Variational Autoencoders

Vinay Setty
vinay.j.setty@uis.no

University of Stavanger

Information Access & Artificial Intelligence

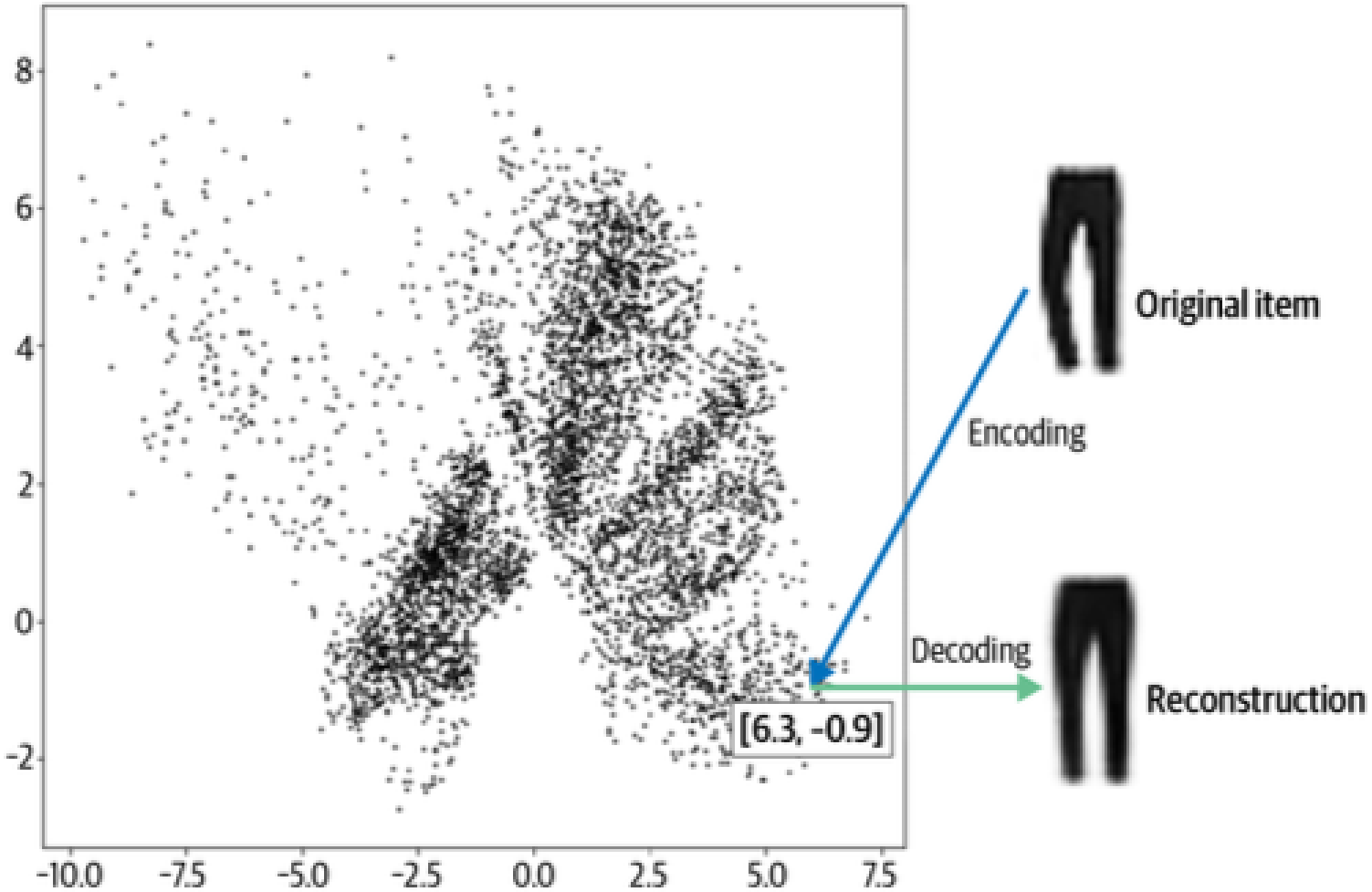
Department of Electrical Engineering and Computer Science
University of Stavanger

January 14, 2026

Overview

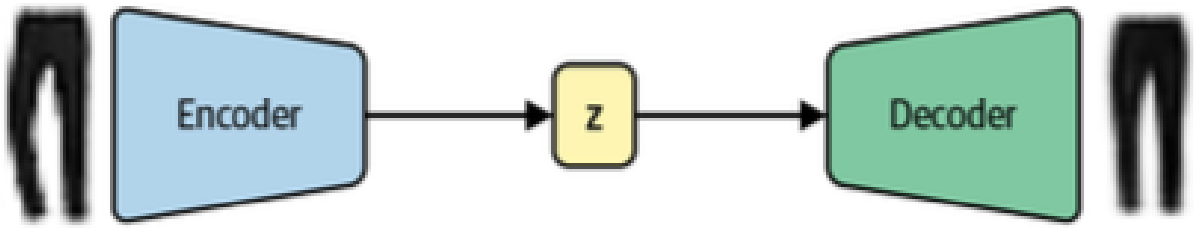
Autoencoders

Autoencoders (cont.)



