Variational Autoencoders

CPSC 540 - Advanced Machine Learning
University of British Columbia

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Motivation

Ordinary autoencoders

- Convolutional layers reduce input data x into latent vector representation z.
- Generate new data: pick a point z in latent space, push through decoder.
- Potential for overfitting.
- Nearby points in latent space can produce different results.

Motivation

Variational Autoencoders (VAEs)

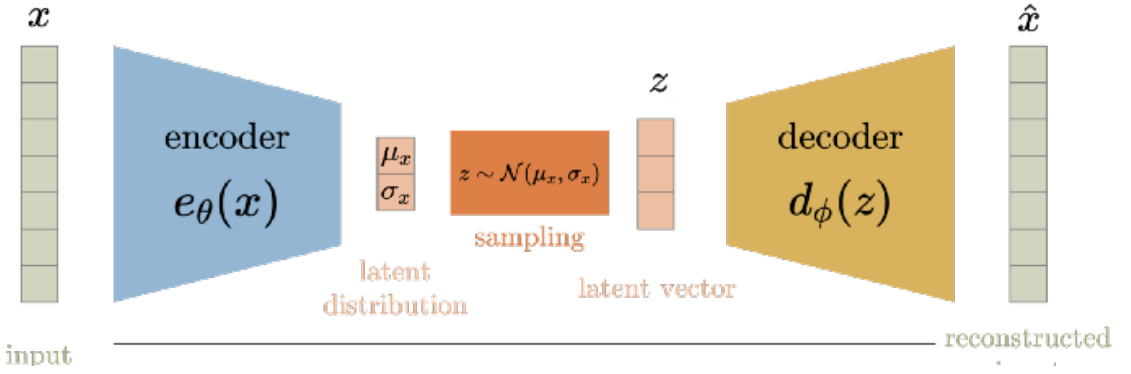
- Represent the latent variable z as a *distribution*

$$z \sim p(z \mid x)$$

- Draw a random sample z, then push it through the decoder.
- Nearby points in latent space produce similar data when pushed through decoder.

Model Definition

- Similar to autoencoders, VAEs have an encoder, decoder, and bottleneck layer.
- The latent vector z is not learned directly.
- Instead the parameters of the distribution are learned.



General framework

- VAEs are deep generative models.
- Use evidence maximization, i.e. maximizing $p(x)$.
- Evidence can be calculated with

$$p(x) = \int p(x \mid z) p(z) \, dz$$

  where the integral is over the possible values of z in the latent space.
- Exponential time to calculate $p(x)$ (must evaluate all configurations).

General framework

Simplifying Assumptions:

- Decoder (likelihood):

$$p_\theta(x \mid z) = \mathcal{N}(f(z, \theta), \sigma^2 I)$$

  Function f to be learned by decoder network weights/biases θ. σ is hyper-parameter.

- Encoder: $p(z \mid x)$ can be approximated by

$$q_\phi(z \mid x) = \mathcal{N}(\mu(x, \phi), \Sigma(x, \phi))$$

  Weights/biases ϕ are learned by encoder network.

- Latent Prior: $p(z) = \mathcal{N}(0, 1)$.

General framework

Q: How can we force $p(z \mid x) \approx q_\phi(z \mid x)$?

A: The Kullback-Leibler (KL) - divergence measures how different two distributions p_1 and p_2 are:

$$\mathcal{KL}(p_1 \mid\mid p_2) := E_{x \sim p_1}(\log(p_1(x)) - \log(p_2(x)))$$

We will try to force $p(z \mid x) \approx q_\phi(z \mid x)$ by minimizing the KL-divergence between them.

