) \\
\stackrel{a}{=}& \nabla_\lambda \left(\mathbb{E}_{\boldsymbol{\epsilon}\sim\mathcal{N}(\mathbf{0},\boldsymbol{I})}\left[\log p_\theta(\boldsymbol{x}, g(\boldsymbol{\epsilon};\boldsymbol{\lambda})) - \log q_{\boldsymbol{\lambda}}(g(\boldsymbol{\epsilon};\boldsymbol{\lambda}))\right]\right) \\
\stackrel{b}{=}& \mathbb{E}_{\boldsymbol{\epsilon}\sim\mathcal{N}(\mathbf{0},\boldsymbol{I})}\left[\nabla_\lambda \left(\log p_\theta(\boldsymbol{x}, g(\boldsymbol{\epsilon};\boldsymbol{\lambda})) - \log q_{\boldsymbol{\lambda}}(g(\boldsymbol{\epsilon};\boldsymbol{\lambda}))\right)\right]
\end{aligned}$$

ELBO Gradients

With Respect to $\boldsymbol{\lambda}$

For the gradient w.r.t to $\boldsymbol{\lambda}$, we have:

$$\begin{aligned}
\nabla_\lambda \,\mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\lambda}) =& \nabla_\lambda \left(\mathbb{E}_{\boldsymbol{z}\sim q_\lambda(\mathbb{Z})}\left[\log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \log q_{\boldsymbol{\lambda}}(\boldsymbol{z})\right]\right) \\
\overset{a}{=}& \nabla_\lambda \left(\mathbb{E}_{\boldsymbol{\epsilon}\sim\mathcal{N}(\mathbf{0},\boldsymbol{I})}\left[\log p_\theta(\boldsymbol{x}, g(\boldsymbol{\epsilon};\boldsymbol{\lambda})) - \log q_{\boldsymbol{\lambda}}(g(\boldsymbol{\epsilon};\boldsymbol{\lambda}))\right]\right) \\
\overset{b}{=}& \mathbb{E}_{\boldsymbol{\epsilon}\sim\mathcal{N}(\mathbf{0},\boldsymbol{I})}\left[\nabla_\lambda \left(\log p_\theta(\boldsymbol{x}, g(\boldsymbol{\epsilon};\boldsymbol{\lambda})) - \log q_{\boldsymbol{\lambda}}(g(\boldsymbol{\epsilon};\boldsymbol{\lambda}))\right)\right] \\
\overset{c}{=}& \frac{1}{K}\sum_{k=1}^{K} \nabla_\lambda \left(\log p_\theta(\boldsymbol{x}, g(\boldsymbol{\epsilon}_k;\boldsymbol{\lambda})) - \log q_{\boldsymbol{\lambda}}(g(\boldsymbol{\epsilon}_k;\boldsymbol{\lambda}))\right)
\end{aligned}$$

ELBO Gradients

With Respect to $\boldsymbol{\lambda}$

For the gradient w.r.t to $\boldsymbol{\lambda}$, we have:

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\overset{b}{=}& \mathbb{E}_{\boldsymbol{\epsilon}\sim\mathcal{N}(\mathbf{0},\boldsymbol{I})}\left[\nabla_\lambda\left(\log p_\theta(\boldsymbol{x},g(\boldsymbol{\epsilon};\boldsymbol{\lambda})) - \log q_{\boldsymbol{\lambda}}(g(\boldsymbol{\epsilon};\boldsymbol{\lambda}))\right)\right]\\
\overset{c}{=}& \frac{1}{K}\sum_{k=1}^{K}\nabla_\lambda\left(\log p_\theta(\boldsymbol{x},g(\boldsymbol{\epsilon}_k;\boldsymbol{\lambda})) - \log q_{\boldsymbol{\lambda}}(g(\boldsymbol{\epsilon}_k;\boldsymbol{\lambda}))\right)
\end{aligned}$$

where:

- $a \Rightarrow$ Reparameterization trick
- $b \Rightarrow q_\lambda(\boldsymbol{z})$ Expectation is with respect to a distribution independent of $\boldsymbol{\lambda}$
- $c \Rightarrow$ Monte-Carlo estimation