Autoencoder Definition

- Learn an identity function with a bottleneck
- Compress data into a low-dimensional latent space
- Reconstruct input from the compressed code



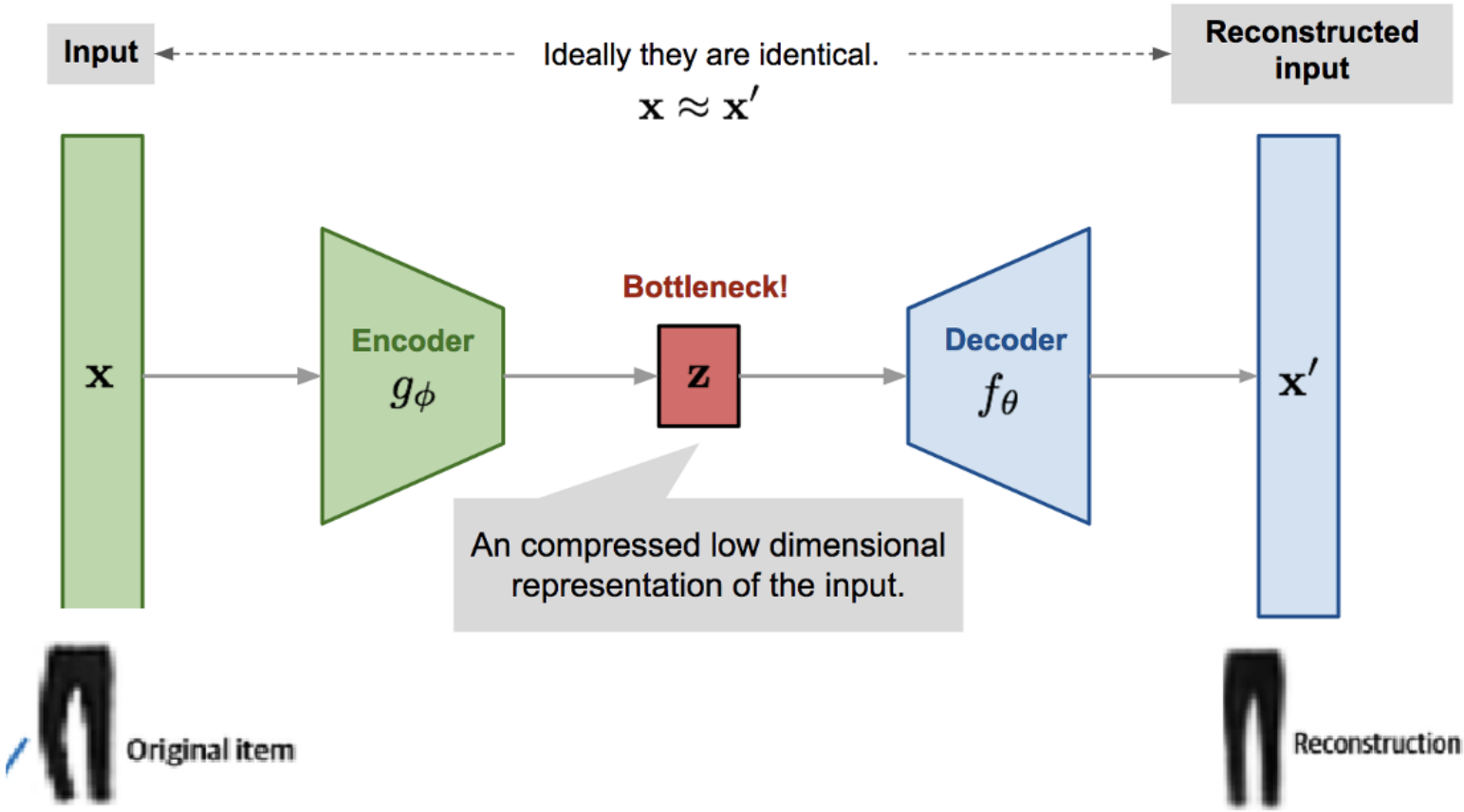
Source: [1]

Autoencoder Definition (cont.)

Notations:

- Dataset: $\mathcal{D} = \{x^{(1)}, x^{(2)}, \ldots, x^{(n)}\}$, $|\mathcal{D}| = n$
- Each sample: $x^{(i)} \in \mathbb{R}^d$, e.g. $x^{(i)} = [x_1^{(i)}, \ldots, x_d^{(i)}]$
- One data point: $x \in \mathcal{D}$
- Reconstruction: x'

Autoencoder Definition (cont.)



