

# Variational Autoencoder - Derivations & Proofs

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## 1 Mathematical Derivations & Proofs

### 1.1 Introduction

A Variational Autoencoder (VAE) is a latent-variable generative model trained by maximizing a tractable lower bound on the log-evidence (marginal likelihood) of the data. The model posits a prior over latent codes  $\mathbf{z}$  and a conditional likelihood (decoder)  $p_{\theta}(\mathbf{x} | \mathbf{z})$ ; inference of the intractable posterior  $p_{\theta}(\mathbf{z} | \mathbf{x})$  is *amortized* by a recognition (encoder) distribution  $q_{\phi}(\mathbf{z} | \mathbf{x})$ . We derive the *Evidence Lower Bound* (ELBO) from first principles, present complete proofs via Jensen's inequality and KL identity, give closed forms for the Gaussian case, and show how the *reparameterization trick* yields low-variance unbiased stochastic gradients.

### 1.2 Data and Notation

We observe a dataset

$$\mathcal{D} = \{\mathbf{x}_i\}_{i=1}^n, \quad \mathbf{x}_i \in \mathbb{R}^d.$$

The VAE specifies:

- A latent prior  $p(\mathbf{z})$  on  $\mathbb{R}^r$  (typically  $\mathcal{N}(\mathbf{0}, \mathbf{I}_r)$ ).
- A decoder (generative model)  $p_{\theta}(\mathbf{x} | \mathbf{z})$  with parameters  $\theta$ .
- An encoder (inference model)  $q_{\phi}(\mathbf{z} | \mathbf{x})$  with parameters  $\phi$ .

Neural parameterizations (one-hidden-layer written for concreteness):

$$\text{Encoder: } q_{\phi}(\mathbf{z} | \mathbf{x}) = \mathcal{N}(\mathbf{z}; \boldsymbol{\mu}_{\phi}(\mathbf{x}), \text{diag}(\boldsymbol{\sigma}_{\phi}^2(\mathbf{x}))),$$

$$\text{Decoder: } p_{\theta}(\mathbf{x} | \mathbf{z}) = \begin{cases} \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_{\theta}(\mathbf{z}), \sigma_x^2 \mathbf{I}_d), & \text{Gaussian output,} \\ \text{Bernoulli}(\mathbf{x}; \boldsymbol{\pi}_{\theta}(\mathbf{z})), & \text{binary output.} \end{cases}$$

Here  $r$  is the latent (bottleneck) dimension;  $d$  is the data dimension.

### Generative Model

We assume that the joint distribution over data and latent variables is given by:

$$p_{\theta}(\mathbf{x}, \mathbf{z}) = p_{\theta}(\mathbf{x} | \mathbf{z}) p(\mathbf{z}).$$

The typical choices are:

- **Prior:**  $p(\mathbf{z})$  is usually chosen as a standard Gaussian

$$p(\mathbf{z}) = \mathcal{N}(\mathbf{z}; \mathbf{0}, \mathbf{I}_d),$$

where  $\mathbf{I}_d$  is the  $d \times d$  identity matrix.

- **Likelihood (Decoder):**  $p_{\theta}(\mathbf{x} | \mathbf{z})$  is a distribution over  $\mathbb{R}^D$ . For real-valued data one may choose a Gaussian

$$p_{\theta}(\mathbf{x} | \mathbf{z}) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_{\theta}(\mathbf{z}), \text{diag}(\boldsymbol{\sigma}_{\theta}^2(\mathbf{z}))),$$

where  $\boldsymbol{\mu}_{\theta}(\mathbf{z}) \in \mathbb{R}^D$  and  $\boldsymbol{\sigma}_{\theta}^2(\mathbf{z}) \in \mathbb{R}_{>0}^D$ . For binary data the likelihood may be modeled as a product of Bernoulli distributions.

### Approximate Posterior (Encoder)

Since the true posterior  $p_{\theta}(\mathbf{z} | \mathbf{x})$  is typically intractable, we introduce an approximate posterior:

$$q_{\phi}(\mathbf{z} | \mathbf{x}),$$

which is also commonly chosen to be Gaussian:

$$q_{\phi}(\mathbf{z} | \mathbf{x}) = \mathcal{N}(\mathbf{z}; \boldsymbol{\mu}_{\phi}(\mathbf{x}), \text{diag}(\boldsymbol{\sigma}_{\phi}^2(\mathbf{x}))).$$

Here:

- The encoder network takes  $\mathbf{x} \in \mathbb{R}^D$  as input and outputs:
  - A mean vector  $\boldsymbol{\mu}_{\phi}(\mathbf{x}) \in \mathbb{R}^d$ ,
  - A variance vector  $\boldsymbol{\sigma}_{\phi}^2(\mathbf{x}) \in \mathbb{R}_{>0}^d$  (or its standard deviation  $\boldsymbol{\sigma}_{\phi}(\mathbf{x}) \in \mathbb{R}_{>0}^d$ ).