ELBO Optimization

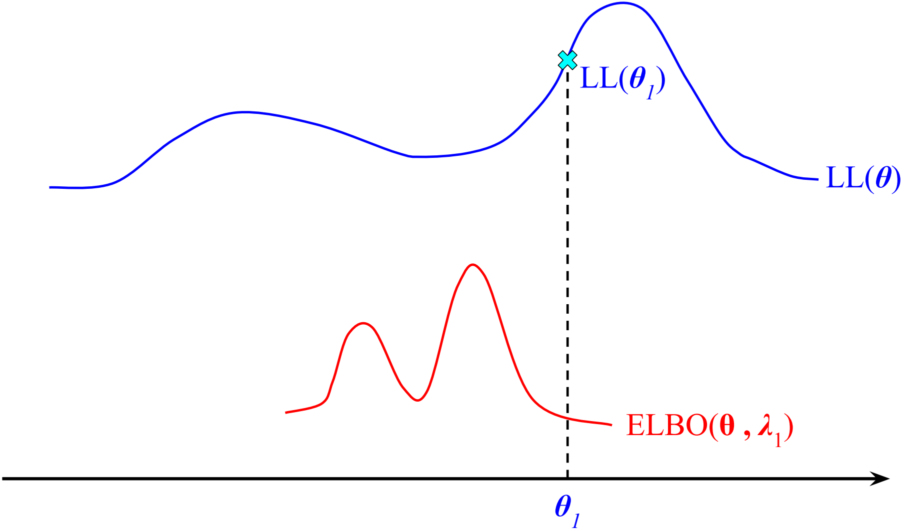

Figure: Starting point $\boldsymbol{\theta}_1$ and $\boldsymbol{\lambda}_1$

ELBO Optimization

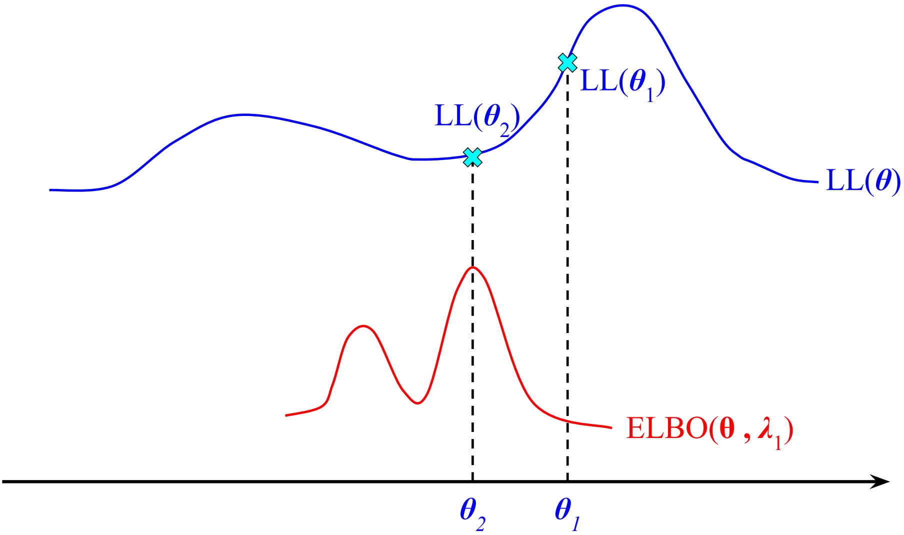

Figure: $\boldsymbol{\theta}_2 = \text{argmax}_{\boldsymbol{\theta}}\, \text{ELBO}(\boldsymbol{\theta}, \boldsymbol{\lambda}_1)$

ELBO Optimization

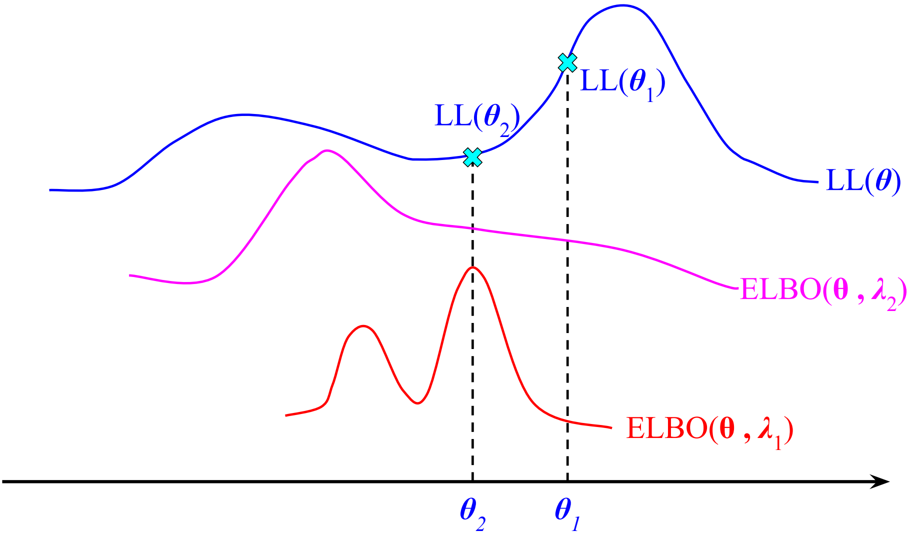

Figure: $\boldsymbol{\lambda}_2 = \mathrm{argmax}_{\boldsymbol{\lambda}}\, \mathrm{ELBO}(\boldsymbol{\theta}_2, \boldsymbol{\lambda})$

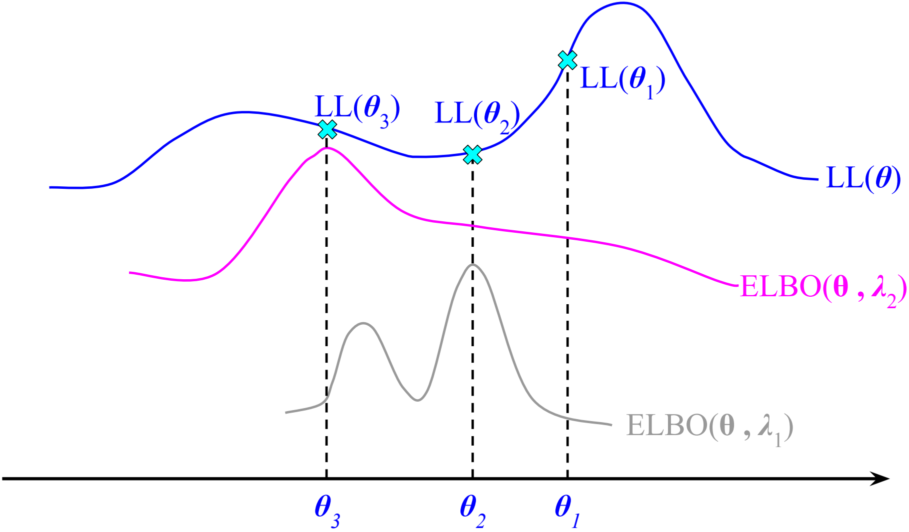

Figure: $\boldsymbol{\theta}_3 = \operatorname{argmax}_{\boldsymbol{\theta}} \mathrm{ELBO}(\boldsymbol{\theta}, \boldsymbol{\lambda}_2)$

Update on our Challenges

Challenge 6

We need to maximize ELBO with respect to $\boldsymbol{\lambda}$. Thus we need the following gradient vector:

- $\nabla_\lambda \, \text{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, \boldsymbol{\lambda})$

Update on our Challenges

Challenge 6

We need to maximize ELBO with respect to $\boldsymbol{\lambda}$. Thus we need the following gradient vector:

- $\nabla_\lambda \operatorname{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, \boldsymbol{\lambda})$

☞ We can use the reparameterization trick to calculate the above gradient.

Update on our Challenges

Challenge 6

We need to maximize ELBO with respect to $\boldsymbol{\lambda}$. Thus we need the following gradient vector:

- $\nabla_\lambda \, \text{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, \boldsymbol{\lambda})$

☞ We can use the reparameterization trick to calculate the above gradient.

