Deep Generative Models: Variational Auto Encoders

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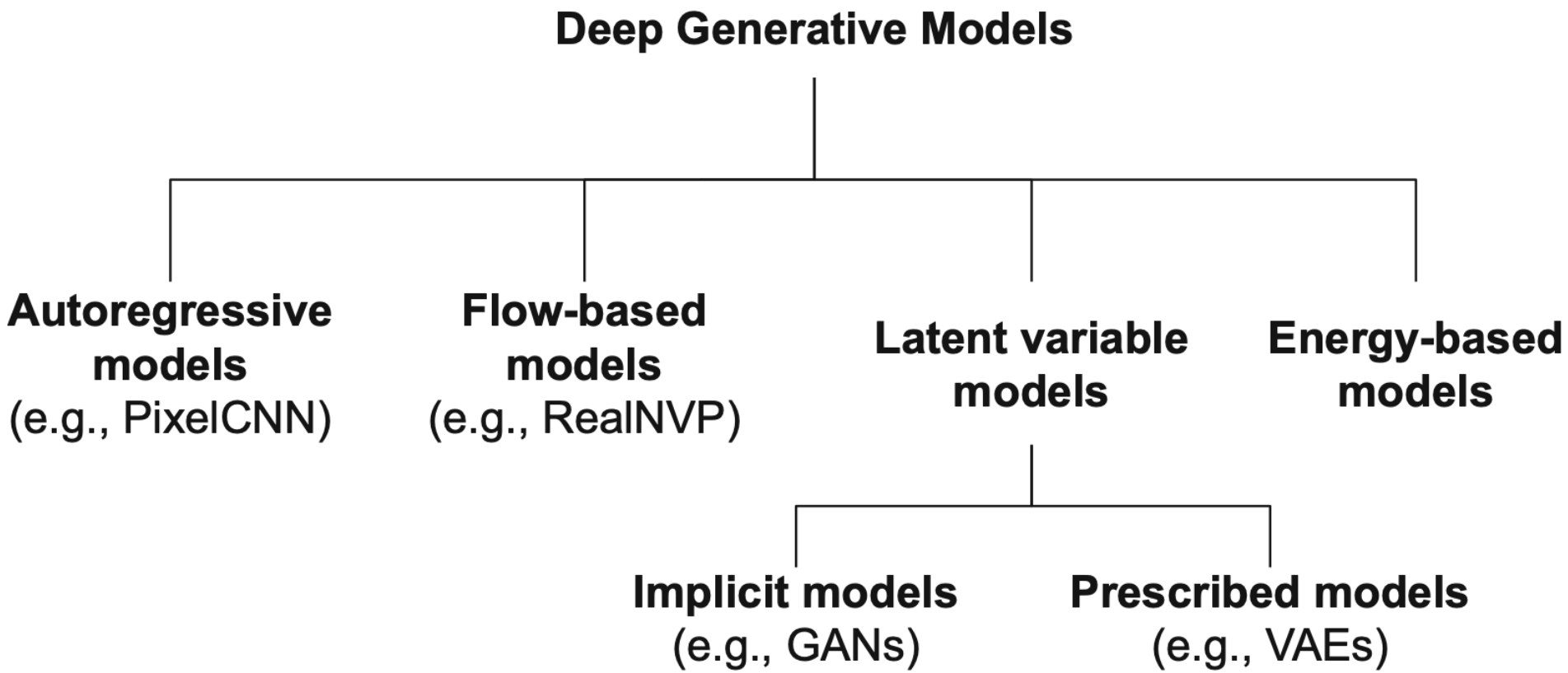
Taxonomy of Generative Models



The story up till now

- **Step 1**: We set out with our original goal of learning a model p_θ that gives maximum likelihood to our datapoints x_i

- **Step 2**: We introduced latent variables z such that $z \sim p(z)$ and $x \mid z \sim p(x \mid z)$, which gave us the marginalization $p(x) = \int p(x \mid z)\, p(z)\, dz$
  - Step 2a: When we supposed $p(z)$ was Gaussian and $p(x \mid z) = N(Wz + b, \sigma^2 I)$, we could solve for (W, b, σ^2) in closed form! This gave us PPCA