## 1.3 Model Formulation and MLE Objective

The joint model is  $p_{\theta}(\mathbf{x}, \mathbf{z}) = p_{\theta}(\mathbf{x} | \mathbf{z}) p(\mathbf{z})$ . Maximum likelihood learning seeks

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

but the integral is generally intractable. VAEs introduce  $q_{\phi}(\mathbf{z} | \mathbf{x})$  to approximate  $p_{\theta}(\mathbf{z} | \mathbf{x})$  and derive a tractable lower bound.

## 1.4 ELBO Derivations (Two Equivalent Proofs)

**(A) Jensen’s inequality (importance trick).** *Proof.* Our goal is to maximize the marginal likelihood (or evidence) of the data:

$$p_{\theta}(\mathbf{x}) = \int_{\mathbb{R}^d} p_{\theta}(\mathbf{x}, \mathbf{z}) d\mathbf{z}.$$

Because this integral is generally intractable, we derive a lower bound on  $\log p_{\theta}(\mathbf{x})$ .

We begin with:

$$\log p_{\theta}(\mathbf{x}) = \log \int_{\mathbb{R}^d} p_{\theta}(\mathbf{x}, \mathbf{z}) d\mathbf{z}.$$

Introduce the approximate posterior  $q_{\phi}(\mathbf{z}|\mathbf{x})$  (which satisfies  $q_{\phi}(\mathbf{z}|\mathbf{x}) > 0$  whenever  $p_{\theta}(\mathbf{x}, \mathbf{z}) > 0$ ):

$$\log p_{\theta}(\mathbf{x}) = \log \int_{\mathbb{R}^d} q_{\phi}(\mathbf{z}|\mathbf{x}) \frac{p_{\theta}(\mathbf{x}, \mathbf{z})}{q_{\phi}(\mathbf{z}|\mathbf{x})} d\mathbf{z}.$$

Since the logarithm is a concave function, Jensen’s inequality yields:

$$\begin{aligned} \log p_{\theta}(\mathbf{x}) &= \log \int q_{\phi}(\mathbf{z} | \mathbf{x}) \frac{p_{\theta}(\mathbf{x}, \mathbf{z})}{q_{\phi}(\mathbf{z} | \mathbf{x})} d\mathbf{z} = \log \mathbb{E}_{q_{\phi}} \left[ \frac{p_{\theta}(\mathbf{x}, \mathbf{z})}{q_{\phi}(\mathbf{z} | \mathbf{x})} \right] \\ &\geq \mathbb{E}_{q_{\phi}} [\log p_{\theta}(\mathbf{x}, \mathbf{z}) - \log q_{\phi}(\mathbf{z} | \mathbf{x})] \triangleq \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \mathbf{x}), \end{aligned} \quad (2)$$

where Eqn. (2) is the *Evidence Lower Bound* (ELBO). All expectations are taken with respect to the approximate posterior  $q_{\phi}(\mathbf{z}|\mathbf{x})$ , where  $\mathbf{z} \in \mathbb{R}^d$ , and the inequality uses concavity of  $\log(\cdot)$ . ■

**(B) KL identity decomposition.** *Proof.* Add and subtract  $\log q_{\phi}(\mathbf{z} | \mathbf{x})$  inside the marginal:

$$\begin{aligned} \log p_{\theta}(\mathbf{x}) &= \mathbb{E}_{q_{\phi}} [\log p_{\theta}(\mathbf{x}, \mathbf{z}) - \log q_{\phi}(\mathbf{z} | \mathbf{x})] + \underbrace{\mathbb{E}_{q_{\phi}} [\log q_{\phi}(\mathbf{z} | \mathbf{x}) - \log p_{\theta}(\mathbf{z} | \mathbf{x})]}_{\text{KL}(q_{\phi}(\mathbf{z}|\mathbf{x}) \parallel p_{\theta}(\mathbf{z}|\mathbf{x}))} \\ &= \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \mathbf{x}) + \text{KL}(q_{\phi}(\mathbf{z} | \mathbf{x}) \parallel p_{\theta}(\mathbf{z} | \mathbf{x})). \end{aligned} \quad (3)$$

Since the KL is nonnegative,  $\mathcal{L}$  is a lower bound tight iff  $q_{\phi} = p_{\theta}$ . ■

**Canonical ELBO form.** Using  $p_{\theta}(\mathbf{x}, \mathbf{z}) = p_{\theta}(\mathbf{x} | \mathbf{z}) p(\mathbf{z})$  in Eqn. (2):

$$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \mathbf{x}) = \mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x})} [\log p_{\theta}(\mathbf{x} | \mathbf{z})] - \text{KL}(q_{\phi}(\mathbf{z} | \mathbf{x}) \parallel p(\mathbf{z})). \quad (4)$$

The first term is a *reconstruction* term; the second regularizes the encoder toward the prior.