Challenge 7

To train a model, we need to maximize the log-likelihood on the dataset $\mathcal{D}$ not an isolated sample $\boldsymbol{x}$.

Section 9

Learning

From Data Point to Dataset

Till now, we found a practical approach to increase the ELBO for a typical sample $\boldsymbol{x}$ as:

$$\log p_\theta(\boldsymbol{x}) \geq \mathrm{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, \boldsymbol{\lambda})$$

From Data Point to Dataset

Till now, we found a practical approach to increase the ELBO for a typical sample $\boldsymbol{x}$ as:

$$\log p_\theta(\boldsymbol{x}) \geq \mathrm{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, \boldsymbol{\lambda})$$

Now assume we have a complete dataset $\mathcal{D} = \{\boldsymbol{x}_i\}_{i=1}^N$. We have the following optimization problem:

$$\boldsymbol{\theta}^\star = \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \frac{1}{N} \sum_{i=1}^{N} \log p_\theta(\boldsymbol{x}_i)$$

Lower Bounding the Objective

We have:

$$\log p_\theta(\boldsymbol{x}_i) \geq \underset{\boldsymbol{\lambda}_i}{\operatorname{argmax}}\ \mathrm{ELBO}(\boldsymbol{x}_i; \boldsymbol{\theta}, \boldsymbol{\lambda}_i)$$

Learning

Lower Bounding the Objective

We have:

$$\log p_\theta(\boldsymbol{x}_i) \geq \underset{\boldsymbol{\lambda}_i}{\operatorname{argmax}}\ \mathrm{ELBO}(\boldsymbol{x}_i; \boldsymbol{\theta}, \boldsymbol{\lambda}_i)$$

$$\Rightarrow \sum_i \log p_\theta(\boldsymbol{x}_i) \geq \sum_i \underset{\boldsymbol{\lambda}_i}{\operatorname{argmax}}\ \mathrm{ELBO}(\boldsymbol{x}_i; \boldsymbol{\theta}, \boldsymbol{\lambda}_i)$$

Lower Bounding the Objective

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$$= \underset{\boldsymbol{\lambda}_1, \ldots \boldsymbol{\lambda}_N}{\operatorname{argmax}} \sum_i \ \text{ELBO}(\boldsymbol{x}_i; \boldsymbol{\theta}, \boldsymbol{\lambda}_i)$$

Learning

Lower Bounding the Objective

We have:

$$\log p_\theta(\boldsymbol{x}_i) \geq \underset{\boldsymbol{\lambda}_i}{\operatorname{argmax}}\ \mathrm{ELBO}(\boldsymbol{x}_i; \boldsymbol{\theta}, \boldsymbol{\lambda}_i)$$

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$$= \underset{\boldsymbol{\lambda}_1, \ldots \boldsymbol{\lambda}_N}{\operatorname{argmax}} \sum_i\ \mathrm{ELBO}(\boldsymbol{x}_i; \boldsymbol{\theta}, \boldsymbol{\lambda}_i)$$

So:

$$\frac{1}{N} \sum_i \log p_\theta(\boldsymbol{x}_i) \geq \underset{\boldsymbol{\lambda}_1, \ldots \boldsymbol{\lambda}_N}{\operatorname{argmax}} \frac{1}{N} \sum_i\ \mathrm{ELBO}(\boldsymbol{x}_i; \boldsymbol{\theta}, \boldsymbol{\lambda}_i)$$

Learning Problem

We see:

$$\frac{1}{N}\sum_i \log p_\theta(\boldsymbol{x}_i) \geq \underset{\boldsymbol{\lambda}_1,\dots\boldsymbol{\lambda}_N}{\operatorname{argmax}} \frac{1}{N}\sum_i \ \mathrm{ELBO}(\boldsymbol{x}_i;\boldsymbol{\theta},\boldsymbol{\lambda}_i)$$

Learning

Learning Problem

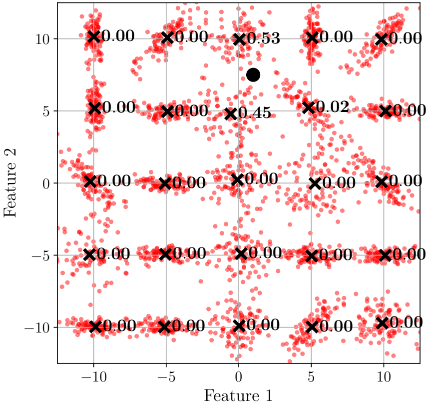
We see:

$$\frac{1}{N}\sum_i \log p_\theta(\boldsymbol{x}_i) \geq \underset{\boldsymbol{\lambda}_1,\ldots\boldsymbol{\lambda}_N}{\operatorname{argmax}} \frac{1}{N}\sum_i \ \mathrm{ELBO}(\boldsymbol{x}_i;\boldsymbol{\theta},\boldsymbol{\lambda}_i)$$

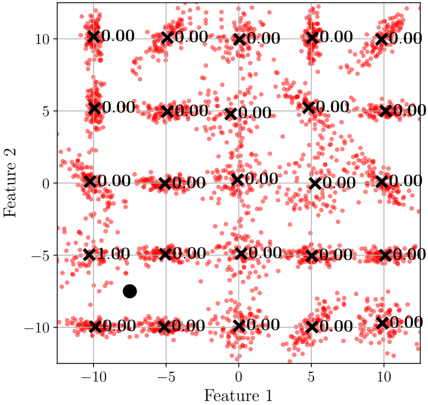
As a result, the learning problem is:

$$\underset{\boldsymbol{\theta}}{\operatorname{argmax}} \underset{\boldsymbol{\lambda}_1,\ldots\boldsymbol{\lambda}_N}{\operatorname{argmax}} \sum_i \ \mathrm{ELBO}(\boldsymbol{x}_i;\boldsymbol{\theta},\boldsymbol{\lambda}_i)$$

Different Sampling Distributions for Different Data Samples



(a) $q(Z|\boldsymbol{x}_1)$



(b) $q(Z|\boldsymbol{x}_2)$

Figure: The model posterior over latent variables for two different samples $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ (so we need one distribution for each sample)