- **Step 3**: We set up variational inference because sadly, not everything in life is Gaussian and linear. This gave us a new objective

$$\max_\theta \log p_\theta(x_i) = \max_\theta \max_{q(\cdot|x_i),\forall i} \sum_{i=1}^{N} \int q(z|x_i) \log \frac{p_\theta(x_i, z)}{q\ (z|x_i)}\, dz$$

  - Step 3a: If $q(z|x)$ is easy to evaluate, we can alternate between optimizing w.r.t. θ with $q(z|x)$ fixed and vice versa, leading to the Expectation Maximization algorithm

The story continues with Variational Autoencoders

- Before introducing VAEs formally, let us decompose ELBO further

$$\max_{\theta} \log p_\theta(x_i) = \max_{\theta} \max_{q} \sum_{i=1}^{N} \int q(z|x_i) \log \frac{p_\theta(x_i, z)}{q(z|x_i)} dz$$

$$\geq \max_{\theta,\psi} \sum_{i} E_{z\sim q_\psi(z|x_i)} \log \frac{p_\theta(x_i, z)}{q_\psi(z|x_i)}$$

Evidence **L**ower **Bo**und (ELBO)

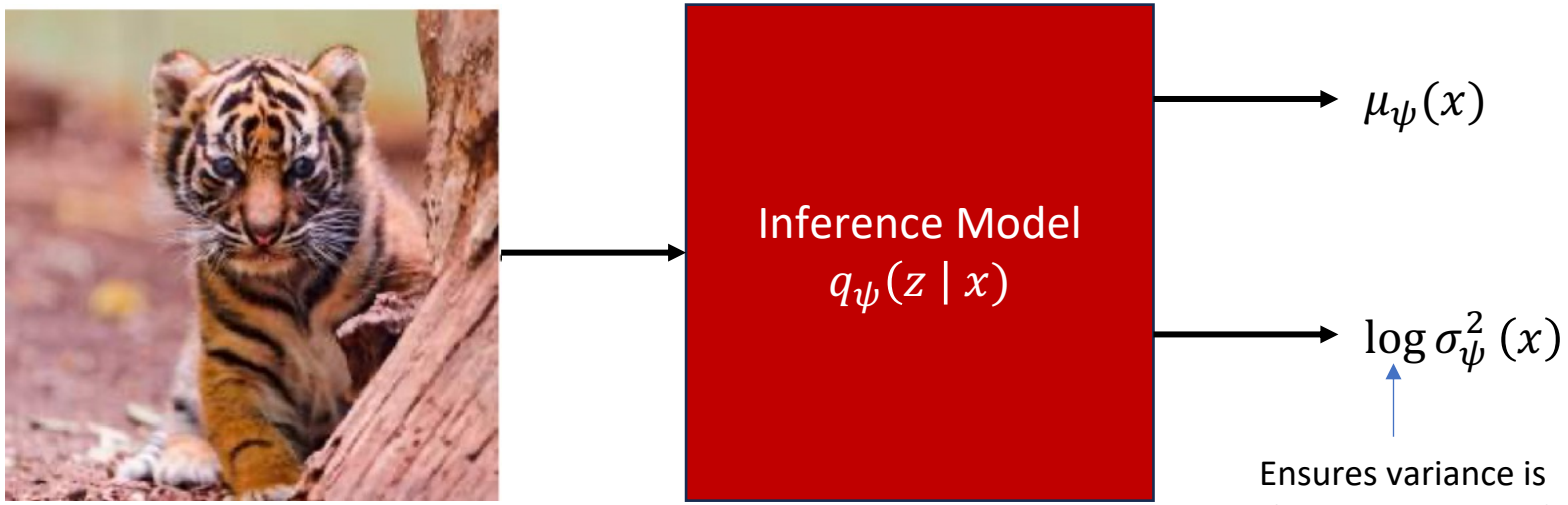
$$= \max_{\theta,\psi} \sum_{i} E_{z\sim q_\psi(z|x_i)} \log p_\theta(x_i|z) \frac{p(z)}{q_\psi(z|x_i)}$$

$$= \max_{\theta,\psi} \sum_{i} E_{z\sim q_\psi(z|x_i)} \log p_\theta(x_i|z) + E_{z\sim q_\psi(z|x_i)} \log \frac{p(z)}{q_\psi(z|x_i)}$$

$$-D_{KL}(q_\psi(z|x)||p(z))$$

Variational AutoEncoders (VAEs): Setup

- We have three models we need to define for VAE model
  1. $q_\psi(z \mid x_i)$ (Inference model): We will define as $q_\psi(z \mid x_i) = N(z; \mu_\psi(x_i), \sigma^2_\psi(x_i)I)$ i.e. a normal distribution with learned mean and covariance