**Dataset ELBO / training objective.**

$$\max_{\boldsymbol{\theta}, \boldsymbol{\phi}} \hat{\mathcal{L}} = \frac{1}{n} \sum_{i=1}^n \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \mathbf{x}_i). \quad (5)$$

## 1.5 Gaussian Encoder: Closed-Form KL and Reparameterization

A key challenge in optimizing the ELBO is that the expectation is taken with respect to a distribution  $q_{\phi}(\mathbf{z}|\mathbf{x})$  that depends on the parameters  $\phi$ . To allow gradient backpropagation through  $\mathbf{z}$ , we reparameterize the sampling process.

Assume  $q_{\phi}(\mathbf{z} | \mathbf{x}) = \mathcal{N}(\mathbf{z}; \boldsymbol{\mu}_{\phi}(\mathbf{x}), \text{diag}(\boldsymbol{\sigma}_{\phi}^2(\mathbf{x})))$  and  $p(\mathbf{z}) = \mathcal{N}(\mathbf{0}, \mathbf{I}_r)$ .

**Closed-form KL.** For diagonal Gaussians  $q = \mathcal{N}(\boldsymbol{\mu}, \text{diag}(\boldsymbol{\sigma}^2))$  vs.  $p = \mathcal{N}(\mathbf{0}, \mathbf{I})$ ,

$$\text{KL}(q\|p) = \frac{1}{2} \sum_{j=1}^r (\mu_j^2 + \sigma_j^2 - \log \sigma_j^2 - 1). \quad (6)$$

If the network outputs  $\boldsymbol{\ell} = \log \boldsymbol{\sigma}^2$ , then  $\sigma_j^2 = \exp(\ell_j)$ , where the log-variance vector  $\boldsymbol{\ell}(\cdot)$  has the identity:  $\boldsymbol{\ell} \triangleq \log \boldsymbol{\sigma}^2$ .

**Reparameterization trick.** Let  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_r)$  be an auxiliary random variable and define the deterministic transform and reparameterize  $\mathbf{z}$  as:

$$\mathbf{z} = \boldsymbol{\mu}_\phi(\mathbf{x}) + \boldsymbol{\sigma}_\phi(\mathbf{x}) \odot \boldsymbol{\epsilon}, \quad (7)$$

where  $\odot$  is the Hadamard product. Then for any integrable  $f$ ,

$$\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[f(\mathbf{z})] = \mathbb{E}_{\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})}[f(\boldsymbol{\mu}_\phi(\mathbf{x}) + \boldsymbol{\sigma}_\phi(\mathbf{x}) \odot \boldsymbol{\epsilon})].$$

This reformulation permits gradients to be computed with respect to  $\phi$  using standard backpropagation.

*Proof.* The pushforward of  $\boldsymbol{\epsilon}$  through the affine map Eqn. (7) is  $\mathcal{N}(\boldsymbol{\mu}_\phi, \text{diag}(\boldsymbol{\sigma}_\phi^2))$ ; equality of expectations follows by change of variables.  $\blacksquare$

**Stochastic ELBO estimator.** With a single Monte Carlo sample  $\boldsymbol{\epsilon}^{(1)}$ ,

$$\hat{\mathcal{L}}(\mathbf{x}) \approx \underbrace{\log p_\theta(\mathbf{x} \mid \boldsymbol{\mu}_\phi(\mathbf{x}) + \boldsymbol{\sigma}_\phi(\mathbf{x}) \odot \boldsymbol{\epsilon}^{(1)})}_{\text{reconstruction term}} - \underbrace{\text{KL}(q_\phi(\mathbf{z} \mid \mathbf{x}) \parallel p(\mathbf{z}))}_{\text{regularization term}}. \quad (8)$$

Gradients w.r.t.  $\boldsymbol{\theta}$  and  $\phi$  can be backpropagated through the deterministic path Eqn. (7), yielding unbiased, low-variance estimates (SGVB).