Autoencoder Definition (cont.)

$$z = g_\phi(x)$$
$$x' = f_\theta(g_\phi(x))$$

- Bottleneck z is the learned representation
- Objective is reconstruction quality, not likelihood modeling
- Good z should capture factors useful for reconstructing x

A common choice (MSE):

$$L_{AE}(\theta, \phi) = \frac{1}{n} \sum_{i=1}^{n} \left(x^{(i)} - f_\theta(g_\phi(x^{(i)})) \right)^2$$

- Cross-entropy often used for binary inputs with sigmoid output
- MSE is typical when outputs are real-valued

Limitations of Autoencoders

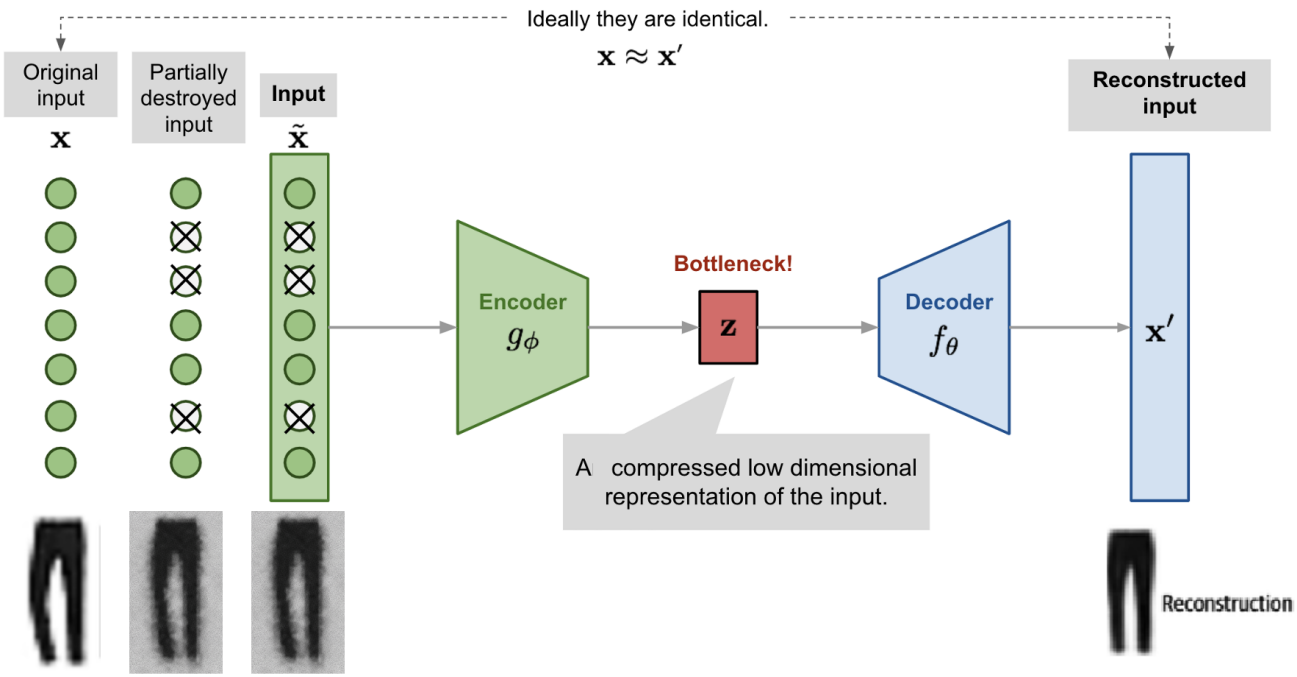
- Autoencoders do not regularize the latent space risking **overfitting**
- Encoded data occupy **disconnected** regions in latent space
- Large empty regions ("**holes**") appear between encoded samples
- Latent points inside these holes do not decode to valid data
- Sampling often passes through holes and fails

Denoising Autoencoder (DAE): Motivation

Plain AE risks learning a trivial identity map if capacity is too high.

DAE prevents this by:

- Corrupting inputs stochastically
- Training the model to reconstruct the clean x



DAE: Corruption process and objective

Corruption:

$$\tilde{x} \sim M_D(\tilde{x}|x)$$

Training objective:

$$L_{DAE}(\theta, \phi) = \frac{1}{n} \sum_{i=1}^{n} \left(x^{(i)} - f_\theta(g_\phi(\tilde{x}^{(i)})) \right)^2$$

- M_D can be masking noise, Gaussian noise, etc.
- Forces the encoder to learn dependencies among input dimensions

