Variational Autoencoders - An Introduction

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Introduction - Autoencoders

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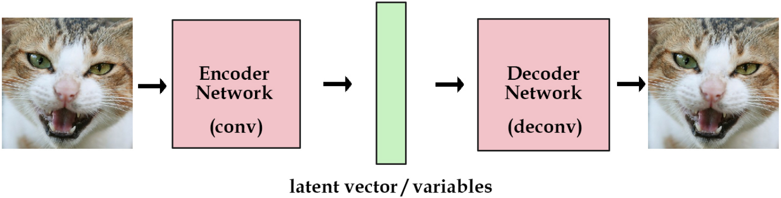

Introduction - Autoencoders

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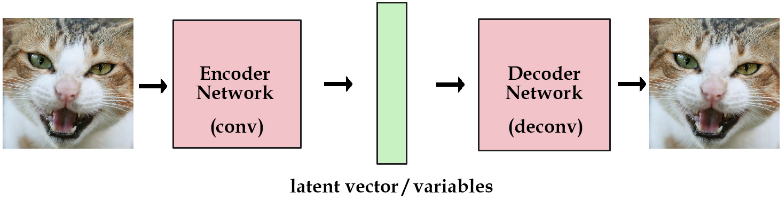

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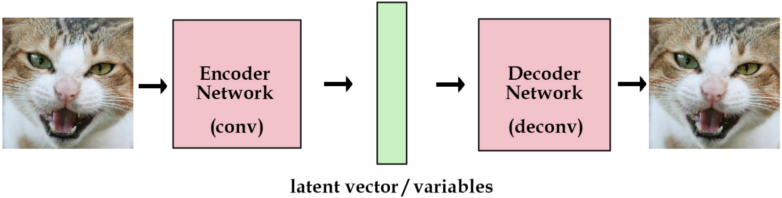
Introduction - Autoencoders

▶



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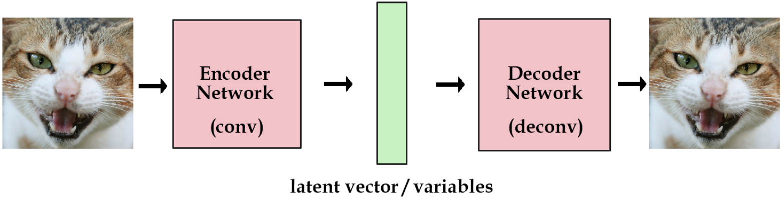
- 

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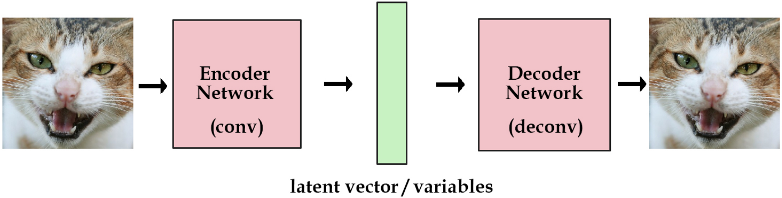
- 

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- Variational: use probabilistic latent encoding

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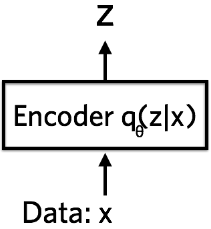
- 

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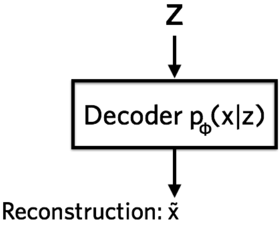
- 

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- Measures how effectively the decoder has learned to reconstruct x given the latent representation z

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- Loss for datapoint x_i:

$$l_i(\theta, \phi) = -\mathbb{E}_{z \sim q_\theta(z|x_i)}\left[\log p_\phi(x_i|z)\right] + KL\left(q_\theta(z|x_i)||p(z)\right)$$

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- Expectation taken over distribution of latent representations

Loss Function

- KL Divergence as regularizer:

$$KL\big(q_\theta(z|x_i)||p(z)\big) = \mathbb{E}_{z\sim q_\theta(z|x_i)}\big[\log q_\theta(z|x_i) - \log p(z)\big]$$