## 1.6 Likelihood Choices and Reconstruction Losses

**Gaussian decoder.** If  $p_\theta(\mathbf{x} \mid \mathbf{z}) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_\theta(\mathbf{z}), \sigma_x^2 \mathbf{I})$  with fixed  $\sigma_x^2 > 0$ , then

$$\log p_\theta(\mathbf{x} \mid \mathbf{Z}) = -\frac{1}{2\sigma_x^2} \|\mathbf{x} - \boldsymbol{\mu}_\theta(\mathbf{Z})\|_2^2 - \frac{d}{2} \log(2\pi\sigma_x^2),$$

so maximizing the ELBO is equivalent (up to constants) to minimizing MSE of the decoder mean plus the KL.

**Bernoulli decoder.** For binary  $\mathbf{x}$  and  $p_\theta(\mathbf{x} \mid \mathbf{Z}) = \text{Bernoulli}(\mathbf{x}; \boldsymbol{\pi}_\theta(\mathbf{Z}))$  with  $\boldsymbol{\pi} = \sigma(\cdot)$ ,

$$\log p_\theta(\mathbf{x} \mid \mathbf{Z}) = -\sum_{j=1}^d \left[ x_j \log \pi_j + (1 - x_j) \log(1 - \pi_j) \right],$$

the (negative) cross-entropy reconstruction term.

## 1.7 Gradients and Proof of Correctness (SGVB)

*Proof.* Write the per-sample ELBO as

$$\mathcal{L}(\boldsymbol{\theta}, \phi; \mathbf{x}) = \mathbb{E}_{\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} \left[ \underbrace{\log p_\theta(\mathbf{x} \mid \mathbf{z}(\mathbf{x}, \boldsymbol{\epsilon}))}_{R(\boldsymbol{\theta}, \phi; \mathbf{x}, \boldsymbol{\epsilon})} \right] - \text{KL}(q_\phi(\mathbf{z} \mid \mathbf{x}) \parallel p(\mathbf{z})).$$

**Decoder gradient.** Since  $R$  depends on  $\theta$  only through  $\log p_\theta$ ,

$$\nabla_\theta \mathcal{L} = \mathbb{E}_\epsilon [\nabla_\theta \log p_\theta(\mathbf{x} \mid \mathbf{z}(\mathbf{x}, \epsilon))] .$$

**Encoder gradient.** The KL has closed-form gradient via Eqn. (6); for the reconstruction term,

$$\nabla_\phi \mathbb{E}_\epsilon [\log p_\theta(\mathbf{x} \mid \mathbf{z}(\mathbf{x}, \epsilon))] = \mathbb{E}_\epsilon \left[ \nabla_{\mathbf{z}} \log p_\theta(\mathbf{x} \mid \mathbf{z}) \frac{\partial \mathbf{z}(\mathbf{x}, \epsilon)}{\partial \phi} \right] ,$$

which is exactly what backpropagation computes through the path  $\mathbf{x} \mapsto (\mu_\phi, \sigma_\phi) \mapsto \mathbf{z} \mapsto \log p_\theta(\mathbf{x} \mid \mathbf{z})$ . Interchanging  $\nabla$  and  $\mathbb{E}$  is justified by dominated convergence (bounded second moments suffice). ■

## 1.8 Relation to MLE and Tightness

Summing Eqn. (3) over  $i$ :

$$\frac{1}{n} \sum_{i=1}^n \log p_\theta(\mathbf{x}_i) = \widehat{\mathcal{L}}(\theta, \phi) + \frac{1}{n} \sum_{i=1}^n \text{KL}(q_\phi(\mathbf{z} \mid \mathbf{x}_i) \parallel p_\theta(\mathbf{z} \mid \mathbf{x}_i)) .$$

Maximizing  $\widehat{\mathcal{L}}$  w.r.t.  $(\theta, \phi)$  jointly increases the likelihood while decreasing the amortized posterior gap; the bound is tight iff  $q_\phi(\mathbf{z} \mid \mathbf{x}_i) = p_\theta(\mathbf{z} \mid \mathbf{x}_i)$  for all  $i$ .