Stochastic Variational Inference (SVI) Learning

Algorithm 1: Stochastic Variational Learning

Input : Dataset $\mathcal{D} = \{\boldsymbol{x}_i\}$

Initialization: $\boldsymbol{\theta}, \boldsymbol{\lambda}_1, \ldots, \boldsymbol{\lambda}_N$

begin

    for $j = 1 : D$ **do**

        Select a Sample $\boldsymbol{x}_i$ from $\mathcal{D}$ randomly

        for $k = 1 : K$ **do**

            $\boldsymbol{\lambda}_i \leftarrow \boldsymbol{\lambda}_i + \eta \nabla_{\boldsymbol{\lambda}_i} \text{ELBO}(\boldsymbol{x}_i; \boldsymbol{\theta}, \boldsymbol{\lambda}_i)$

        end

        $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \mu \nabla_{\theta} \text{ELBO}(\boldsymbol{x}_i; \boldsymbol{\theta}, \boldsymbol{\lambda}_i)$

    end

end

Output : $\boldsymbol{\theta}$

Update on our Challenges

Challenge 7

To train a model, we need to maximize the log-likelihood on the dataset $\mathcal{D}$, not an isolated sample $\boldsymbol{x}$.

Update on our Challenges

Challenge 7

To train a model, we need to maximize the log-likelihood on the dataset $\mathcal{D}$, not an isolated sample $\boldsymbol{x}$.

☞ We derive the objective for the complete dataset as:

$$\underset{\boldsymbol{\theta}}{\operatorname{argmax}} \underset{\boldsymbol{\lambda}_1,\ldots\boldsymbol{\lambda}_N}{\operatorname{argmax}} \sum_i \operatorname{ELBO}(\boldsymbol{x}_i; \boldsymbol{\theta}, \boldsymbol{\lambda}_i)$$

Update on our Challenges

Challenge 7

To train a model, we need to maximize the log-likelihood on the dataset $\mathcal{D}$, not an isolated sample $\boldsymbol{x}$.

☞ We derive the objective for the complete dataset as:

$$\underset{\boldsymbol{\theta}}{\operatorname{argmax}} \underset{\boldsymbol{\lambda}_1, \ldots \boldsymbol{\lambda}_N}{\operatorname{argmax}} \sum_i \operatorname{ELBO}(\boldsymbol{x}_i; \boldsymbol{\theta}, \boldsymbol{\lambda}_i)$$

Challenge 8

As we can see in the above optimization problem, the number of parameters is not scalable with the dataset size. Each training sample adds one $\boldsymbol{\lambda}$ vector to the optimization problem.

Section 10

Amortization

Amortization

Scalability of SVI

Using the SVI, we can solve the following maximization problem:

$$\boldsymbol{\theta}^\star, \boldsymbol{\lambda}_1^\star, \boldsymbol{\lambda}_2^\star, \ldots, \boldsymbol{\lambda}_N^\star = \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \underset{\boldsymbol{\lambda}_1, \ldots \boldsymbol{\lambda}_N}{\operatorname{argmax}} \sum_i \operatorname{ELBO}(\boldsymbol{x}_i; \boldsymbol{\theta}, \boldsymbol{\lambda}_i)$$

Amortization

Scalability of SVI

Using the SVI, we can solve the following maximization problem:

$$\boldsymbol{\theta}^\star, \boldsymbol{\lambda}_1^\star, \boldsymbol{\lambda}_2^\star, \ldots, \boldsymbol{\lambda}_N^\star = \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \underset{\boldsymbol{\lambda}_1, \ldots \boldsymbol{\lambda}_N}{\operatorname{argmax}} \sum_i \operatorname{ELBO}(\boldsymbol{x}_i; \boldsymbol{\theta}, \boldsymbol{\lambda}_i)$$

Amortization is a type of parameter sharing to achieve scalability with respect to dataset size.

Amortization

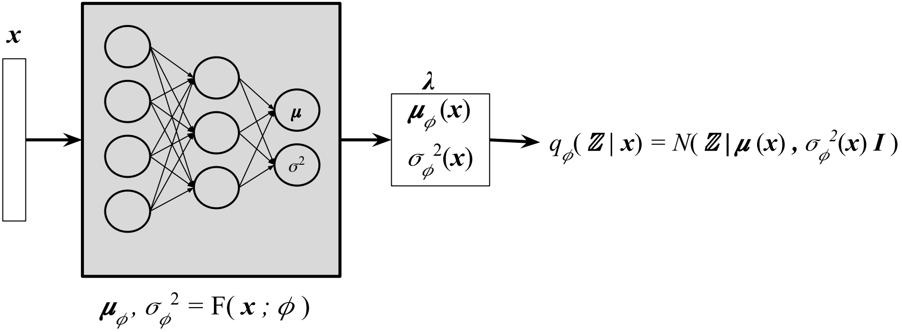


Figure: Amortization: The parameters of neural network $F(\cdot;\cdot)$ is shared between all the training samples.

Amortization

Notation Update

By using the Amortization technique, $\boldsymbol{\phi}$ the parameters of F are shared between all training data samples. So instead of $\text{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, \boldsymbol{\lambda})$ we use:

$$\text{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, \boldsymbol{\phi}) = \mathbb{E}_{\boldsymbol{z} \sim q_{\phi}(\mathbb{Z}|\boldsymbol{x})} \left[\log \left(\frac{p_{\theta}(\boldsymbol{x}, \boldsymbol{z})}{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \right) \right]$$

Amortization

Notation Update

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Amortized Inference

Using Amortization, the ELBO for sample $\boldsymbol{x}_i$ can be written as:

$$\text{ELBO}(\boldsymbol{x}_i;\boldsymbol{\theta},\boldsymbol{\phi}) = \mathbb{E}_{\boldsymbol{z}\sim q_{\phi}(\mathbb{Z}|\boldsymbol{x}_i)}\left[\log p_{\theta}(\boldsymbol{x},\boldsymbol{z}) - \log q_{\phi}(\boldsymbol{z}|\boldsymbol{x}_i)\right]$$

