Variational Autoencoders on MNIST

ELBO Derivation, KL Annealing, and CVAE Extension (v2)

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Generative AI and Diffusion Models

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Project Objectives

1. **Derive the ELBO** from first principles with closed-form KL for Gaussians
2. **Implement a Convolutional VAE** on MNIST with 2D latent space
3. **Track reconstruction vs KL** separately, implement KL annealing
4. **Visualize**: latent space, latent traversals, interpolations
5. **Extend to CVAE** for controlled digit generation

ELBO Derivation

Starting from intractable marginal likelihood, we derived:

Evidence Lower Bound

$$\log p(x) \geq \mathcal{L} = \underbrace{\mathbb{E}_{q_\phi(z|x)}[\log p_\theta(x|z)]}_{\text{Reconstruction (BCE)}} - \underbrace{\mathrm{KL}(q_\phi(z|x) \| p(z))}_{\text{Regularization}}$$

Closed-form KL for Gaussian encoder $q = \mathcal{N}(\mu, \sigma^2)$ and prior $p = \mathcal{N}(0, I)$:

$$\mathrm{KL}(q \| p) = \frac{1}{2} \sum_{j=1}^{d} \left(\mu_j^2 + \sigma_j^2 - \log \sigma_j^2 - 1 \right)$$

ELBO — Proof of Lower Bound

Start from the marginal log-likelihood:

$$\log p_\theta(x) = \log \int p_\theta(x|z)p(z)\,dz$$

Introduce an arbitrary approximate posterior $q_\phi(z|x)$ and rewrite:

$$\begin{aligned}\log p_\theta(x) &= \log \int q_\phi(z|x)\frac{p_\theta(x|z)p(z)}{q_\phi(z|x)}\,dz \\ &= \log \mathbb{E}_{q_\phi(z|x)}\left[\frac{p_\theta(x|z)p(z)}{q_\phi(z|x)}\right]\end{aligned}$$

Apply Jensen's inequality (log is concave):

$$\begin{aligned}\log p_\theta(x) &\geq \mathbb{E}_{q_\phi(z|x)}\left[\log \frac{p_\theta(x|z)p(z)}{q_\phi(z|x)}\right] \\ &= \mathbb{E}_{q_\phi(z|x)}[\log p_\theta(x|z)] + \mathbb{E}_{q_\phi(z|x)}\left[\log \frac{p(z)}{q_\phi(z|x)}\right] \\ &= \mathbb{E}_{q_\phi(z|x)}[\log p_\theta(x|z)] - \mathrm{KL}(q_\phi(z|x)\|p(z))\end{aligned}$$

This establishes $\log p_\theta(x) \geq \mathcal{L}(\theta,\phi;x)$.

ELBO — Gradients / Derivative

We optimize parameters θ (decoder) and ϕ (encoder) by maximizing the ELBO. The ELBO for a single datum is:

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

Gradient w.r.t. decoder parameters θ (decoder appears only in $p_\theta(x|z)$):

$$\begin{aligned} \nabla_\theta \mathcal{L} &= \nabla_\theta \mathbb{E}_{q_\phi(z|x)}[\log p_\theta(x|z)] \\ &= \mathbb{E}_{q_\phi(z|x)}\left[\nabla_\theta \log p_\theta(x|z)\right]. \end{aligned}$$

In practice estimate by Monte Carlo: sample $z \sim q_\phi(z|x)$ via reparameterization $z = \mu_\phi(x) + \sigma_\phi(x) \odot \epsilon$. Gradient w.r.t. encoder parameters ϕ uses reparameterization to push gradient through samples:

$$\nabla_\phi \mathcal{L} = \nabla_\phi \mathbb{E}_{\epsilon \sim \mathcal{N}(0,I)}\left[\log p_\theta(x|\mu_\phi + \sigma_\phi \odot \epsilon)\right] - \nabla_\phi \mathrm{KL}(q_\phi \| p)$$

where the KL term has closed-form gradients: $\partial_{\mu_j} \mathrm{KL} = \mu_j$, $\partial_{\sigma_j} \mathrm{KL} = \sigma_j - 1/\sigma_j$.