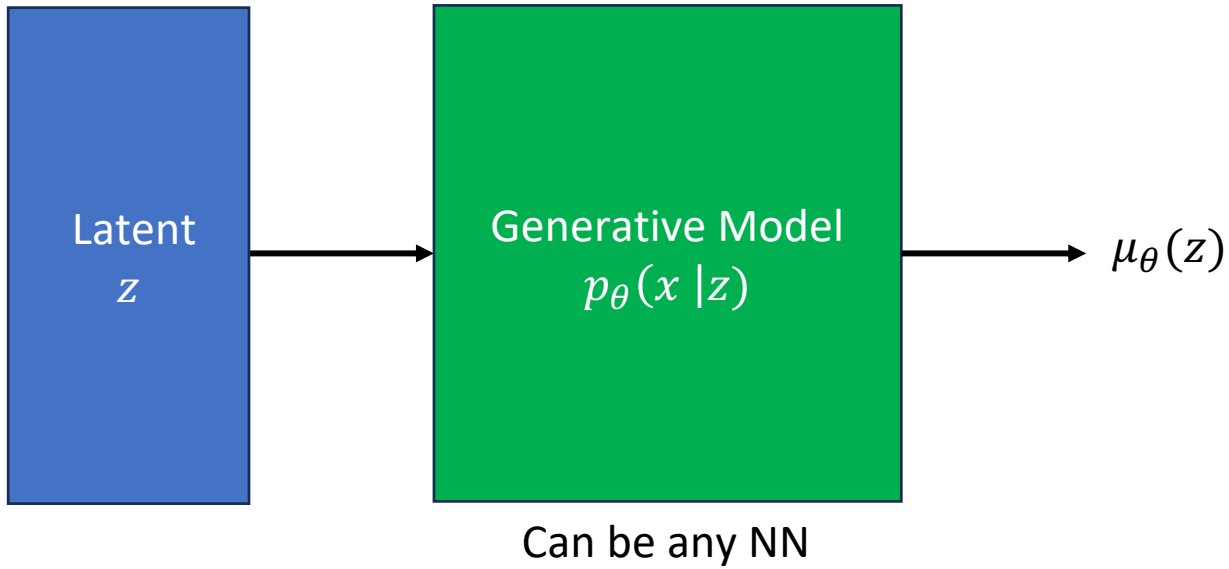
  2. $p(z)$ (Prior): We will define prior for latent variables as $p(z) = N(0, I)$

Variational AutoEncoders (VAEs): Setup

- We have three models we need to define for VAE model

  3. $\mathrm{p}_\theta(\mathrm{x} \mid \mathrm{z})$ (Generative model): We will define as $p_\theta(x \mid z) = N(z; \mu_\theta(z), \eta^2 I)$ i.e. a normal distribution with learned mean and variance

     - Note this can be defined in many different ways, yielding different models (such as a categorical distribution over 255 values of each pixel)