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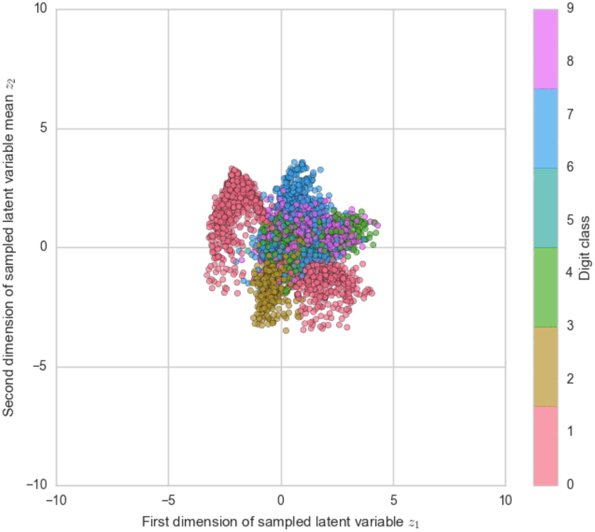
- Otherwise could "memorize" the data and map each observed datapoint to a distinct region of space

MNIST latent variable space



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- Output of $q_\theta(z|x)$ is vector of μ's and vector of σ's

Summary

- Deep Learning objective is to minimize the loss function:

$$L(\theta, \phi) = \sum_{i=1}^{N} \Big(-\mathbb{E}_{z \sim q_\theta(z|x_i)} \big[\log p_\phi(x_i|z) \big] + KL\big(q_\theta(z|x_i) || p(z)\big) \Big)$$

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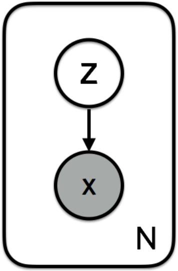
- Graphical model:



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- Which choice of λ gives the 'best' $q_\lambda(z|x)$?
- KL divergence measures information lost when using q_λ to approximate p
- Choose λ to minimize $KL\big(q_\lambda(z|x)||p(z|x)\big) = KL\big(q_\lambda||p\big)$

Probabilistic Model Perspective

- $$\begin{aligned} KL\big(q_\lambda || p\big) &:= \mathbb{E}_{z\sim q_\lambda}\big[\log q_\lambda(z|x) - \log p(z|x)\big] \\ &= \mathbb{E}_{z\sim q_\lambda}\big[\log q_\lambda(z|x)\big] - \mathbb{E}_{z\sim q_\lambda}\big[\log p(x,z)\big] \\ &\qquad + \log p(x) \end{aligned}$$

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- Still contains $p(x)$ term! So cannot compute directly
- But $p(x)$ does not depend on λ, so still hope

Probabilistic Model Perspective

- Define **E**vidence **L**ower **BO**und:

$$ELBO(\lambda) := \mathbb{E}_{z \sim q_\lambda}\big[\log p(x, z)\big] - \mathbb{E}_{z \sim q_\lambda}\big[\log q_\lambda(z|x)\big]$$

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- Then

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- So minimizing $KL\big(q_\lambda || p\big)$ w.r.t. λ is equivalent to maximizing $ELBO(\lambda)$

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- Since no two datapoints share latent variables, we can write:

$$ELBO(\lambda) = \sum_{i=1}^{N} ELBO_i(\lambda)$$

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- Where

$$ELBO_i(\lambda) = \mathbb{E}_{z \sim q_\lambda(z|x_i)}\big[\log p(x_i, z)\big] - \mathbb{E}_{z \sim q_\lambda(z|x_i)}\big[\log q_\lambda(z|x_i)\big]$$

Probabilistic Model Perspective

- We can rewrite the term $ELBO_i(\lambda)$:

$$
\begin{aligned}
ELBO_i(\lambda) &= \mathbb{E}_{z\sim q_\lambda(z|x_i)}\Big[\log p(x_i, z)\Big] - \mathbb{E}_{z\sim q_\lambda(z|x_i)}\Big[\log q_\lambda(z|x_i)\Big] \\
&= \mathbb{E}_{z\sim q_\lambda(z|x_i)}\Big[\log p(x_i|z) + \log p(z)\Big] \\
&\qquad - \mathbb{E}_{z\sim q_\lambda(z|x_i)}\Big[\log q_\lambda(z|x_i)\Big] \\
&= \mathbb{E}_{z\sim q_\lambda(z|x_i)}\Big[\log p(x_i|z)\Big] \\
&\qquad - \mathbb{E}_{z\sim q_\lambda(z|x_i)}\Big[\log q_\lambda(z|x_i) - \log p(z)\Big] \\
&= \mathbb{E}_{z\sim q_\lambda(z|x_i)}\Big[\log p(x_i|z)\Big] - KL\Big(q_\lambda(z|x_i)||p(z)\Big)
\end{aligned}
$$