Amortization

Algorithm 2: Amortized Stochastic Variational Inference

Input : Dataset $\mathcal{D} = \{\boldsymbol{x}_i\}$
Initialization: $\boldsymbol{\theta}, \boldsymbol{\phi}$
begin
  for $j = 1 : D$ **do**
    Select a Sample $\boldsymbol{x}_i$ from $\mathcal{D}$ randomly
    $\boldsymbol{\phi} \leftarrow \boldsymbol{\phi} + \eta \nabla_{\boldsymbol{\phi}} \mathrm{ELBO}(\boldsymbol{x}_i; \boldsymbol{\theta}, \boldsymbol{\phi})$
    $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \mu \nabla_{\theta} \mathrm{ELBO}(\boldsymbol{x}_i; \boldsymbol{\theta}, \boldsymbol{\phi})$
  end
end
Output : $\boldsymbol{\theta}, \boldsymbol{\phi}$

Section 11

Revisiting Objective Function

Variational Autoencoder

Revisiting ELBO

We can reformulate ELBO as:

$$\text{ELBO}(\boldsymbol{x}; \boldsymbol{\theta}, \boldsymbol{\phi}) = \mathbb{E}_{\boldsymbol{z} \sim q_\phi(\mathbb{Z}|\boldsymbol{x})} \left[\log p_\theta(\boldsymbol{x}, \boldsymbol{z}) - \log q_\phi(\boldsymbol{z}|\boldsymbol{x}) \right]$$

Revisiting ELBO

We can reformulate ELBO as:

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$$= \mathbb{E}_{\boldsymbol{z}\sim q_\phi(\mathbb{Z}|\boldsymbol{x})}\left[\underbrace{\log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \log p_\theta(\boldsymbol{z})}_{\log p_\theta(\boldsymbol{x}|\boldsymbol{z})} + \underbrace{\log p_\theta(\boldsymbol{z}) - \log q_\phi(\boldsymbol{z}|\boldsymbol{x})}_{-\log \frac{q_\phi(\boldsymbol{z}|\boldsymbol{x})}{p_\theta(\boldsymbol{z})}}\right]$$

Variational Autoencoder

Revisiting ELBO

We can reformulate ELBO as:

$$
\begin{aligned}
\mathrm{ELBO}(\boldsymbol{x};\boldsymbol{\theta},\boldsymbol{\phi}) &= \mathbb{E}_{\boldsymbol{z}\sim q_\phi(\mathbb{Z}|\boldsymbol{x})}\left[\log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \log q_\phi(\boldsymbol{z}|\boldsymbol{x})\right] \\
&= \mathbb{E}_{\boldsymbol{z}\sim q_\phi(\mathbb{Z}|\boldsymbol{x})}\left[\underbrace{\log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \log p_\theta(\boldsymbol{z})}_{\log p_\theta(\boldsymbol{x}|\boldsymbol{z})} + \underbrace{\log p_\theta(\boldsymbol{z}) - \log q_\phi(\boldsymbol{z}|\boldsymbol{x})}_{-\log \frac{q_\phi(\boldsymbol{z}|\boldsymbol{x})}{p_\theta(\boldsymbol{z})}}\right] \\
&= \mathbb{E}_{\boldsymbol{z}\sim q_\phi(\mathbb{Z}|\boldsymbol{x})}\left[\log p_\theta(\boldsymbol{x}|\boldsymbol{z})\right] - \mathrm{KL}\left(q_\phi(\boldsymbol{z}|\boldsymbol{x})\|p_\theta(\boldsymbol{z})\right)
\end{aligned}
$$

Variational Autoencoder Overview

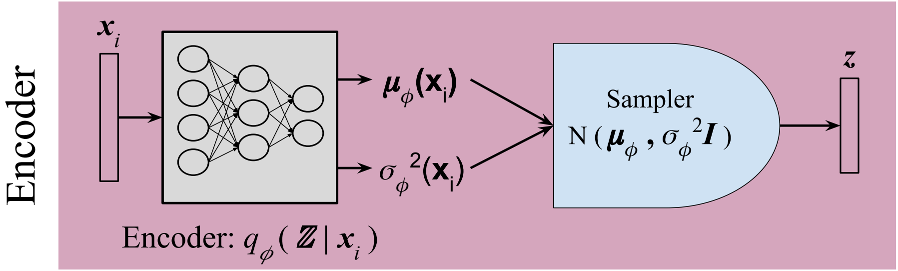

Figure: Encoding

Variational Autoencoder Overview

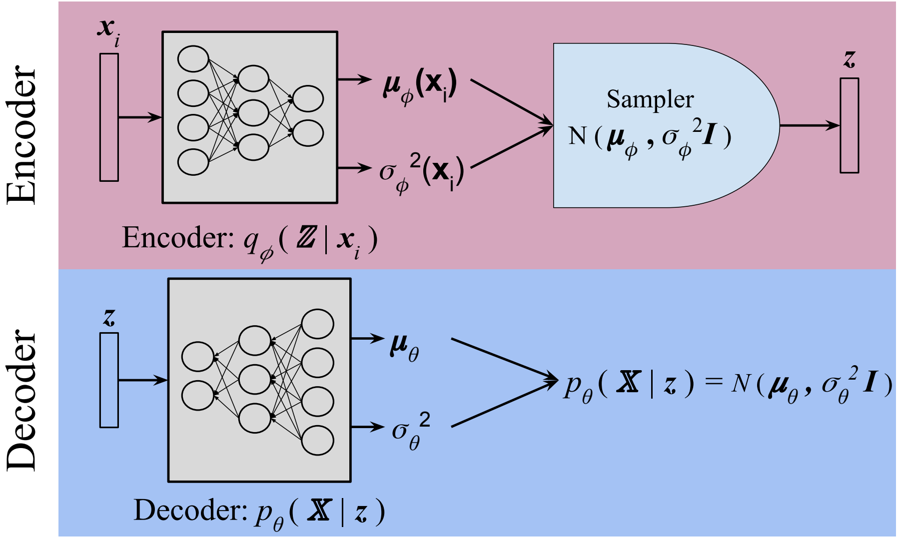

Figure: Encoding and Decoding

Revisiting ELBO

Let's focus on the first term:

$$\mathbb{E}_{\boldsymbol{z} \sim q_\phi(\mathbb{Z}|\boldsymbol{x}_i)} \left[\log p_\theta(\boldsymbol{x}_i|\boldsymbol{z})\right]$$

Variational Autoencoder

Revisiting ELBO

Let's focus on the first term:

$$\mathbb{E}_{\boldsymbol{z}\sim q_\phi(\mathbb{Z}|\boldsymbol{x}_i)}\left[\log p_\theta(\boldsymbol{x}_i|\boldsymbol{z})\right]$$

Conceptually, we have:

- Select a training sample $\boldsymbol{x}_i$.