Loss Function

Want to learn best μ and Σ for encoder distribution $q_\phi(z \mid x^i) = \mathcal{N}(\mu(x^i, \phi), \Sigma(x^i, \phi))$:

$$q^*_\phi(z \mid x) = \text{argmin}_\phi \, \mathcal{KL}(q_\phi(z \mid x) \mid\mid p(z \mid x))$$

Intractable due to $p(x)$ term which shows up in KL-divergence:

$$\mathcal{KL}(q_\phi(z \mid x) \mid\mid p(z \mid x)) = E_{z \sim q_\phi(z \mid x)}[\log(q_\phi(z \mid x)) - \log(p(x, z)) + \log(p(x))]$$

Loss Function

Instead, maximize the evidence $p(x)$. After some manipulation (to be done on the assignment):

$$\mathcal{KL}(q_\phi(z \mid x) \mid\mid p(z \mid x)) = E_{z \sim q_\phi(z \mid x)}[\log(q_\phi(z \mid x)) - \log(p(x, z))] + \log(p(x))$$

Solving for $\log(p(x))$:

$$\log(p(x)) = E_{z \sim q_\phi(z \mid x)}[\log(p(x, z)) - \log(q_\phi(z \mid x))] + \mathcal{KL}(q_\phi(z \mid x) \mid\mid p(z \mid x))$$

Loss Function

(Continued) Log-evidence to be maximized:

$$\log(p(x)) = E_{z\sim q_\phi(z\mid x)}[\log(p(x,z)) - \log(q_\phi(z\mid x))] + \mathcal{KL}(q_\phi(z\mid x)\mid\mid p(z\mid x))$$

- Expectation term on RHS is called "ELBO" function.
- Issue: $p(x)$ still appears in KL term like before! (Hard to calculate).
- However, we can now safely ignore the KL term. Why?
- KL-divergence is nonnegative, so $\log(p(x)) \geq$ ELBO.
- Our goal is to maximize ELBO, which therefore will increase $\log(p(x) \geq$ ELBO!

"MLE"

ELBO can be manipulated (to be done on assignment) into the following form:

$$\text{ELBO}_i(\theta, \phi) = E_{z \sim q_\phi(z \mid x^i)}[\log(p_\theta(x^i \mid z))] - \mathcal{KL}(q_\phi(z \mid x^i) \mid\mid p(z))$$

The negative of this is the loss for a single training example i.

- "Evidence Lower BOund" - Satisfies $\text{ELBO}(x) \leq \log(p(x))$.
- Instead of maximizing $\log(p(x))$ directly like in MLE (intractable), maximize ELBO.
- Can be viewed as *modified* or *approximate* "MLE".

Interpretation of the Loss Function

Loss function:

$$-\text{ELBO}_i(\theta, \phi) = -E_{z \sim q_\phi(z \mid x^i)}[\log(p_\theta(x^i \mid z))] + \mathcal{KL}(q_\phi(z \mid x^i) \mid\mid p(z))$$

Interpretation:

- First term: reconstruction error (minimize NLL expected under our distribution q_ϕ).
  - Remember $p_\theta(x^i \mid z) = \mathcal{N}(f(z, \theta), \sigma^2)$
  - $\log(p_\theta(x^i \mid z)) = (x^i - f(z, \theta))^2 + \text{Constant}$ (reconstruction error)
- Second term: regularization (minimize KL-divergence).

The Role of Regularization

Regularization is provided by the $\mathcal{KL}(q_\phi(z \mid x^i) \mid\mid p(z))$ term.

- KL-divergence penalizes $q_\phi(z \mid x)$ for getting too far from $p(z) = \mathcal{N}(0, 1)$).
- Without KL regularization, model learns Gaussians $q_\phi(z \mid x)$ with very low variance
- Low variance Gaussian is just a "spike" at a particular point in latent space.
- This makes it practically deterministic, like an ordinary autoencoder.
- This regularization is how VAEs prevent this overfitting.