Variational Autoencoders: Training

Datapoint x_i

Inference Model
$q_\psi(z \mid x_i)$

μ

$\log \sigma^2$

Sample
$z \sim$
$N(z \mid \mu_\psi(x_i), \sigma^2_\psi(x_i) I)$

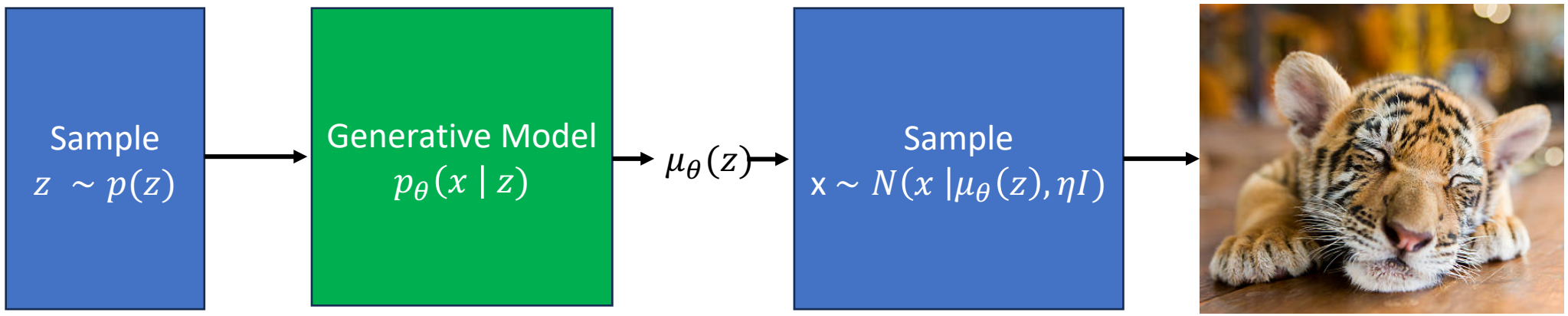
Generative Model
$p_\theta(x \mid z)$

$\mu_\theta(z)$

ELBO Objective
$\mathrm{E}_{z \sim q_\psi(z \mid x)}[\log p_\theta(x \mid z) - KL(q_\psi(z \mid x) || p(z)]$

Variational Autoencoders after Training

- Suppose we have learned VAE using the ELBO loss (details to follow).
- Then, as a generative model, we just sample $z \sim p(z)$ and use the fixed generative model $p_\theta(x \mid z)$



Computing the ELBO Loss

$$L_{\theta,\psi}(x) := \mathbb{E}_{z\sim q_\psi(z\,|x)}\ \log p_\theta(x\,|z) + \mathbb{E}_{z\sim q_\psi(z\,|\,x)} \log \frac{p(z)}{q_\psi(z\,|x)}$$

- Term 1 (Reconstruction Error)
  - Because $p_\theta(x|z) = \mathcal{N}(x|\mu_\theta(z), \eta I)$, we have $\log p_\theta(x|z) = -\frac{1}{2\eta}\left|\left|x - \mu_\theta(z)\right|\right|_2^2 + const.$
  - We can approximate the expectation over $z \sim q_\psi(z\,|x)$ by an average over $q_\psi(z\,|x)$
  - Recall that the expectation of a function $f(X)$ w.r.t. a random variable $X \sim p$ can be approximated from i.i.d. samples $x_i \sim p$, $i = 1, \ldots, N$, via Monte Carlo averages

$$\mathbb{E}_{X\sim p}[f(X)] = \int\ f(x)p(x)dx \approx \frac{1}{N}\sum f(x_i)$$

  - Applying the above formula to M i.i.d. samples $z_j \sim q_\psi(Z\ |\ x)$ we get

$$\mathbb{E}_{Z\sim q_\psi}[\log p_\theta(X\ |\ Z)] \approx \frac{1}{M}\sum \log p_\theta(\,x\ |\ z_j\,) = \frac{1}{2\eta M}\sum\ ||x - \mu_\theta(z_j)||_2^2$$

Computing the ELBO Loss

$$L_{\theta,\psi}(x) := \mathbb{E}_{z\sim q_\psi(z\,|x)}\ \log p_\theta(x\,|z) + \mathbb{E}_{z\sim q_\psi(z\,|\,x)} \log \frac{p(z)}{q_\psi(z\,|x)}$$

- Term 2 (Regularization to Prior)
  - Because $\mathbb{E}_{z\sim q_\psi(z|x)} \log \frac{p(z)}{q_\psi(z|x)} = -D_{KL}(q_\psi(z|x)||p(z))$, $q_\psi(z|x) = N(z|\mu_\psi(x), \sigma_\psi^2(x)I)$, $p(z) = N(0, I)$, the second term is a KL divergence between two d-dimensional Gaussians, which has a closed form solution

$$KL(N(\mu_1, \sigma_1^2 I)||N(\mu_2, \sigma_2^2 I)) = \log\left(\frac{\sigma_2}{\sigma_1}\right) - \frac{d}{2} + \frac{d\sigma_1^2 + ||\mu_1 - \mu_2||_2^2}{2\sigma_2^2}$$

  - Applying the above formula to our VAE model yields,

$$KL\big(q_\psi(z\,|x)||p(z)\big) = -\log\Big(\sigma_\psi(x)\Big) + \frac{d\sigma_\psi^2(x) + ||\mu_\psi(x)\,||_2^2}{2} + constant$$

  - Note this term does not require any sampling w.r.t. z because the expectation is computed in closed form thanks for the KL formula for Gaussians.