Architecture & Training Setup

Convolutional VAE:

- Encoder: Conv layers $\rightarrow$ 2D latent $(\mu, \log \sigma^2)$
- Decoder: Linear $\rightarrow$ ConvTranspose layers
- Reparameterization: $z = \mu + \sigma \odot \epsilon$

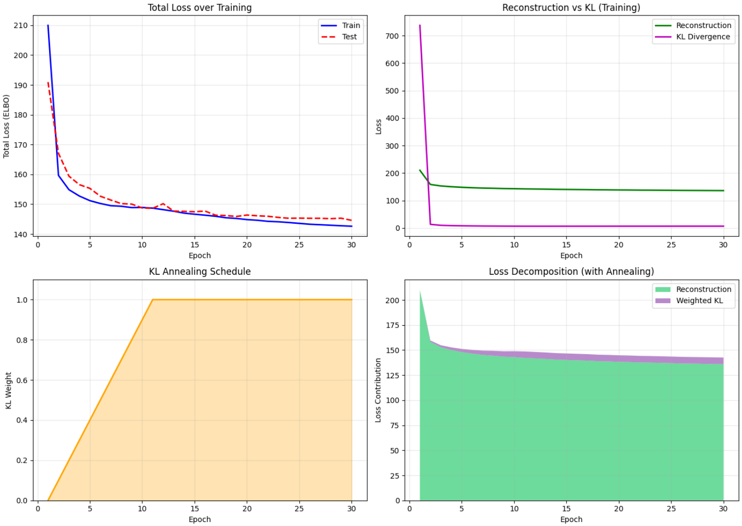
KL Annealing:

$$\beta(t) = \min\left(1, \frac{t}{10}\right)$$

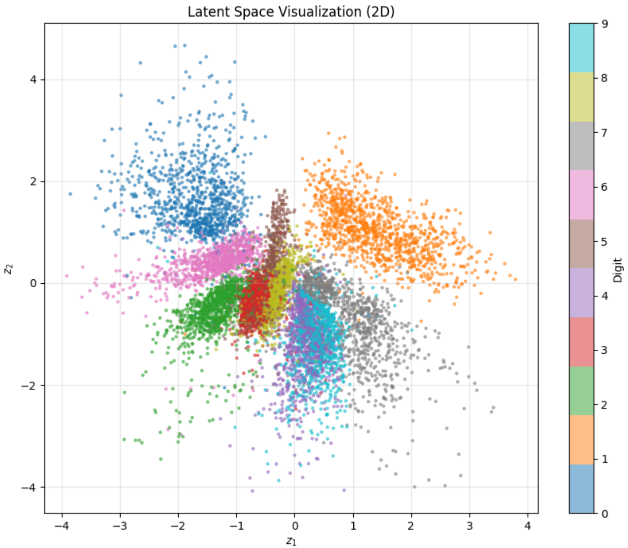
Prevents posterior collapse

Parameter	**Value**
Latent dim	2
Batch size	128
Learning rate	10^{-3}
Optimizer	Adam
Epochs	30
KL warmup	10 epochs

VAE Training Curves



Latent Space Visualization

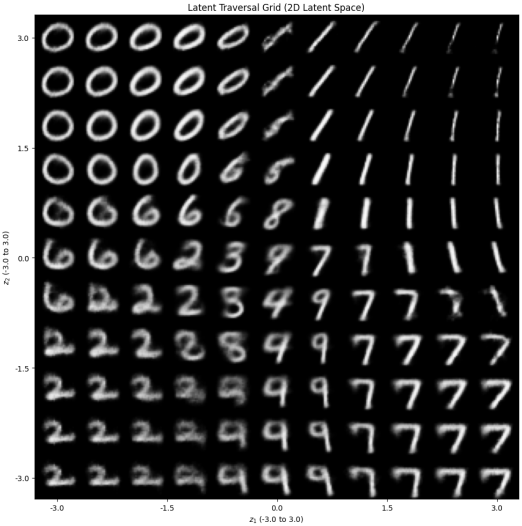


Observations:

- Clear clustering by digit class
- Similar digits nearby (4/9, 3/8, 1/7)
- Smooth, continuous manifold
- Matches $\mathcal{N}(0, I)$ prior

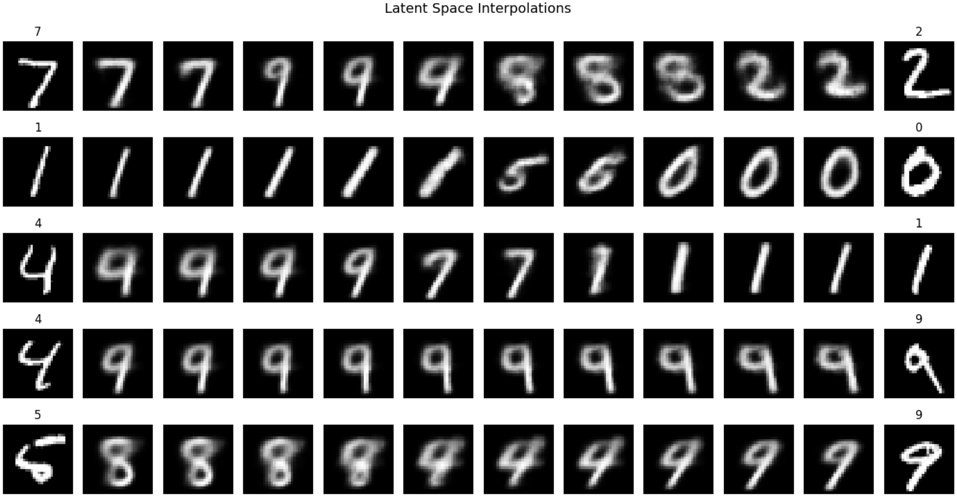
Key insight:
Organization emerges from reconstruction alone — no labels used!