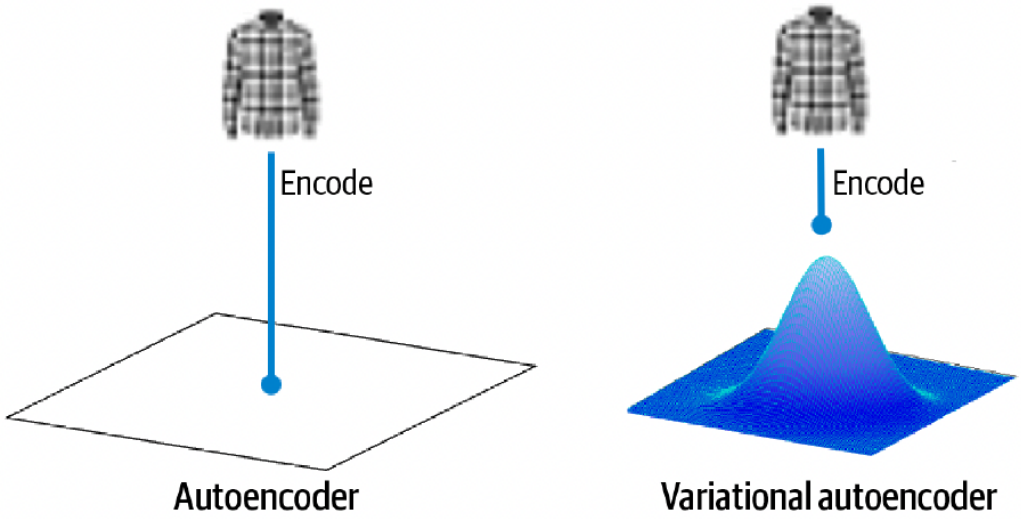
VAE: Shift in viewpoint

VAE is rooted in variational Bayesian inference:

- Instead of mapping $x \rightarrow z$ deterministically, map to a distribution
- Latent variables have a prior and generate data via a likelihood

VAE: Intuition

VAE: Intuition (cont.)



Source: [2]

VAE: Prior, likelihood, posterior

- Prior: $p_\theta(z)$
- Likelihood: $p_\theta(x|z)$
- Posterior: $p_\theta(z|x)$ (intractable in general)

Generation story:

1. Sample $z \sim p_{\theta^*}(z)$
2. Generate $x \sim p_{\theta^*}(x|z)$

VAE: Maximum likelihood objective

Optimize parameters to maximize probability of real data:

$$\theta^* = \arg\max_\theta \prod_{i=1}^{n} p_\theta(x^{(i)})$$

Often in log space:

$$\theta^* = \arg\max_\theta \sum_{i=1}^{n} \log p_\theta(x^{(i)})$$

Marginal likelihood:

$$p_\theta(x^{(i)}) = \int p_\theta(x^{(i)}|z) p_\theta(z)\, dz$$

- Integral over all z is expensive
- Introduce an approximation $q_\phi(z|x)$

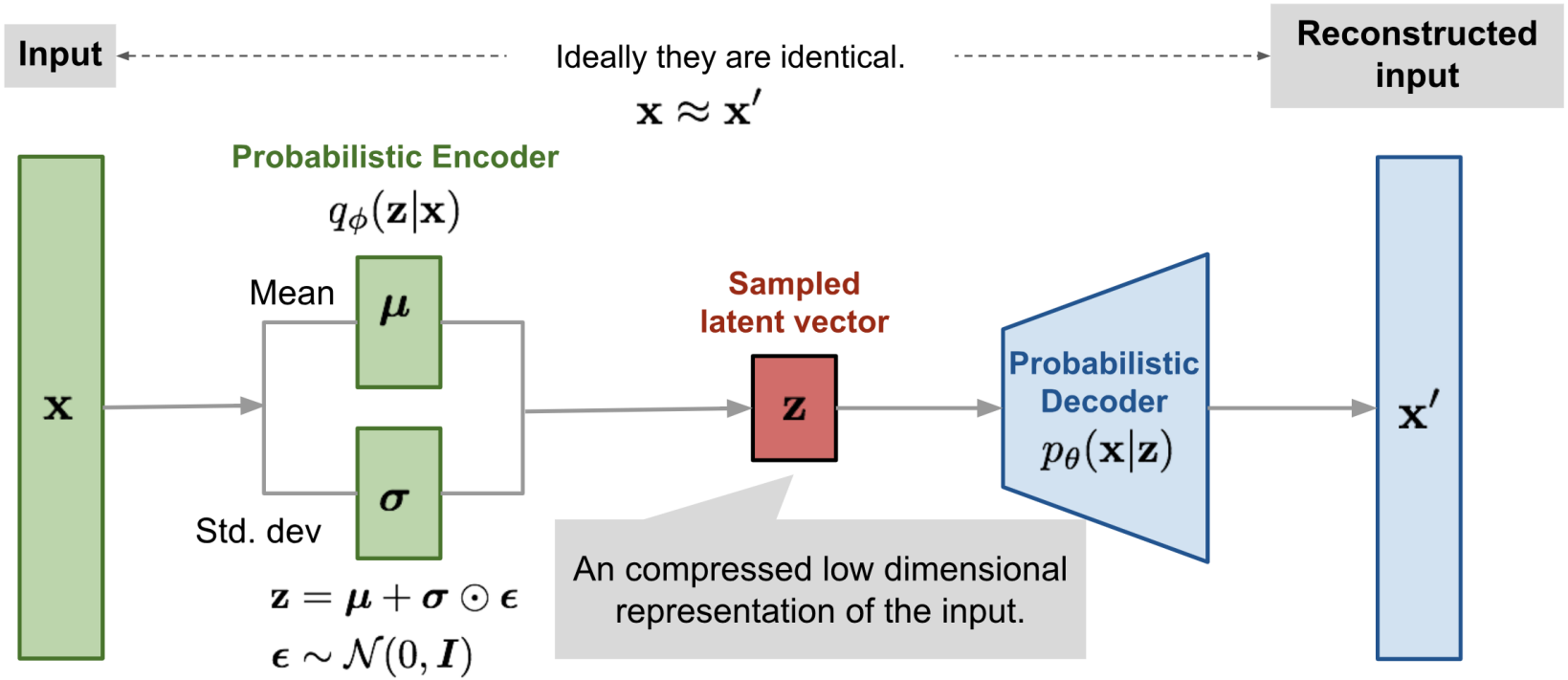
VAE: Approximate posterior (probabilistic encoder)