## 1.9 Algorithm (VAE Training via SGVB)

1. **Input:** data  $\{\mathbf{x}_i\}$ , latent dimension  $r$ , prior  $p(\mathbf{z})$ , decoder family  $p_\theta(\mathbf{x} \mid \mathbf{z})$ , encoder family  $q_\phi(\mathbf{z} \mid \mathbf{x})$ .
2. **Initialize** parameters  $(\theta, \phi)$  (e.g., Xavier/He).
3. **Repeat** over mini-batches  $\mathcal{B}$ :
  - (a) For each  $\mathbf{x} \in \mathcal{B}$ , compute encoder outputs  $(\mu_\phi(\mathbf{x}), \ell_\phi(\mathbf{x}))$  and set  $\sigma_\phi = \exp(\frac{1}{2}\ell_\phi)$ .
  - (b) Sample  $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_r)$  and set  $\mathbf{z} = \mu_\phi(\mathbf{x}) + \sigma_\phi(\mathbf{x}) \odot \epsilon$ .
  - (c) Compute reconstruction log-likelihood  $\log p_\theta(\mathbf{x} \mid \mathbf{z})$  and KL via Eqn. (6); average over the batch to obtain  $\widehat{\mathcal{L}}_{\mathcal{B}}$ .
  - (d) Backpropagate  $\nabla_{\theta, \phi}(-\widehat{\mathcal{L}}_{\mathcal{B}})$  and update with SGD/Adam.
4. **Output:** learned generative model  $p_\theta(\mathbf{x} \mid \mathbf{z})$ ; inference model  $q_\phi(\mathbf{z} \mid \mathbf{x})$ .

## 1.10 Extensions (Brief)

**$\beta$ -VAE.** Replace the KL term by  $\beta$  KL:

$$\mathcal{L}_\beta = \mathbb{E}_q[\log p_\theta(\mathbf{x} \mid \mathbf{z})] - \beta \text{KL}(q_\phi(\mathbf{z} \mid \mathbf{x}) \parallel p(\mathbf{z})) ,$$

trading off reconstruction and regularization (information bottleneck interpretation).

**Conditional VAE (cVAE).** For side information  $\mathbf{y}$ , model  $p_\theta(\mathbf{x} \mid \mathbf{z}, \mathbf{y})$  and  $q_\phi(\mathbf{z} \mid \mathbf{x}, \mathbf{y})$ ; the ELBO conditions on  $\mathbf{y}$ .

**Discrete latents.** Use a continuous relaxation (GumbelSoftmax/Concrete) for categorical  $\mathbf{z}$  to enable reparameterized gradients.

**Importance-weighted ELBO (IWAE).** Tighter bound with  $K$  samples:  $\log p(\mathbf{x}) \geq \mathbb{E} \left[ \log \frac{1}{K} \sum_{k=1}^K \frac{p_\theta(\mathbf{x}, \mathbf{z}^{(k)})}{q_\phi(\mathbf{z}^{(k)} \mid \mathbf{x})} \right]$ .

### 1.11 Summary of Variables and Their Dimensions

- $\mathbf{x}_i \in \mathbb{R}^d$ : observed data vector.
- $\mathbf{z} \in \mathbb{R}^r$ : latent code; prior  $p(\mathbf{z}) = \mathcal{N}(\mathbf{0}, \mathbf{I}_r)$ .
- Encoder  $q_\phi(\mathbf{z} | \mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}_\phi(\mathbf{x}), \text{diag}(\boldsymbol{\sigma}_\phi^2(\mathbf{x})))$  with outputs  $\boldsymbol{\mu}_\phi(\mathbf{x}) \in \mathbb{R}^r$ ,  $\boldsymbol{\sigma}_\phi^2(\mathbf{x}) \in \mathbb{R}^r$ .
- Decoder  $p_\theta(\mathbf{x} | \mathbf{z})$ : Gaussian (mean  $\boldsymbol{\mu}_\theta(\mathbf{z}) \in \mathbb{R}^d$ , variance  $\sigma_x^2$ ) or Bernoulli (probs  $\boldsymbol{\pi}_\theta(\mathbf{z}) \in (0, 1)^d$ ).
- ELBO  $\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \mathbf{x}) = \mathbb{E}_q[\log p_\theta(\mathbf{x} | \mathbf{z})] - \text{KL}(q||p)$  (scalar).
- Reparameterization:  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_r)$ ,  $\mathbf{z} = \boldsymbol{\mu}_\phi + \boldsymbol{\sigma}_\phi \odot \boldsymbol{\epsilon}$ .

### 1.12 Summary

From first principles, VAEs perform maximum likelihood learning for latent-variable models by optimizing the ELBO Eqn. (4), obtained either by Jensen's inequality or by a KL decomposition Eqn. (3). With a Gaussian encoder and standard normal prior, the KL admits the closed form Eqn. (6). The reparameterization trick Eqn. (7) converts expectations over  $q_\phi(\mathbf{z} | \mathbf{x})$  into expectations over a fixed noise source, enabling unbiased low-variance gradient estimates (SGVB) and end-to-end training with backpropagation. Likelihood choices determine the reconstruction term (Gaussian  $\leftrightarrow$  MSE; Bernoulli  $\leftrightarrow$  cross-entropy). Extensions like  $\beta$ -VAE, cVAE, discrete latents, and IWAE follow from the same variational principles.