Maximizing ELBO: How to Optimize?

- **ELBO objective**: We want to solve the following optimization problem:

$$\max_{\theta,\psi} \sum_i L_{\theta,\psi}(x_i) = \sum_i E_{z\sim q_\psi(z\,|x_i)} \log \frac{p_\theta(x_i, z)}{q_\psi(z\,|x_i)}$$

- **Simple idea**: Just alternate gradient ascent wrt θ, ψ on objective function

$$\theta_{k+1} = \theta_k + \alpha \frac{\delta L}{\delta \theta}(\theta_k, \psi_k)$$

$$\psi_{k+1} = \psi_k + \alpha \frac{\delta L}{\delta \psi}(\theta_k, \psi_k)$$

Stochastic Optimization of ELBO wrt θ

- **Issue**: Computing ∇_θ (ELBO) is not easy because of expectation w.r.t. latent z.
- **Solution**: Compute an unbiased estimator

$$\nabla_\theta L_{\theta,\psi}(x) = \nabla_\theta E_{z\sim q_\psi(z\,|x)}\left[\log(p_\theta(x\,|z))\right] + E_{z\sim q_\psi(z\,|\,x)}\left[\log\left(\frac{p(z)}{q_\psi(z\,|x)}\right)\right]$$

$$= E_{z\sim q_\psi(z\,|x)}[\nabla_\theta \log p_\theta(x|z)]$$

$$= -\frac{1}{2\eta} E_{z\sim q_\psi(z\,|x)} \nabla_\theta \left|\left|x\ - \mu_\theta(z)\right|\right|_2^2$$

- We can take sample averages to compute an unbiased estimator
  - For each datapoint x, compute $q_\psi(z\,|x)$ through encoder, which gives $\mu_\psi(x), \sigma_\psi^2(x)$
  - Sample $z_j \sim N\left(\mu_\psi(x), \sigma_\psi^2(x)I\right)$, find $\mu_\theta\left(z_j\right)$ through decoder
  - Estimate gradient from M samples: $\nabla_\theta L_{\theta,\psi}(x) \approx -\frac{1}{2\eta M}\sum_j \nabla_\theta \left|\left|x - \mu_\theta\left(z_j\right)\right|\right|_2^2$

Stochastic Optimization of ELBO wrt ψ

- Here, we cannot just switch gradient and expectation because both are wrt to ψ

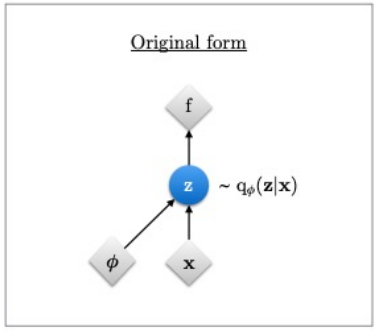
$$\nabla_\psi E_{z\sim q_\psi(z|x)}[\log p_\theta(x\,,z) - \log q_\psi(z\,|x)] \neq E_{z\sim q_\psi(z|x)}\nabla_\psi[\log p_\theta(x,z) - \log q_\psi(z\,|x)]$$

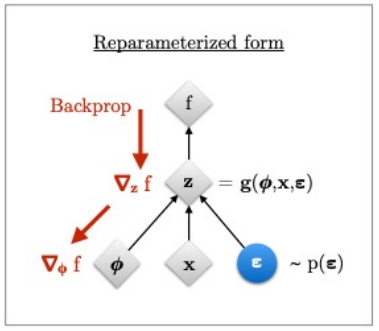
- Reparameterization trick
  - Because $q_\psi(z|x) = N(z;\mu_\psi(x),\sigma_\psi(x)I)$, we can rewrite samples $z\sim q_\psi(z\,|x)$ as

$$z_\psi = g(\epsilon,\psi,x) = \mu_\psi(x) + \sigma_\psi(x)\epsilon \quad \text{for} \quad \epsilon\sim N(0,I)$$