Introduce:

$$q_\phi(z|x)$$

- $q_\phi(z|x)$ approximates the intractable $p_\theta(z|x)$
- Makes inference amortized: one network predicts distribution params from x
- Structure resembles AE:
  - Decoder: $p_\theta(x|z)$
  - Encoder: $q_\phi(z|x)$

VAE Architecture



KL Divergence: Intuition

What is KL divergence?

$$D_{KL}(q \,\|\, p) = \mathbb{E}_q \left[\log \frac{q(z)}{p(z)} \right]$$

- Measures how much a distribution q deviates from a reference distribution p
- Always non-negative
- Equal to zero only when $q = p$
- Not symmetric and not a distance

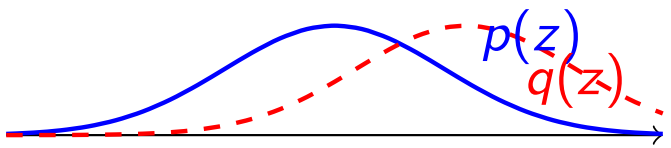
KL Divergence: Intuition (cont.)

Intuition

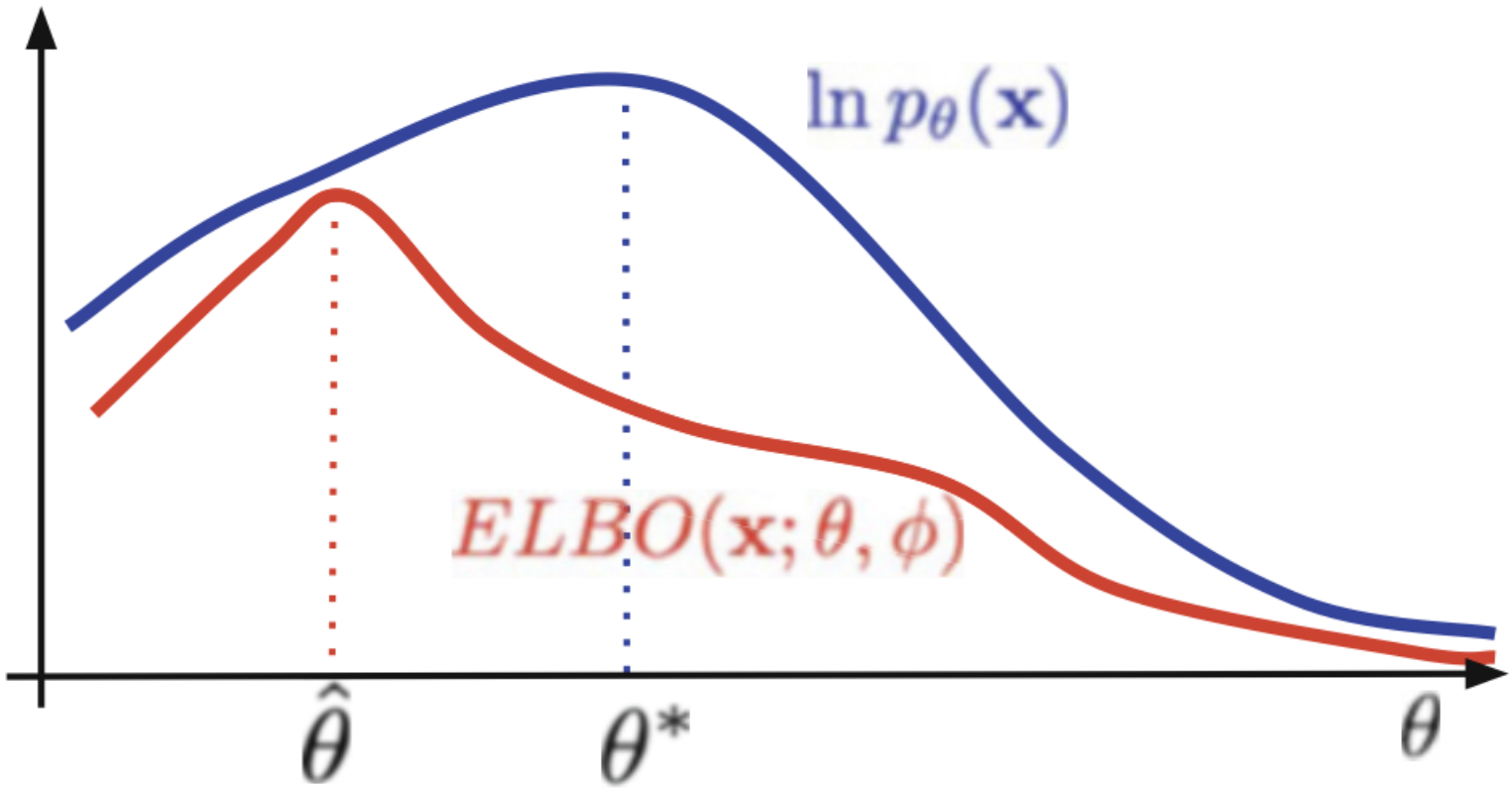
- Think of p as the rule you agreed to follow
- q is what you actually do
- KL divergence is the *penalty for breaking the rule*
- Larger mismatch means higher cost

