On the Latent Space of Deep Generative Models

Honors Thesis Presentation

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August 2018

Outline

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Deep Generative Models

- "[Generative Adversarial Networks], and the variations that are now being proposed is the most interesting idea in the last 10 years in ML, in my opinion." - Yann LeCun (courtesy of Quora post)

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- Sample noise from distribution (draw a latent vector), pass through a function (typically a neural net), and get meaningful output (some image)

Variational Autoencoders

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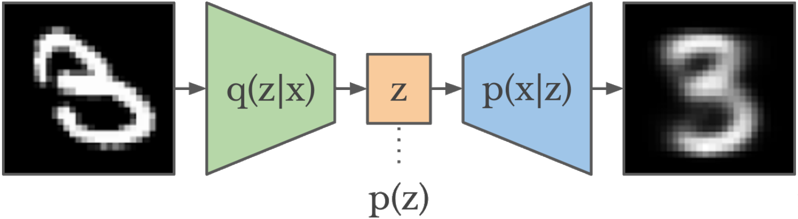
  - On average, how lossy is the compression that the VAE is performing?
  - Use ℓ_2 distance between two images

VAE Architecture



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[1] Diagram courtesy of Danijar Hafner.

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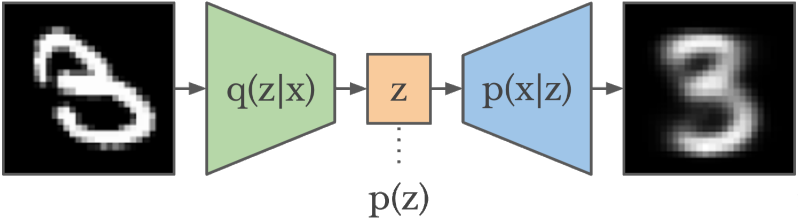

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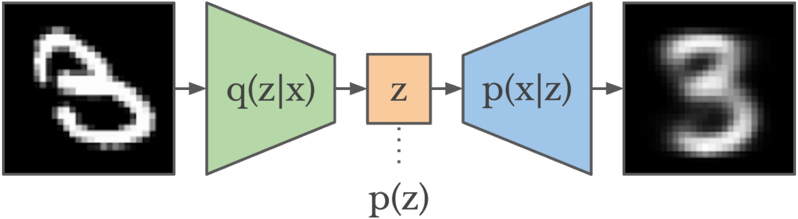

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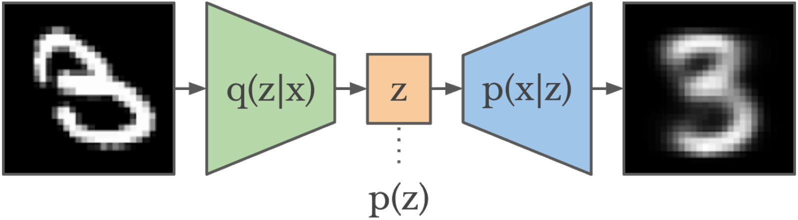

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- Generator tries to fool discriminator by producing realistic outputs
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- Formulated as min-max game

Problems

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Generally, theoretical understanding of deep generative models is still lacking.

Outline

Deep Generative Model

Definition (Deep Generative Model)

A *deep generative model* is a (possibly randomized) function, denoted g, that accepts some vector $z \in \mathbb{R}^d$ for some d as input and outputs some image $I \in \mathcal{I}$, where $\mathcal{I}$ represents the space of images.

Encoder

Definition (Encoder)

An *encoder* is a (possibly randomized) function, denoted f, that accepts some input image $I \in \mathcal{I}$ (where, again $\mathcal{I}$ is the space of images) and outputs some vector $z \in \mathbb{R}^d$.