Variational Autoencoder

Revisiting ELBO

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Conceptually, we have:

- Select a training sample $\boldsymbol{x}_i$.
- Generate the approximate posterior over the latent vector given $\boldsymbol{x}_i$

Revisiting ELBO

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Conceptually, we have:

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- Generate the approximate posterior over the latent vector given $\boldsymbol{x}_i$
- Sample $\boldsymbol{z}$ from the approximate posterior

Variational Autoencoder

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Conceptually, we have:

- Select a training sample $\boldsymbol{x}_i$.
- Generate the approximate posterior over the latent vector given $\boldsymbol{x}_i$
- Sample $\boldsymbol{z}$ from the approximate posterior
- Generate the model posterior over $\mathbb{X}$ given $\boldsymbol{z}$ or $p_\theta(\mathbb{X}|\boldsymbol{z})$

Variational Autoencoder

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Conceptually, we have:

- Select a training sample $\boldsymbol{x}_i$.
- Generate the approximate posterior over the latent vector given $\boldsymbol{x}_i$
- Sample $\boldsymbol{z}$ from the approximate posterior
- Generate the model posterior over $\mathbb{X}$ given $\boldsymbol{z}$ or $p_\theta(\mathbb{X}|\boldsymbol{z})$

A good model is one where $\log p_\theta(\boldsymbol{x}_i|\boldsymbol{z})$ is maximized.

Revisiting ELBO

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Variational Autoencoder

Revisiting ELBO

Let's focus on the first term:

$$\mathbb{E}_{\boldsymbol{z} \sim q_\phi(\mathbb{Z}|\boldsymbol{x}_i)} \left[\log p_\theta(\boldsymbol{x}_i|\boldsymbol{z})\right]$$

In terms of formulations, we have:

$$\log p_\theta(\boldsymbol{x}_i|\boldsymbol{z}) = \log \mathcal{N}(\boldsymbol{x}_i|\boldsymbol{\mu}_\theta, \sigma_\theta^2 \boldsymbol{I})$$

Variational Autoencoder

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$$\begin{aligned}\log p_\theta(\boldsymbol{x}_i|\boldsymbol{z}) &= \log \mathcal{N}(\boldsymbol{x}_i|\boldsymbol{\mu}_\theta, \sigma_\theta^2\boldsymbol{I})\\ &= -\frac{D}{2}\log(2\pi\sigma_\theta^2) - \frac{1}{2\sigma_\theta^2}\|\boldsymbol{x}_i - \boldsymbol{\mu}_\theta\|_2^2\end{aligned}$$

Revisiting ELBO

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Note that:

- The optimization w.r.t. $\boldsymbol{\theta}$ is straightforward.

Variational Autoencoder

Revisiting ELBO

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$$\mathbb{E}_{\boldsymbol{z}\sim q_\phi(\mathbb{Z}|\boldsymbol{x}_i)}\left[\log p_\theta(\boldsymbol{x}_i|\boldsymbol{z})\right]$$

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$$\begin{aligned}\log p_\theta(\boldsymbol{x}_i|\boldsymbol{z}) &= \log \mathcal{N}(\boldsymbol{x}_i|\boldsymbol{\mu}_\theta, \sigma_\theta^2 \boldsymbol{I}) \\ &= -\frac{D}{2}\log(2\pi\sigma_\theta^2) - \frac{1}{2\sigma_\theta^2}\|\boldsymbol{x}_i - \boldsymbol{\mu}_\theta\|_2^2\end{aligned}$$

Note that:

- The optimization w.r.t. $\boldsymbol{\theta}$ is straightforward.
- The optimization w.r.t. $\boldsymbol{\phi}$ needs reparameterization trick.

Variational Autoencoder with Reparameterization Trick

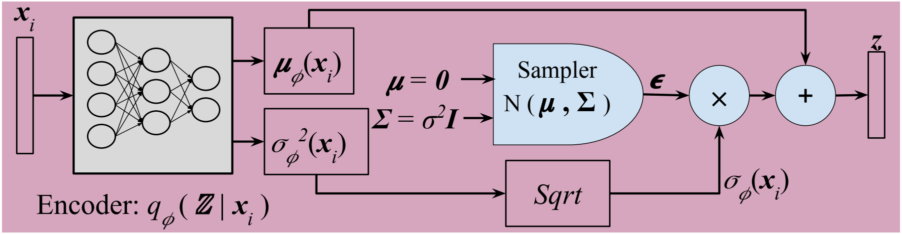

Figure: Encoding with Reparameterization Trick

Variational Autoencoder with Reparameterization Trick

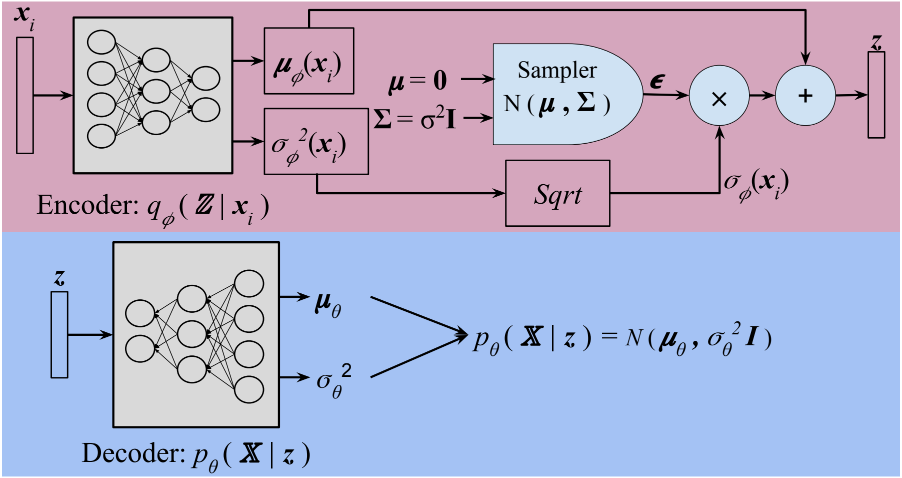

Figure: Encoding and Decoding

Revisiting ELBO

Now let's move on to the second term:

$$-\operatorname{KL}\left(q_\phi(\mathbb{Z}|\boldsymbol{x}_i)\|p_\theta(\mathbb{Z})\right)$$