Example (VAE context)

- $p(z) = \mathcal{N}(0, I)$ is the prior
- $q(z|x)$ is the encoder distribution
- KL penalizes latent codes that drift too far from zero or become too narrow



Evidence Lower Bound (ELBO)



Source: [3]

ELBO derivation via Jensen (amortized VI)

Start from the marginal likelihood:

$$p(x) = \int p(x|z)\, p(z)\, dz = \mathbb{E}_{z\sim p(z)}[p(x|z)] \approx \frac{1}{K}\sum_{k=1}^{K} p(x|z_k), \quad z_k \sim p(z).$$

Introduce an auxiliary distribution $q_\phi(z)$:

$$\ln p(x) = \ln \int \frac{q_\phi(z)}{q_\phi(z)} p(x|z)p(z)\, dz = \ln \mathbb{E}_{z\sim q_\phi(z)}\left[\frac{p(x|z)p(z)}{q_\phi(z)}\right].$$

Apply Jensen:

$$\ln p(x) \geq \mathbb{E}_{z\sim q_\phi(z)}\Big[\ln p(x|z) + \ln p(z) - \ln q_\phi(z)\Big].$$

Amortize with $q_\phi(z|x)$:

$$\ln p(x) \geq \mathbb{E}_{z\sim q_\phi(z|x)}[\ln p_\theta(x|z)] - \mathbb{E}_{z\sim q_\phi(z|x)}[\ln q_\phi(z|x) - \ln p(z)]\,.$$

$$\boxed{\mathcal{L}_{\text{ELBO}}(x;\theta,\phi) = \mathbb{E}_{q_\phi(z|x)}[\ln p_\theta(x|z)] - D_{KL}(q_\phi(z|x)\|p(z))}$$

Alternative ELBO derivation

$$\ln p_\theta(x) = \mathbb{E}_{z\sim q_\phi(z|x)}[\ln p_\theta(x)] \tag{1}$$

$$= \mathbb{E}_{z\sim q_\phi(z|x)}\left[\ln \frac{p_\theta(z|x)p_\theta(x)}{p_\theta(z|x)}\right] \tag{2}$$

$$= \mathbb{E}_{z\sim q_\phi(z|x)}\left[\ln \frac{p_\theta(x|z)p(z)}{p_\theta(z|x)}\right] \tag{3}$$

$$= \mathbb{E}_{z\sim q_\phi(z|x)}\left[\ln \frac{p_\theta(x|z)p(z)\,q_\phi(z|x)}{p_\theta(z|x)\,q_\phi(z|x)}\right] \tag{4}$$

$$= \mathbb{E}_{z\sim q_\phi(z|x)}\left[\ln p_\theta(x|z) - \ln \frac{q_\phi(z|x)}{p(z)} + \ln \frac{q_\phi(z|x)}{p_\theta(z|x)}\right] \tag{5}$$

$$= \mathbb{E}_{z\sim q_\phi(z|x)}[\ln p_\theta(x|z)] - D_{KL}(q_\phi(z|x)\|p(z)) + D_{KL}(q_\phi(z|x)\|p_\theta(z|x))\,. \tag{6}$$

ELBO and the KL gap to the true posterior

$$\ln p_\theta(x) = \mathbb{E}_{z\sim q_\phi(z|x)}\left[\ln p_\theta(x|z) - \ln \frac{q_\phi(z|x)}{p(z)} + \ln \frac{q_\phi(z|x)}{p_\theta(z|x)}\right] \tag{7}$$

$$= \mathbb{E}_{z\sim q_\phi(z|x)}[\ln p_\theta(x|z)] - D_{KL}(q_\phi(z|x)\|p(z)) + D_{KL}(q_\phi(z|x)\|p_\theta(z|x))\,. \tag{8}$$

$$\ln p_\theta(x) = \underbrace{\mathbb{E}_{q_\phi(z|x)}[\ln p_\theta(x|z)] - D_{KL}(q_\phi(z|x)\|p(z))}_{\text{ELBO}} + \underbrace{D_{KL}(q_\phi(z|x)\|p_\theta(z|x))}_{\geq 0}\,. \tag{9}$$

Key point: The term $D_{KL}(q_\phi(z|x)\|p_\theta(z|x))$ measures the gap between the variational posterior and the *true* posterior. Since $p_\theta(z|x)$ is intractable and the KL divergence is always non-negative, this term cannot be minimized directly and does not affect optimization. Maximizing the ELBO is therefore equivalent to maximizing a lower bound on $\ln p_\theta(x)$.