Class

Definition (Class)

Suppose we are given a classifier into K classes $c : \mathcal{I} \to [K]$ that accepts as input an image and outputs a class label which is an integer index in $[K] := \{i\}_{i=1}^{K}$. Then, the *class* of an image I under c is given by:

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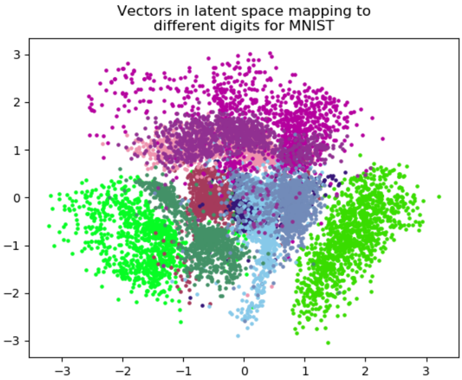
In words, K_i is the subset of the latent space that is classified into label i when a point $z \in K_i$ is passed through g and subsequently classified by c.

Latent Hole

Definition (Latent Hole)

A *hole* is a point $z \in \mathbb{R}^d$ such that there does not exist an image I in the data manifold for which $f(I) = z$.

Examples


Vectors in latent space mapping to
different digits for MNIST
3
2
1
0
−1
−2
−3
−3
−2
−1
0
1
2
3

Class Radius

Definition (Class Radius)

Consider the probability vector $p \in \mathbb{R}^K$ such that:

$$p_i \propto \nu\left(K_i\right)$$

Then, the *class radius* is the expected distance from a random point $z \sim p$ in some class to the closest point in a different class. Specifically, define $r(z)$ below, and let $c(g(z)) = i$:

$$r(z) := \inf_{z' \in \bigcup_{j \neq i} K_j} \left\| z - z' \right\|$$

Then the class radius is simply:

$$\mathop{\mathbb{E}}_{z \sim p}\left[r(z)\right]$$

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  - Attempted resolution: bring classes closer to each other and cover more probability (our empirical contribution)

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Assumptions

Probability Decay

$$\|p\|_\infty \leq \min\left(\frac{1}{5}, h(K) \in \left[\Omega\left(\frac{1}{K}\right), o(1)\right]\right)$$

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Partition of Latent Space

$$\bigcup_{i=1}^{K} K_i = \mathbb{R}^d$$

- Every latent vector maps to some image in the data manifold

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Class Radius to Diversity

Theorem

Under the aforementioned assumptions, we have the following regarding the expected class radius of each image in the latent space of our generative model:

$$\mathbb{E}\left[r(z)\right] \leq \frac{\log\left(4\pi \log\left(1/\left\|p\right\|_2^2\right)\right)}{\sqrt{2\log\left(1/\left\|p\right\|_2^2\right)}}$$

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- Upper bound depends *only* on $\|p\|_2^2$

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$\|p\|_2^2$ as a Measure of Diversity

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I have a bunch of socks in a drawer distributed according to p. If I draw two socks, what is the probability that they are of the same type?

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- $\sum p_i^2 = \|p\|_2^2$

$||p||_2^2$ as a Measure of Diversity

Definition (α-order Rényi Entropy)

$$H_\alpha(p) = \frac{1}{1-\alpha} \log \left(\sum_{i=1}^{K} p_i^\alpha \right)$$

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Special Case: Collision Entropy

$$H_2(p) = -\log \left(\sum p_i^2 \right) = \log \left(\frac{1}{\|p\|_2^2} \right)$$

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Fact (Maximum Entropy Distribution)

For all α, the distribution maximizing the α-order Rényi Entropy is the uniform distribution, yielding:

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$$\mathbb{E}[r(z)] \leq \frac{\log(4\pi \log(K))}{\sqrt{2\log(K)}}$$

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3. Massage a little
   - Our contribution

Some Details

(Slightly rewritten) Result from Fawzi et al. (2018)

$$\mathbb{E}\left[r(z)\right] \leq \sum_{i=1}^{K} \Phi^{-1}(p_i) \cdot p_i + \frac{e^{-\Phi^{-1}(p_i)^2/2}}{\sqrt{2\pi}}$$