Variational Autoencoder

Revisiting ELBO

Now let's move on to the second term:

$$-\,\mathrm{KL}\left(q_\phi(\mathbb{Z}|\boldsymbol{x}_i)\|p_\theta(\mathbb{Z})\right)$$

After training and at the end of the day:

- $q_\phi(\mathbb{Z}|\boldsymbol{x}_i), i = 1, \ldots, N$ be near the prior distribution $p_\theta(\mathbb{Z})$ in KLD sense.

Variational Autoencoder

Revisiting ELBO

Now let's move on to the second term:

$$-\operatorname{KL}\left(q_\phi(\mathbb{Z}|\boldsymbol{x}_i)\|p_\theta(\mathbb{Z})\right)$$

After training and at the end of the day:

- $q_\phi(\mathbb{Z}|\boldsymbol{x}_i), i = 1, \ldots, N$ be near the prior distribution $p_\theta(\mathbb{Z})$ in KLD sense.

What does it imply?

Variational Autoencoder

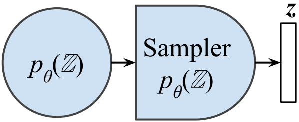

Figure: Encoding with Reparameterization Trick

Variational Autoencoder

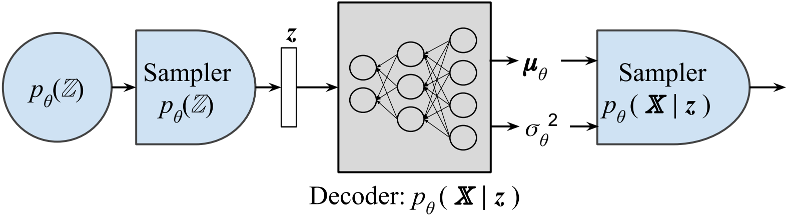

Figure: Encoding with Reparameterization Trick

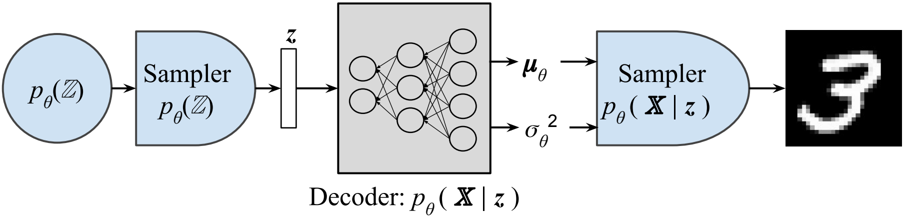

Figure: Encoding with Reparameterization Trick

Section 12

Attribute Vectors in Code Space

Concept

SW: Smiling Woman
NW: Neutral Woman
SM: Smiling Man
NM: Neutral Man

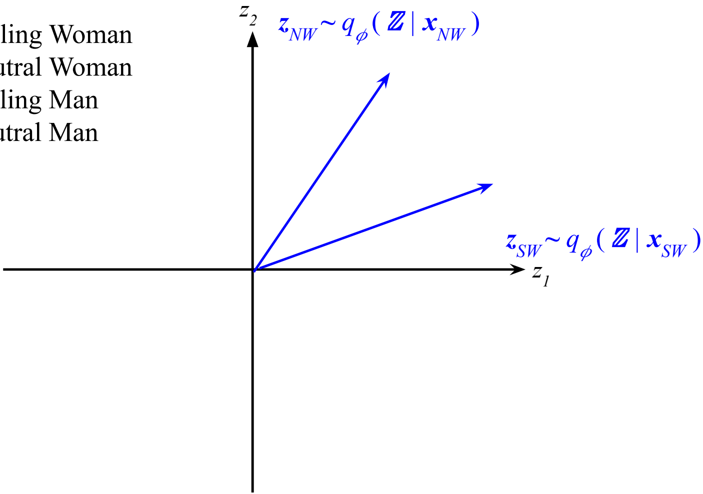