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- How do we relate λ to ϕ and θ seen earlier?
- We can parameterize approximate posterior $q_\theta(z|x, \lambda)$ by a network that takes data x and outputs parameters λ
- Parameterize the likelihood $p(x|z)$ with a network that takes latent variables and outputs parameters to the data distribution $p_\phi(x|z)$
- So we can re-write

$$ELBO_i(\theta, \phi) = \mathbb{E}_{z \sim q_\theta(z|x_i)}\big[\log p_\phi(x_i|z)\big] - KL\big(q_\theta(z|x_i)||p(z)\big)$$

Probabilistic Model Objective

- Recall the Deep Learning objective derived earlier. We want to minimize:

$$L(\theta, \phi) = \sum_{i=1}^{N} \Big(- E_{z \sim q_\theta(z|x_i)} \big[\log p_\phi(x_i|z) \big] + KL\big(q_\theta(z|x_i) || p(z)\big) \Big)$$

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- The objective just derived for the Probabilistic Model was to maximize:

$$ELBO(\theta, \phi) = \sum_{i=1}^{N} \Big(\mathbb{E}_{z \sim q_\theta(z|x_i)} \big[\log p_\phi(x_i|z) \big] - KL\big(q_\theta(z|x_i) || p(z)\big) \Big)$$

- They are equivalent!

Applications - Image generation

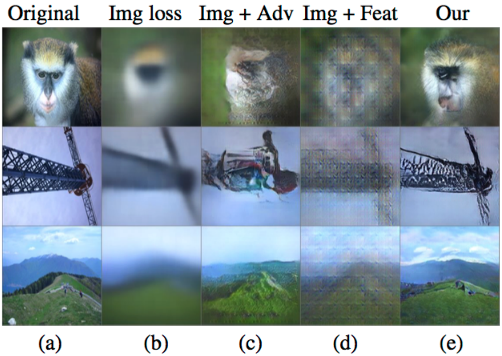


Figure 1: Reconstructions from AlexNet FC6 with different components of the loss.

A. Dosovitskiy and T. Brox. Generating images with perceptual similarity metrics based on deep networks. *arXiv preprint arXiv*:1602.02644, 2016.

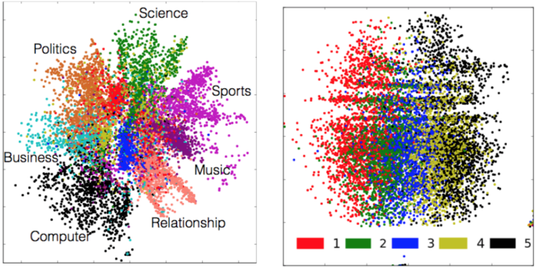
Applications - Caption generation

a man with a snowboard next to a man with glasses | a big black dog standing on the grass | a player is holding a hockey stick | a desk with a keyboard | a man is standing next to a brown horse | a box full of apples and oranges

Figure 2: Examples of generated caption from unseen images on the validation dataset of ImageNet.

Y. Pu, Z. Gan, R. Henao, X. Yuan, C. Li, A. Stevens, and L. Carin. Variational autoencoder for deep learning of images, labels and captions. In NIPS, 2016.

Applications - Semi-/Un-supervised document classification



(a) Yahoo (b) Yelp

Figure 3: Visualizations of learned latent representations.

Z. Yang, Z. Hu, R. Salakhutdinov, and T. Berg-Kirkpatrick. Improved variational autoencoders for text modeling using dilated convolutions. In *Proceedings of The 34rd International Conference on Machine Learning*, 2017.

Applications - Pixel art videogame characters

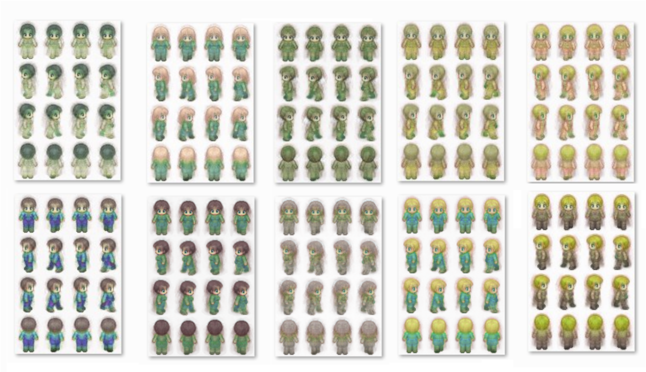


Figure 6: Samples of the generated characters

https://mlexplained.wordpress.com/category/generative-models/vae/.

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- Thank you. Questions?