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Rewrite some:

$$\sum_{i=1}^{K} \Phi^{-1}(p_i) \cdot p_i + \frac{e^{-\Phi^{-1}(p_i)^2/2}}{\sqrt{2\pi}} \leq \sum_{i=1}^{K} p_i \left(\frac{\log\left(4\pi \log\left(1/p_i\right)\right)}{\sqrt{2\log\left(1/p_i\right)}} \right)$$

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Use concavity of:

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Then Jensen:

$$\mathbb{E}\left[r(z)\right] \leq g\left(\sum_{i=1}^{K} p_i \cdot p_i\right) = g\left(\|p\|_2^2\right) = \boxed{\frac{\log\left(4\pi \log\left(1/\|p\|_2^2\right)\right)}{\sqrt{2\log\left(1/\|p\|_2^2\right)}}}$$

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Test for Diversity

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Solution

Compare $\mathbb{E}[r(z)]$ for g_1 and g_2; claim that the generator with higher class radius is less diverse.

Unfortunately, computing $\mathbb{E}[r(z)]$ might be more difficult than computing $\|p\|_2^2$ unless K is extremely large

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- If g is L-Lipschitz, then on average, you don't have to perturb too much in image space:

$$L \cdot \frac{\log\left(4\pi \log\left(1/\left\|p\right\|_2^2\right)\right)}{\sqrt{2\log\left(1/\left\|p\right\|_2^2\right)}}$$

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- Under the probability decay assumption, above approaches 0 as the number of classes K grows arbitrarily large

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Regularize with $\omega\left(\cdot, \cdot\right)$ summed over many pairs of images. To force ω to be low, enforce Lipschitz constant via network weight clipping.

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- Regularizer (batch size b; set $\lambda = 30$):

$$\lambda \cdot \sum_{i=1}^{b/2} \omega\left(I_i, I_{i+b/2}\right)$$

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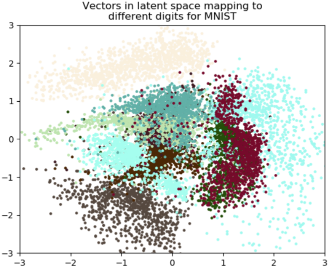
- Vanilla VAE objective
- Regularizer (batch size b; set $\lambda = 30$):

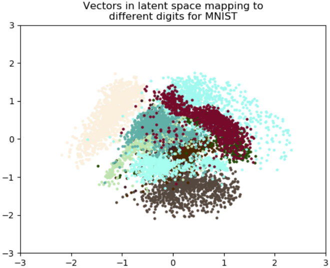
$$\lambda \cdot \sum_{i=1}^{b/2} \omega\left(I_i, I_{i+b/2}\right)$$

- Clip weights to $[-0.3, 0.3]$

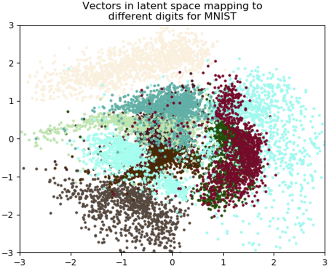
Outline

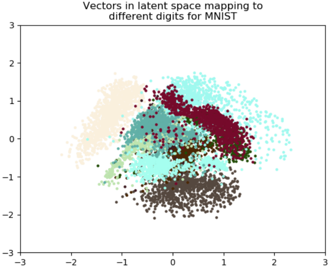
Geometric Implications





Geometric Implications





Conclusion: Modified VAE makes classes come closer to one another but decreases probability mass of space covered

Sample Quality

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Conclusion: Modified VAE does not change quality of generated samples noticeably

Interpretation of Results

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Problem

For future: Devise an optimization objective that favors both closer classes and better coverage of the latent space.

Conclusion

Summary

We care about coverage of the latent space.

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- As previously identified, this is indicative of the model having better learned the data manifold.

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We want to leverage these findings empirically.

- Develop optimization procedures to achieve these properties
- Test generative models for diversity
- Meta-Problem: Theoretically understand generative models better

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