Latent Traversal Grid



Traversing z_1 vs z_2: z_1 (horizontal) controls slant/rotation; z_2 (vertical) controls thickness/scale.

Latent Interpolations



Linear interpolation between encoded digit pairs. Smooth transitions validate the continuous, well-structured latent space.

CVAE Extension: Conditional Generation

Modification: Condition encoder and decoder on class label c

$$\mathcal{L}_{\text{CVAE}} = \mathbb{E}_{q_\phi(z|x,c)}[\log p_\theta(x|z,c)] - \mathrm{KL}(q_\phi(z|x,c)\|p(z))$$

Implementation:

- Embedding the label to $\times 28 \times 28$
- Concatenate with image as extra channels
- Class-independent prior: $p(z) = \mathcal{N}(0, I)$

Result: Latent space encodes *style*, label provides *class identity*

CVAE ELBO

Condition on label c; objective per datum (x, c):

$$\mathcal{L}_{\text{CVAE}}(\theta, \phi; x, c) = \mathbb{E}_{q_\phi(z|x,c)}[\log p_\theta(x|z, c)] - \mathrm{KL}(q_\phi(z|x, c) \| p(z)).$$

Proof of lower bound follows identical steps with all densities conditioned on c:

$$\begin{aligned} \log p_\theta(x|c) &= \log \int p_\theta(x|z, c)p(z)\, dz \\ &= \log \mathbb{E}_{q_\phi(z|x,c)} \left[\frac{p_\theta(x|z, c)p(z)}{q_\phi(z|x, c)} \right] \\ &\geq \mathbb{E}_{q_\phi(z|x,c)} \left[\log \frac{p_\theta(x|z, c)p(z)}{q_\phi(z|x, c)} \right] = \mathcal{L}_{\text{CVAE}}. \end{aligned}$$

Gradients: similar decomposition as VAE; decoder gradient

$$\nabla_\theta \mathcal{L}_{\text{CVAE}} = \mathbb{E}_{q_\phi(z|x,c)} \left[\nabla_\theta \log p_\theta(x|z, c) \right]$$

Encoder gradients use reparameterization with the conditional encoder $\mu_\phi(x, c), \sigma_\phi(x, c)$ and the closed-form KL.

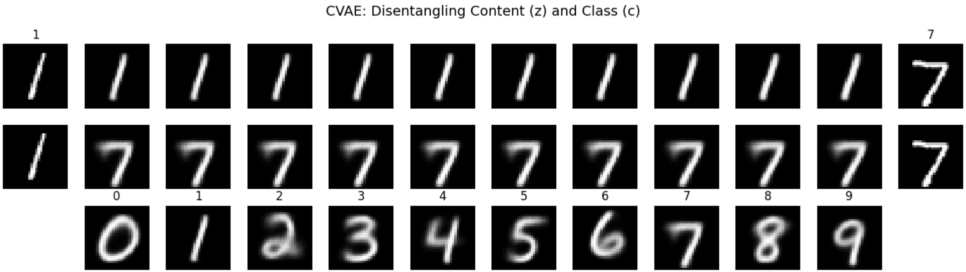
VAE vs CVAE: Quantitative Comparison

Model	Recon. Loss	KL	Total Loss
VAE	138.00	6.59	144.59
CVAE	124.36	4.80	129.16
Improvement	**9.9%**	**27.2%**	**10.7%**

Why CVAE performs better:

- Decoder doesn't need to infer class from $z \Rightarrow$ simpler task
- Latent space focuses purely on style variations
- More compact representation (lower KL)

CVAE: Disentanglement Demonstration



Row 1-2: Same z interpolation with different class labels (1 vs 7). **Row 3:** Fixed z, varying class 0-9 $\Rightarrow$ style transfer across all digits.

Key Findings

1. **ELBO provides principled training objective**
   - Reconstruction + regularization trade-off
   - Closed-form KL enables efficient optimization
2. **KL annealing is essential**
   - Without it: posterior collapse, KL $\rightarrow 0$
   - 10-epoch warmup gave balanced training
3. **VAE learns meaningful structure unsupervised**
   - Class clustering, smooth interpolations
4. **CVAE achieves explicit disentanglement**
   - 9.9% better reconstruction, controlled generation

Thank You!

Questions?

Code available in accompanying Jupyter notebook