The Role of Regularization

Figure: Latent distributions. Left: no regularization. Right: regularization. Source: https://towardsdatascience.com/understanding-variational-autoencoders-vaes-f70510919f73

- Each x^i gets its own Gaussian distribution $q_\phi(z \mid x^i)$.
- On left: learned Gaussians are sharp and far apart from each other.
- Overfitting - Nonsense data generated from latent vectors between distributions.
- On right: broader distributions. Keeps the distributions close together.
- Latent vectors between distributions produce more realistic data.

Training

Loss function:

$$-\text{ELBO}_i(\theta, \phi) = -E_{z \sim q_\phi(z \mid x^i)}[\log(p_\theta(x^i \mid z))] + \mathcal{KL}(q_\phi(z \mid x^i) \mid\mid p(z))$$

How do we train? Remember our simplifying assumptions:

- $q_\phi(z \mid x^i) = \mathcal{N}(\mu(x^i, \phi), \sigma^2(x^i, \phi))$
- $p_\theta(x^i \mid z) = \mathcal{N}(f(z, \phi), \sigma^2)$
- $p(z) = \mathcal{N}(0, 1)$

Training

Loss function:

$$-\text{ELBO}_i(\theta, \phi) = -E_{z \sim q_\phi(z \mid x^i)}[\log(p_\theta(x^i \mid z))] + \mathcal{KL}(q_\phi(z \mid x^i) \mid\mid p(z))$$

Computing first term on RHS:

- Draw a few (or sometimes just one) samples

$$z \sim q_\phi(z \mid x^i)$$

- Approximate the expectation using Monte Carlo.

Training

Loss function:

$$-\text{ELBO}_i(\theta, \phi) = -E_{z \sim q_\phi(z \mid x^i)}[\log(p_\theta(x^i \mid z))] + \mathcal{KL}(q_\phi(z \mid x^i) \mid\mid p(z))$$

Computing second term on RHS:

- Just the KL-divergence between two Gaussians.
- Has a closed form:

$$\begin{aligned}&\mathcal{KL}(\mathcal{N}(\mu_1, \Sigma_1) \mid\mid \mathcal{N}(\mu_2, \Sigma_2)) \\ &\quad = \frac{1}{2}\left(\text{Tr}(\Sigma_2^{-1}\Sigma_1) + (\mu_2 - \mu_1)^T\Sigma_2^{-1}(\mu_2 - \mu_1) - k + \log\left(\frac{|\Sigma_2|}{|\Sigma_1|}\right)\right)\end{aligned}$$

where k is the dimension of the distributions.

Training

Loss function:

$$-\text{ELBO}_i(\theta, \phi) = -E_{z \sim q_\phi(z \mid x^i)}[\log(p_\theta(x^i \mid z))] + \mathcal{KL}(q_\phi(z \mid x^i) \mid\mid p(z))$$

Problem:

- Drawing samples $z \sim q_\phi(z \mid x^i)$ to estimate the expectation on RHS.
- This is not a differentiable step.
- Can't backpropagate error for SGD!

Reparametrization Trick

Solution: Final step is to use the reparametrization trick:

- Draw a sample $\varepsilon \sim \mathcal{N}(0, 1)$.
- $z = A\varepsilon + \mu$ will be distributed as $\mathcal{N}(\mu, A^T A)$.
- Use Cholesky decomposition $\Sigma = A^T A$ to get the desired A.
- This is a differentiable step! All the randomness comes from ε.
- Remember

$$q_\phi(z \mid x) = \mathcal{N}(\mu(x, \phi), \Sigma(x, \phi))$$

so $A(x^i, \phi)$ and $\mu(x^i, \phi)$ depend on network parameters.

