Variational Autoencoders

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Overview

Introduction

Denoising Autoencoder

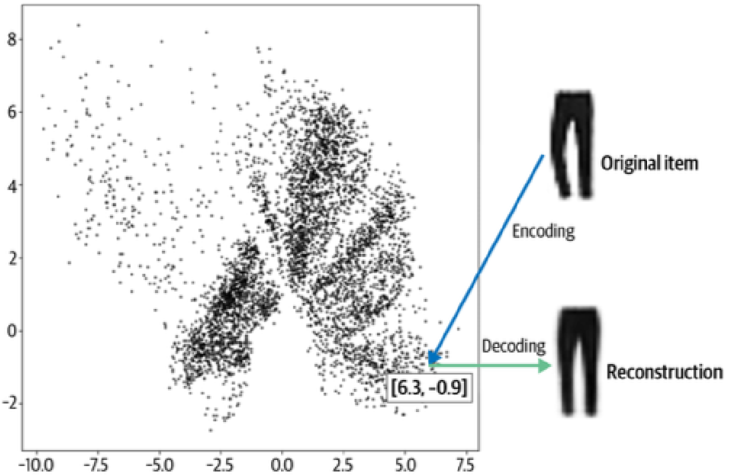
Variational Autoencoder

- ELBO
- Reparameterization Trick

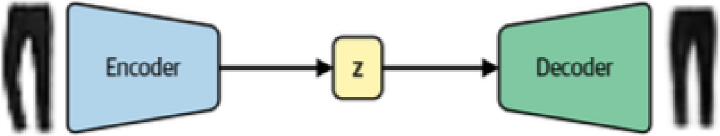
β–VAE

Autoencoders

Autoencoders (cont.)



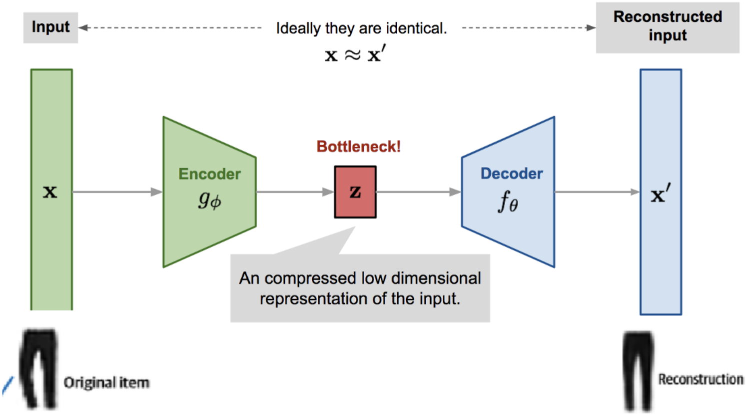
- Learn an identity function with a bottleneck
- Compress data into a low-dimensional latent space
- Reconstruct input from the compressed code



Source: [1] Notations

Autoencoder Definition (cont.)

- 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'


Input
Ideally they are identical.
$\mathbf{x} \approx \mathbf{x}'$
Reconstructed input
$\mathbf{x}$
Encoder
g_ϕ
Bottleneck!
$\mathbf{z}$
Decoder
f_θ
$\mathbf{x}'$
An compressed low dimensional representation of the input.
Original item
Reconstruction

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

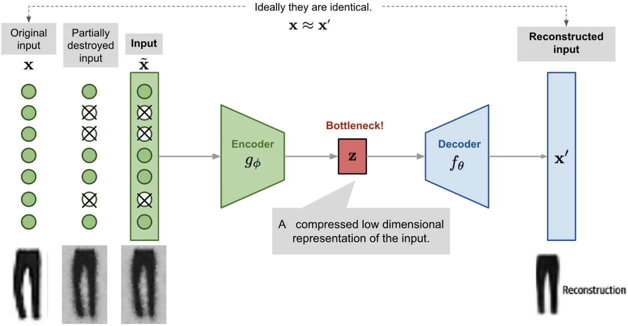
- Autoencoders do not regularize the latent space risking **overfitting**
- Encoded data occupy **disconnected** regions in latent space
- Large empty regions (“**holes**”) appear between encoded samples
- Latent points inside these holes do not decode to valid data
- Sampling often passes through holes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

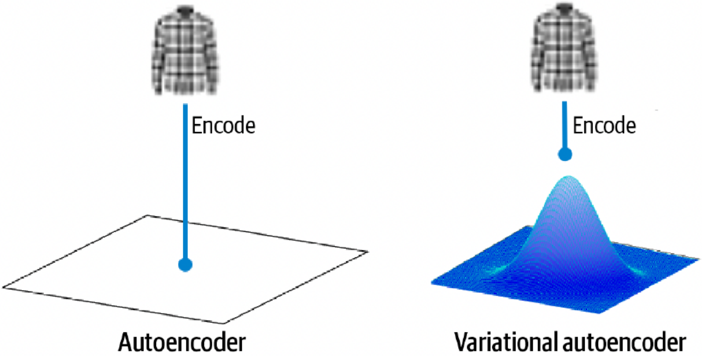
VAE is rooted in variational Bayesian inference:

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

fig_vae_graphical_model.png

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 $q_\phi(z|x)$

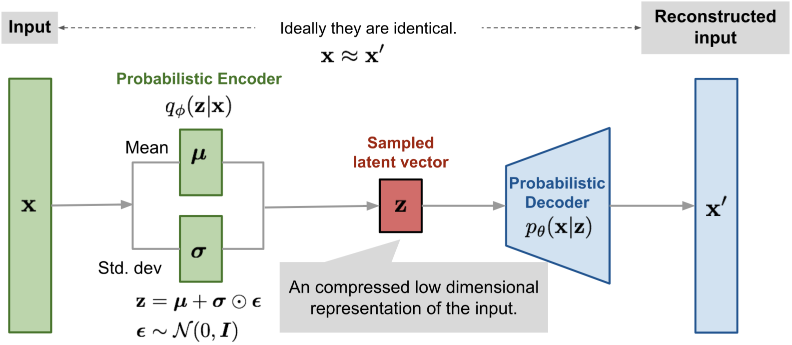
VAE: Approximate posterior (probabilistic encoder)

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?

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

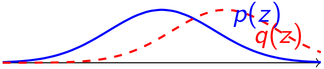
- Measures how much a distribution q deviates from a reference distribution p
- Always non-negative
- Equal to zero only when $q = p$
- Not symmetric and not a distance

Intuition

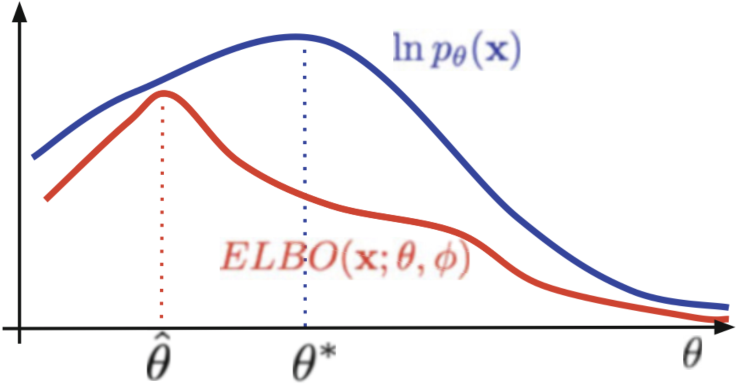
- Think of p as the rule you agreed to follow
- q is what you actually do
- KL divergence is the *penalty for breaking the rule*
- Larger mismatch means higher cost

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: Step-by-step derivation (1)

Start:

$$D_{KL}(q_\phi(z|x) \| p_\theta(z|x)) = \int q_\phi(z|x) \log \frac{q_\phi(z|x)}{p_\theta(z|x)} \, dz$$

Use $p(z|x) = \frac{p(z,x)}{p(x)}$:

$$= \int q_\phi(z|x) \log \frac{q_\phi(z|x) p_\theta(x)}{p_\theta(z,x)} \, dz$$

$$= \int q_\phi(z|x) \left(\log p_\theta(x) + \log \frac{q_\phi(z|x)}{p_\theta(z,x)} \right) dz$$

Because $\int q(z|x)dz = 1$:

$$= \log p_\theta(x) + \int q_\phi(z|x) \log \frac{q_\phi(z|x)}{p_\theta(z,x)} dz$$

Because $p(z,x) = p(x|z)p(z)$:

$$= \log p_\theta(x) + \int q_\phi(z|x) \log \frac{q_\phi(z|x)}{p_\theta(x|z)p_\theta(z)} dz$$

ELBO: Step-by-step derivation (3)

Convert integral to expectation:

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

So:

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

Rearrange:

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

Define VAE loss (as given):

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

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

- First term: reconstruction (negative log-likelihood)
- Second term: regularization toward prior

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

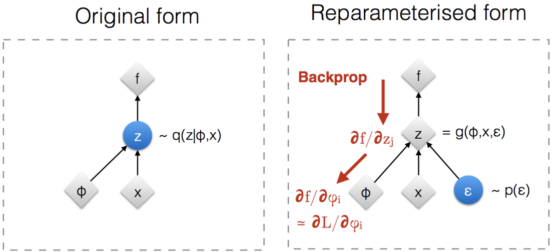
The reconstruction term uses sampling:

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

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




: Deterministic node

: Random node

[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

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.

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 (as given)

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

[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.