  - With this change of variables, we can rewrite the gradient of the loss as:

$$\nabla_\psi L_{\theta,\psi}(x) = \nabla_\psi E_{z\sim q_\psi(z\,|x)}\left[\log p_\theta\left(x,z_\psi\right) - \log q_\psi\left(z_\psi\,|x\right)\right]$$
$$= \nabla_\psi E_{\epsilon\sim N(0,I)}\left[\log p_\theta\left(x,z_\psi\right) - \log q_\psi\left(z_\psi\,|x\right)\right]$$

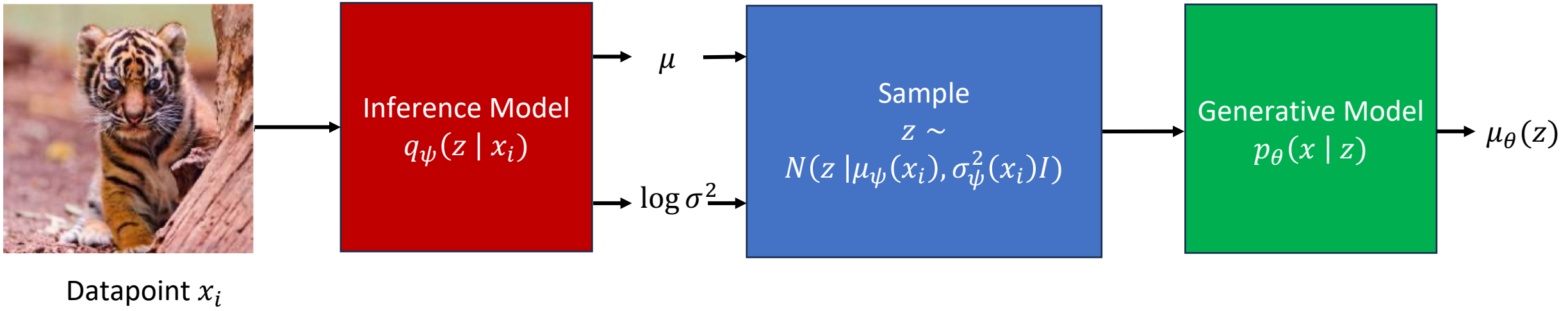




Gradient and expectation can now be switched! So as before, we compute an unbiased estimator by sampling many ϵ

Putting it all together

- Variational Autoencoder
  - We modelled inference and generative model as deep networks
  - We interpreted ELBO as an expected reconstruction error plus a KL-regularization to prior
  - Then, we rewrote the sampling in the latent space using the reparameterization trick
  - Finally, we derived stochastic gradient estimates to optimize the ELBO and learn a VAE



VAE's in Action

- $q_\psi(z\,|x) = N(z\,|\mu_\psi(x), \sigma^2_\psi(x))$
- $p(z) = N(z|0, I)$
- $p_\theta(x\,|z) = Categorical\,(x\,|\pi_\theta\,(z))$ Note this is different from the model considered up till now!

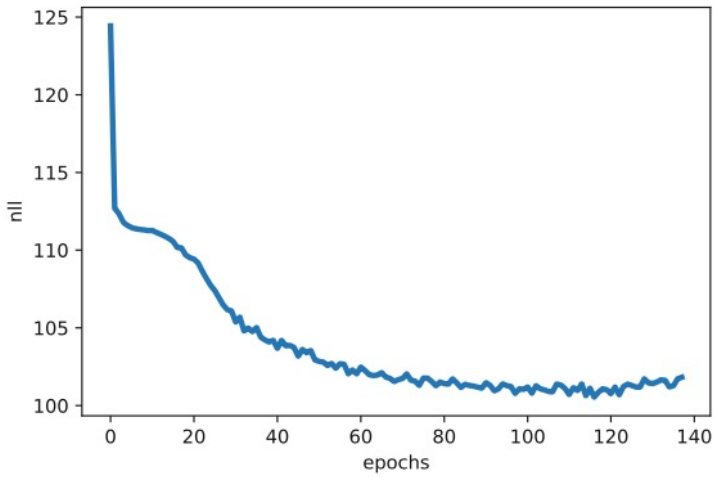
- Encoder network: $x \in R^D$ -> Linear(D, 256) -> LeakyReLU -> Linear (256, $2d$) -> split into $\mu \in R^d, \log \sigma^2 \in R^d$