Reparametrization Trick

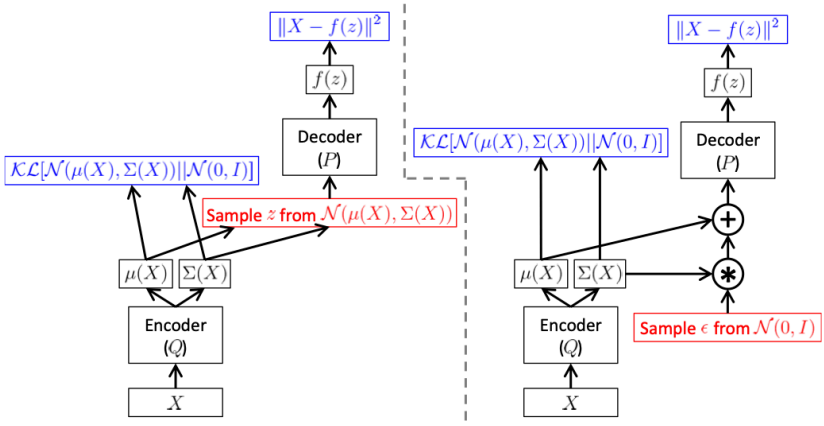


Figure: Left: Without reparametrization trick. Right: with reparametrization trick. Source: https://arxiv.org/pdf/1606.05908.pdf

Inference: Generating New Samples

- Latent space can be used to generate new samples.
- Goal is to generate data that looks like training, but is different.
- Simply sample a random z and push it through the decoder.
- Hopefully looks like new sample thanks to regularization term $\mathcal{KL}(q_\phi(z \mid x) \mid\mid p(z))$.

Inference: Generating New MNIST Samples

Figure: MNIST digits created with a VAE. Source: https://arxiv.org/pdf/1312.6114.pdf

- Look like slightly blurry digits. This is a drawback of VAEs.
- The noise from sampling z tends to produce blurry images compared to GANs.

Inference: Generating New Chemical Samples

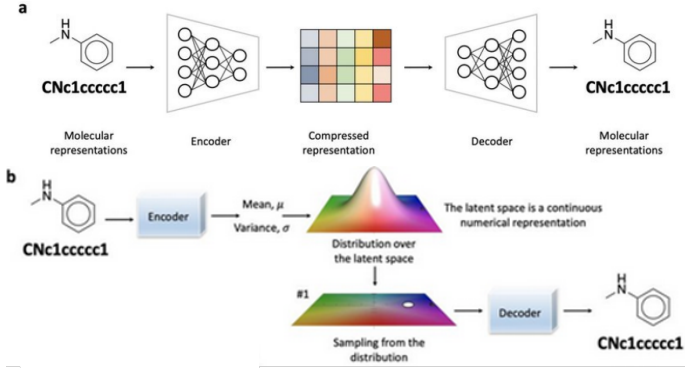


Figure: Creating new molecules similar to a given molecule. a) normal autoencoder. b) variational autoencoder. Source: https://www.researchgate.net/figure/The-autoencoder-and-the-variational-autoencoder-a-An-autoencoder-encodes-input$_fig3_343786548$

Application: Retina Disease

retina-VAE: Variationally Decoding the Spectrum of Macular Disease

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- Uses VAE to gain insights into macular disease.
- Generated 3,000 "patient profile vector" samples x^i using simulated clinical data.
- Trained a VAE with 3-dimensional latent space.
- Found 14 well-defined clusters when plotting the latent vectors.
- Classified clusters using k-means.
- Different clusters might respond better to different treatments.

Application: Retina Disease

Figure: Left: normal retina. Right: macular degeneration. Source: https://arxiv.org/pdf/1907.05195.pdf

Application: Retina Disease

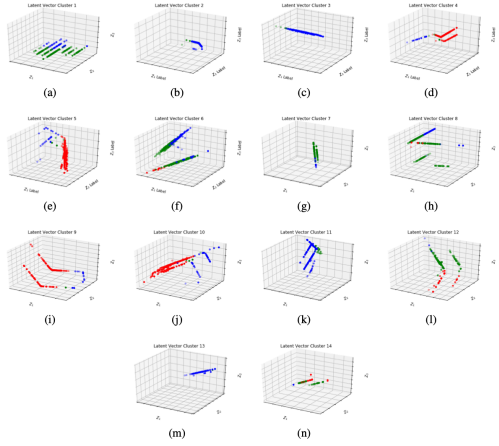

Figure: 14 clusters of the 3d latent vectors sampled from $q_\phi(z \mid x)$. Source: https://arxiv.org/pdf/1907.05195.pdf