Figure: Encoding of *Neutral Woman* and *Smiling Woman* images

Concept

SW: Smiling Woman
NW: Neutral Woman
SM: Smiling Man
NM: Neutral Man

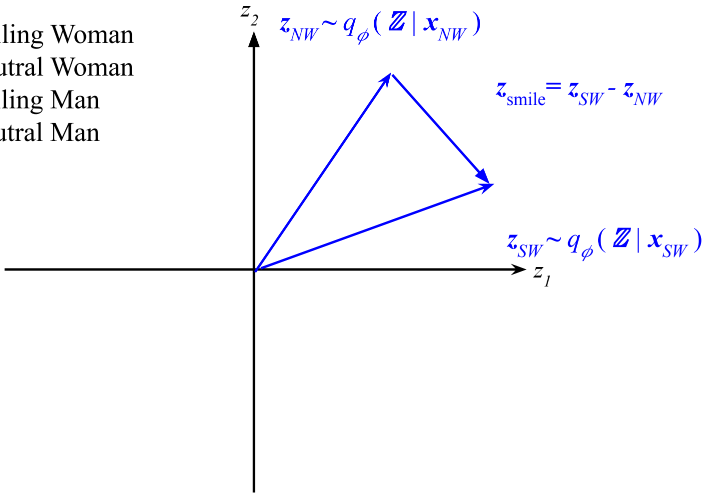

Figure: Calculating the attribute vector of *Smile* in latent space

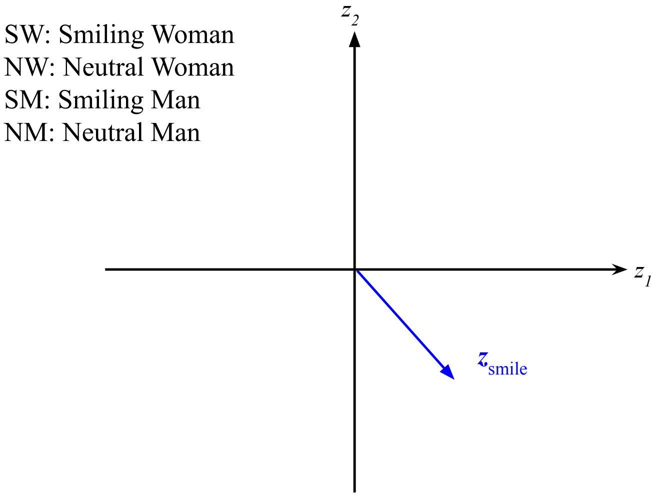

Figure: *Smile* attribute vector

Concept

SW: Smiling Woman
NW: Neutral Woman
SM: Smiling Man
NM: Neutral Man

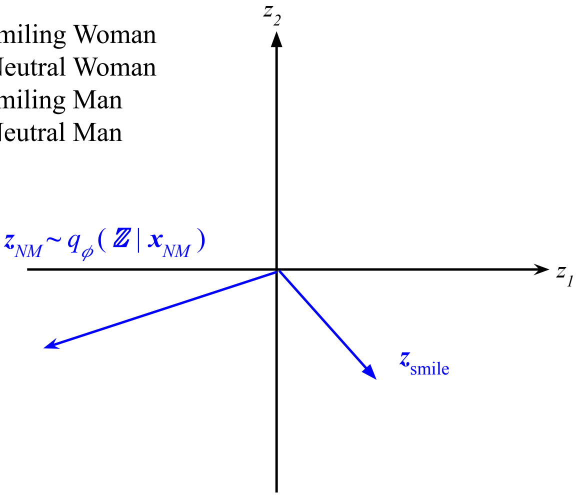

Figure: Encoding of *Neutral Man* image

Concept

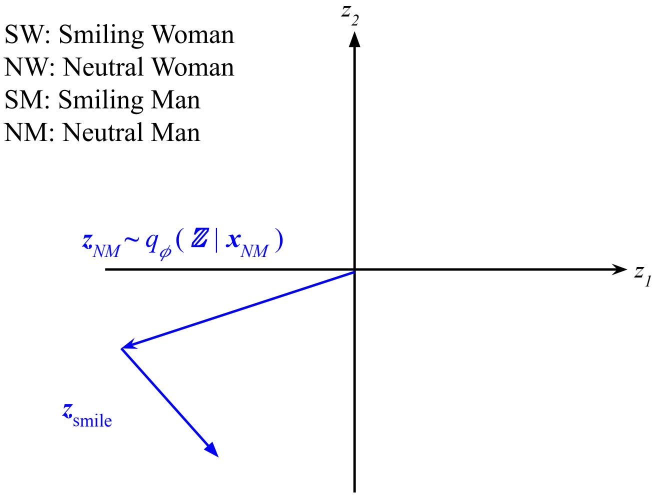

Figure: Adding *Smile* attribute vector to *Neutral Man* latent vector

Concept

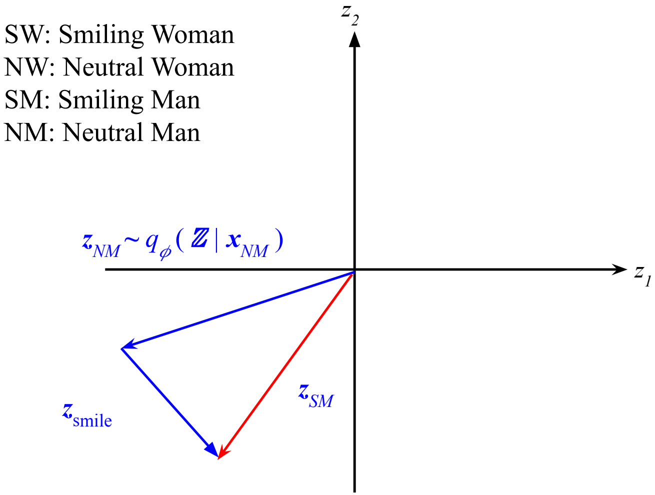

Figure: The latent vector of *Smiling Man*

Sample of Using Attribute Vectors

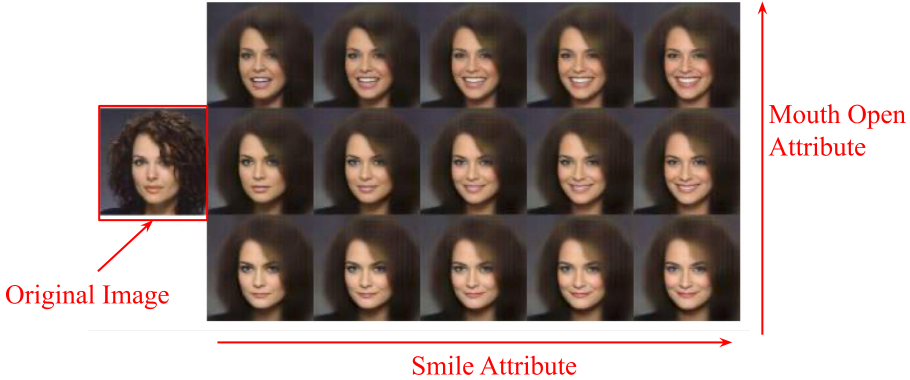

Figure: Application of attribute vectors in real worl application of face images (source: [2])

List of Abbreviations

Complete	Abbreviation
Evidence Lower-BOund	ELBO
Gaussian Mixture Model	GMM
Kullback–Leibler	KL
Left-Hand Side	LHS
Log-Likelihood	LL
Right-Hand Side	RHS
Stochastic Variational Inference	SVI
Variational AutoEncoder	VAE

References I

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