- Decoder network: $z \in R^d$ -> Linear(d, 256) -> LeakyReLU -> Linear(256, D) -> softmax

VAE's for Generation of MNIST Digits

A

B



C

Fig. 4.4 An example of outcomes after the training: (**a**) Randomly selected real images. (**b**) Unconditional generations from the VAE. (**c**) The validation curve during training

Typical Issues with VAEs

- ELBO: $\ln p(\mathbf{x}) = \underbrace{\mathbb{E}_{\mathbf{z}\sim q_\psi(\mathbf{z}|\mathbf{x})}[\ln p_\theta(\mathbf{x} \mid \mathbf{z})] - KL\left[q_\psi(\mathbf{z} \mid \mathbf{x}) \parallel p(\mathbf{z})\right]}_{ELBO} + \underbrace{KL\left[q_\psi(\mathbf{z} \mid \mathbf{x}) \parallel p_\theta(\mathbf{z} \mid \mathbf{x})\right]}_{\geq 0}$
- Posterior collapse
  - If the decoder is so powerful that it treats z as noise, then $\forall_{\mathbf{x}} q_\phi(\mathbf{z} \mid \mathbf{x}) = p(\mathbf{z})$
- Mismatch between prior $p(\boldsymbol{z})$ and aggregated posterior $q_\phi(\mathbf{z}) = \frac{1}{N}\sum_i q_\psi(\mathbf{z} \mid \mathbf{x}_i)$
  - Prior assigns high probability but aggregated posterior assigns low probability, or other way around.
  - Sampling from such regions provides unrealistic latent values and the decoder produces images of very low quality.
- Out-of-distribution samples

Aggregated posterior

Fig. 4.5 An example of the aggregated posterior. Individual points are encoded as Gaussians in the 2D latent space (magenta), and the mixture of variational posteriors (the aggregated posterior) is presented by contours