Bayesian Variational Autoencoders

- BVAEs place a prior over the network parameters θ.
- Estimate the marginal likelihood using

$$p(\tilde{x} \mid x) \propto \int \int p_\theta(\tilde{x} \mid z) p(z) p(\theta \mid x) \, dz d\theta$$

- There are various tricks for implementing BVAEs. See e.g. `https://arxiv.org/pdf/1912.05651.pdf`.
- Can perform better on outlier detection tasks than ordinary VAEs.

Modification: β-VAEs

- β-VAEs are a generalization of VAEs.
- Hyperparameter β controls regularization strength:

$$\text{Loss} = -E_{z \sim q_\phi(z \mid x^i)}[\log(p_\theta(x^i \mid z))] + \beta \mathcal{KL}(q_\phi(z \mid x^i) \mid\mid p(z))$$

- β-VAEs allow for training with a special emphasis on *disentanglement*.

Disentanglement

- Phenomenon where latent vector components are highly interpretable.
- Changing one component of a latent vector only affects one part of output data.
- Well-chosen β values (typically $\beta > 1$) lead to increased disentanglement.

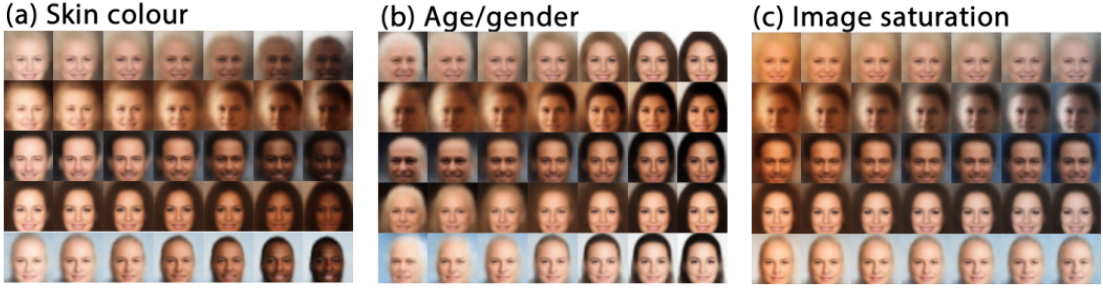

Figure: Changes to one component of the latent vector z produce interpretable changes in the output data.

Supervised Variational Autoencoders

- In supervised learning, the decoder is not used.
- Given new data $\hat{x}$, we encode it as a latent distribution $q_\phi(z \mid \hat{x})$.
- We can then connect bottleneck to an output layer of our choosing.
- For example, could use a categorical estimator in final layer

$$p(y \mid x) = \text{Categorical}(y \mid \pi_\phi(\mu(\hat{x}, \phi), \Sigma(\hat{x}, \phi), \hat{x}))$$

where π_ϕ is a probability vector learned by the network.

Supervised Variational Autoencoders

(a) Row collision. (b) Untraversable obstacle. (c) Traversable obstacle.

Figure: Supervised VAE used in a self-driving toy car trained for anomaly detection in terrain types using LiDAR data. Source: https://arxiv.org/pdf/2012.08637.pdf

Summary

- VAEs are deep generative models.
- Same architecture are autoencoders, but uses latent distribution.
- Regularization from KL-divergence allows for more realistic sampling.
- Use the reparametrization trick so that all steps are differentiable.
- With some effort, can achieve interpretability through disentanglement.
- Downside: the random nature of the latent vectors tends to lead to "blurrier" samples compared to GANs.