ELBO: Why "lower bound"

$$-L_{VAE} = \log p_\theta(x) - D_{KL}(q_\phi(z|x) \| p_\theta(z|x))$$

log

$p_\theta(x)$ because KL divergence is non-negative.

- Maximizing ELBO is maximizing a lower bound on $\log p_\theta(x)$
- Also minimizes the gap between approximate and true posterior

Reparameterization trick: The problem

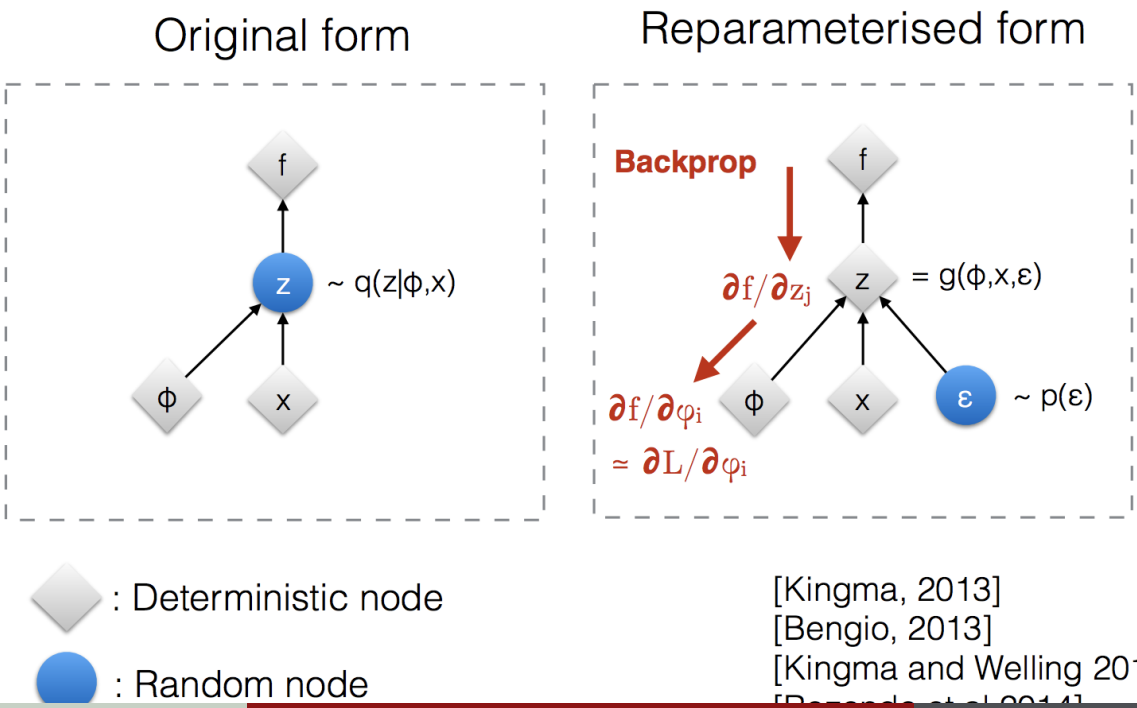
The reconstruction term uses sampling:

$$z \sim q_\phi(z|x)$$

Sampling is stochastic, so naive backpropagation does not work.

Goal:

- Express sampling as a deterministic transform of noise
- Push randomness into an auxiliary variable independent of ϕ



[Kingma, 2013]
[Bengio, 2013]
[Kingma and Welling 2014]

Reparameterization trick: General form

Write the random variable as:

$$z = T_\phi(x, \epsilon)$$

where:

- ϵ is auxiliary independent noise
- T_ϕ is a differentiable transformation parameterized by ϕ

Reparameterization trick: Gaussian case (as given)

Assume diagonal Gaussian:

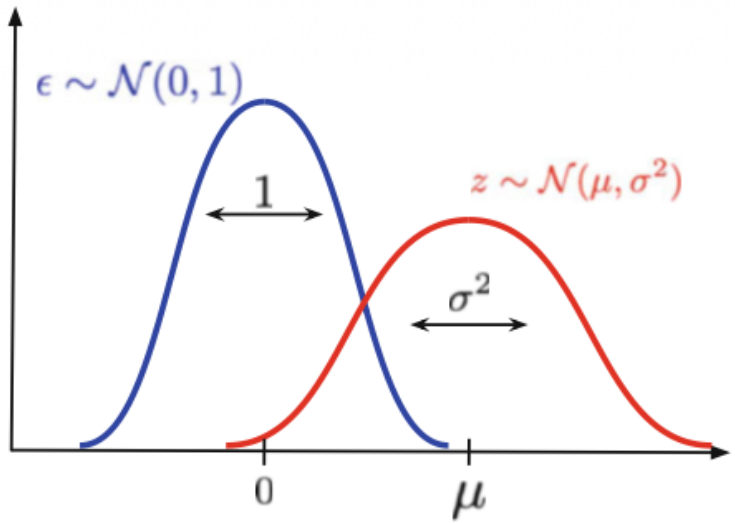
$$z \sim q_\phi(z|x^{(i)}) = \mathcal{N}(z; \mu^{(i)}, \sigma^{2(i)} I)$$

Then:

$$z = \mu + \sigma \odot \epsilon, \quad \text{where } \epsilon \sim \mathcal{N}(0, I)$$

$\odot$ denotes element-wise product.

- Learn μ and σ via encoder network outputs
- Gradients pass through μ, σ while randomness stays in ϵ



Core Limitations of VAEs

- Loose likelihood estimation due to the ELBO gap
- Posterior collapse with expressive decoders: Approximate posterior matches the prior and the latent variables carry little to no information about the data
- Latent space holes caused by prior–aggregated posterior mismatch: Mismatch between the aggregated posterior and the assumed prior, usually a standard Gaussian
- Weak out-of-distribution detection
- Trade-off between reconstruction faithfulness and regularization

Optimization and Representation Issues

- ELBO optimization does not guarantee informative latents: No meaningful semantic structure of latent variables.
- Powerful decoders can ignore latent variables entirely
- Fixed simple priors (e.g, isotropic Gaussian) impose suboptimal latent geometry
- Disentanglement is not ensured without additional inductive bias

Architectural Variants of VAEs

- β-VAE and information-theoretic objectives
- Hierarchical VAEs for multi-scale latent structure
- Discrete VAEs using Gumbel–Softmax or gradient estimators
- Hyperspherical and hyperbolic latent spaces

Improving VAEs: Priors and Posteriors

- Learnable priors: VampPrior, mixture priors, flow-based priors
- Expressive posteriors via normalizing flows
- Adversarially learned aggregated posteriors
- Resampling and hierarchical priors to reduce latent mismatch

β–VAE: Disentanglement intuition

A representation is disentangled if:

- Each latent variable is sensitive to one generative factor
- Relatively invariant to other factors

Examples of factors in faces:

- skin color, hair color, hair length, emotion, glasses, etc.

β–VAE increases pressure toward factorized, efficient latent codes.

β–VAE: Constrained objective

Optimization problem:

$$\max_{\phi,\theta} \mathbb{E}_{x\sim\mathcal{D}}\left[\mathbb{E}_{z\sim q_\phi(z|x)} \log p_\theta(x|z)\right]$$

subject to:

$$D_{KL}(q_\phi(z|x)\|p_\theta(z)) < \delta$$

β–VAE: Lagrangian form

Define Lagrangian:

$$F(\theta, \phi, \beta) = \mathbb{E}_{z \sim q_\phi(z|x)} \log p_\theta(x|z) - \beta \left(D_{KL}(q_\phi(z|x) \| p_\theta(z)) - \delta \right)$$

Expand:

$$= \mathbb{E}_{z \sim q_\phi(z|x)} \log p_\theta(x|z) - \beta D_{KL}(q_\phi(z|x) \| p_\theta(z)) + \beta\delta$$

Lower bound:

$$\geq \mathbb{E}_{z \sim q_\phi(z|x)} \log p_\theta(x|z) - \beta D_{KL}(q_\phi(z|x) \| p_\theta(z))$$

β–VAE: Loss function (as given)

$$L_{\beta VAE}(\phi, \beta) = -\mathbb{E}_{z \sim q_\phi(z|x)} \log p_\theta(x|z) + \beta D_{KL}(q_\phi(z|x) \| p_\theta(z))$$

- $\beta = 1$ recovers VAE
- $\beta > 1$ strengthens the bottleneck constraint
- Tradeoff: reconstruction quality vs disentanglement pressure

Summary

- VAEs are flexible but fragile under naive design choices
- Many failures stem from weak inductive bias in ELBO training
- Modern VAE variants focus on priors, hierarchy, and inference
- Architectural bias is as important as objective design

Bibliography

[1] L. Weng, "From autoencoder to beta-vae," *lilianweng.github.io*, 2018. [Online]. Available: https://lilianweng.github.io/posts/2018-08-12-vae/.

[2] D. Foster, *Generative deep learning*. " O'Reilly Media, Inc.", 2022.

[3] J. M. Tomczak, *Deep Generative Modeling*, 2nd ed. Springer Cham, 2024, ISBN: 978-3-031-64086-5. DOI: 10.1007/978-3-031-64087-2. [Online]. Available: https://link.springer.com/book/10.1007/978-3-031-64087-2.