$$q_\psi(\mathbf{z}) = \frac{1}{N}\sum_i q_\psi(\mathbf{z} \mid \mathbf{x}_i)$$

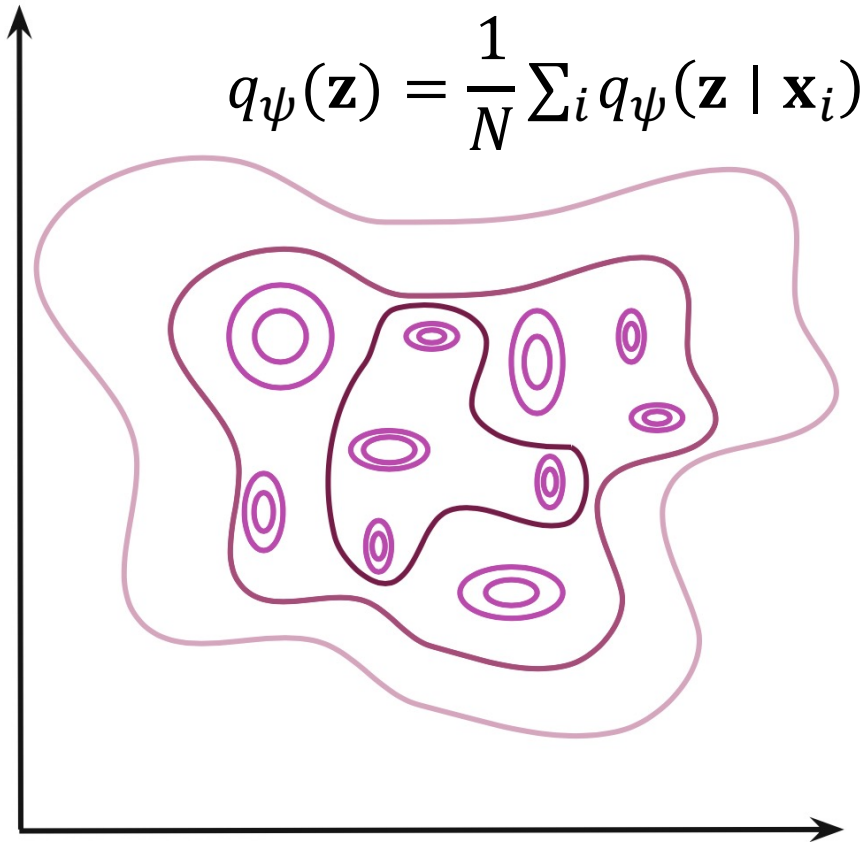
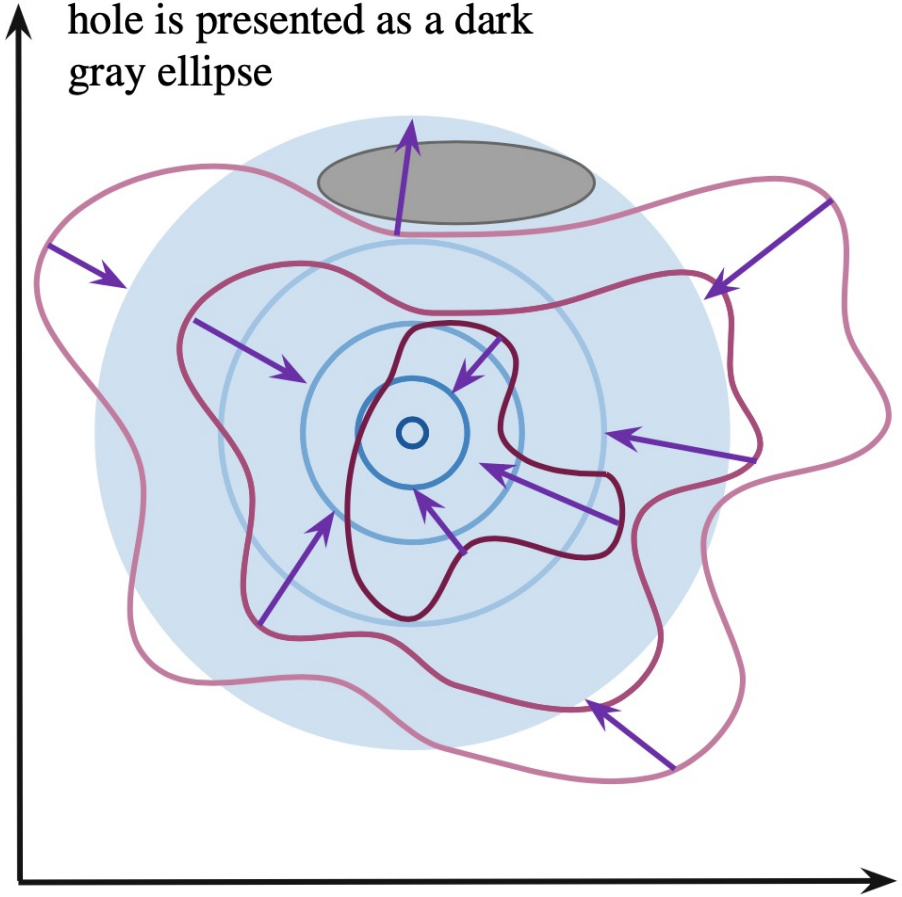


Fig. 4.6 An example of the effect of the cross-entropy optimization with a non-learnable prior. The aggregated posterior (purple contours) tries to match the non-learnable prior (in blue). The purple arrows indicate the change of the aggregated posterior. An example of a hole is presented as a dark gray ellipse



Improving VAEs

- The ELBO consists of two parts: first, the reconstruction error

$$RE \triangleq \mathbb{E}_{\mathbf{x}\sim p_{\text{data}}(\mathbf{x})}\left[\mathbb{E}_{q_\psi(\mathbf{z}|\mathbf{x})}[\ln p_\theta(\mathbf{x} \mid \mathbf{z})]\right]$$

- Then the regularization term between the encoder and the prior

$$\begin{aligned}\Omega \quad &\triangleq \mathbb{E}_{\mathbf{x}\sim p_{\text{data}}(\mathbf{x})}\left[\mathbb{E}_{q_\psi(\mathbf{z}|\mathbf{x})}\left[\ln p(\mathbf{z}) - \ln q_\psi(\mathbf{z} \mid \mathbf{x})\right]\right] \\ &= -KL\left[q_\psi(\mathbf{z}) \parallel p(\mathbf{z})\right] + \mathbb{H}\left[q_\psi(\mathbf{z} \mid \mathbf{x})\right]\end{aligned}$$

- For a Gaussian, the entropy is maximized when sigma -> infinity