Evaluating Generative Models

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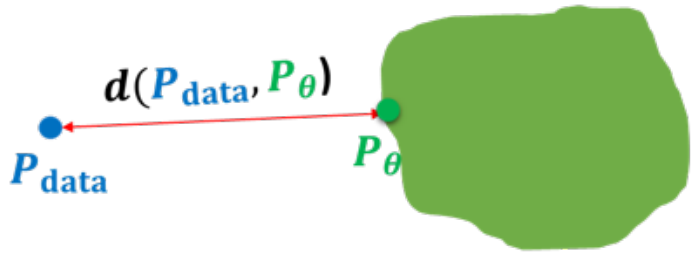
Lecture 15

Announcements

- Assignment 3 is due this Sunday..
- We will have a guest lecture next Wednesday

Background

$\mathbf{x}_i \sim P_{\text{data}}$
$i = 1, 2, \ldots, n$



Story so far

- Representation: Latent variable vs. fully observed
- Objective function and optimization algorithm: Many divergences and distances optimized via likelihood-free (two sample test) or likelihood based methods

Plan for today: Evaluating generative models

Evaluation

- Evaluating generative models can be very tricky
- **Key question**: What is the task that you care about?
  - Classical generative modeling tasks?
    - Density estimation
    - Sampling/generation
    - Latent representation learning
  - More than one task? Custom downstream task?
    - Semisupervised learning
    - Image translation
    - Compressive sensing
- In any research field, evaluation drives progress. How do we evaluate generative models?

Lecture Outline

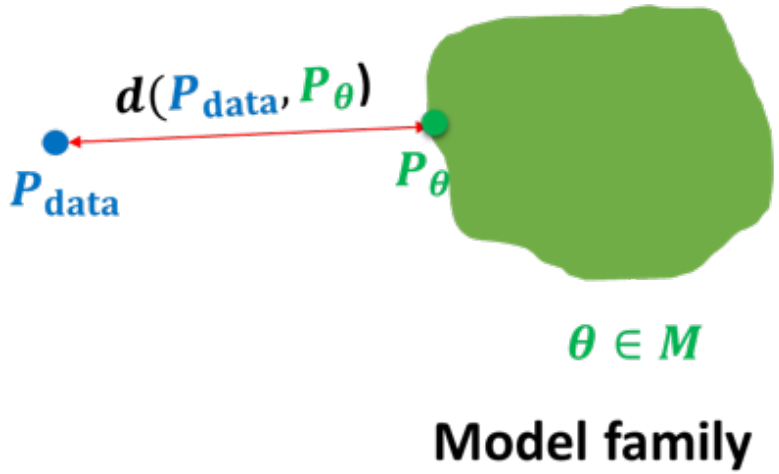
1. Density Esimation
   - Overfitting & Underfitting
   - Importance Sampling
   - Kernel Density Estimation
2. Evaluating Sample Quality
   - Inception Scores
   - Frechet Inception Distance
   - Kernel Inception Distance
3. Evaluating Latent Variables
   - Supervised Clustering
   - Compression
   - Disentanglement

Recall: Density Estimation

Density estimation is the task of learning the full distribution so that later we can answer *any* probabilistic inference query

- We want to construct P_θ as "close" as possible to P_{data} (recall we assume we are given a dataset $\mathcal{D}$ of samples from P_{data})

$$x_i \sim P_{\text{data}}$$
$$i = 1, 2, \ldots, n$$



- We can use an objective $d(P_{\text{data}}, P_\theta)$ that captures "closeness" between $P_{\text{data}}, P_\theta$
- In practice, we use the KL divergence, which is equivalent (up to a constant) to maximum likelihood.

Evaluating Density Estimation

Density estimation is the task of learning a good model p_θ that approximates p_{data}. Afterwards, we can use p_θ for any task.

- In practice, we evaluate models using the KL divergence, which is equivalent (up to a constant) to maximum likelihood.

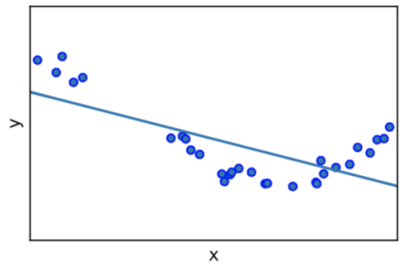
It's straightforward to evaluate models with tractable likelihoods

- Split dataset into train, validation, test sets
- Evaluate gradients based on train set
- Tune hyperparameters (e.g., learning rate, neural network architecture) based on validation set
- Evaluate generalization by reporting likelihoods on test set

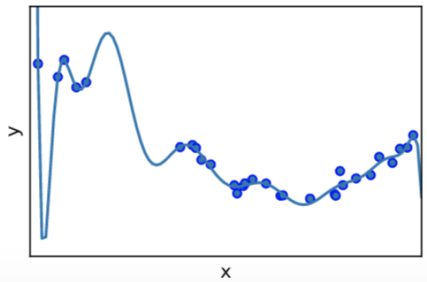
Overfitting vs. Underfitting

We evaluate densities on a test set to assess generalization and detect overfitting.

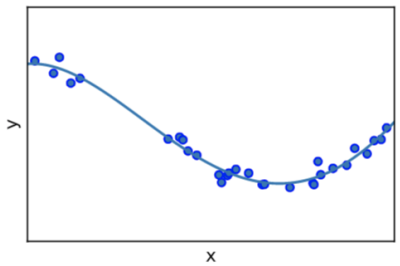
- Density can be wrong due to underfitting (bias) and overfitting (variance).
- Examples of underfitting:
  - Linear function
  - Mixture of Gaussians on dog images



- Examples of overfitting:
  - High degree polynomial
  - Memorizing the training set



- Example of a good fit
  - Low degree polynomial
  - Well-tuned generative model



Density Estimation Without Tractable Likelihoods

Not all models have tractable likelihoods e.g., VAEs, GANs, energy based models. What do we do in such cases?

- For **VAEs**, we can compare evidence lower bounds (ELBO) to log-likelihoods.
- For **energy-based models** and **VAEs**, we can perform (annealed) importance sampling to estimate the density directly.
- For implicit models (e.g., **GANs**), we can estimate the density from samples using non-parametric kernel density estimation.

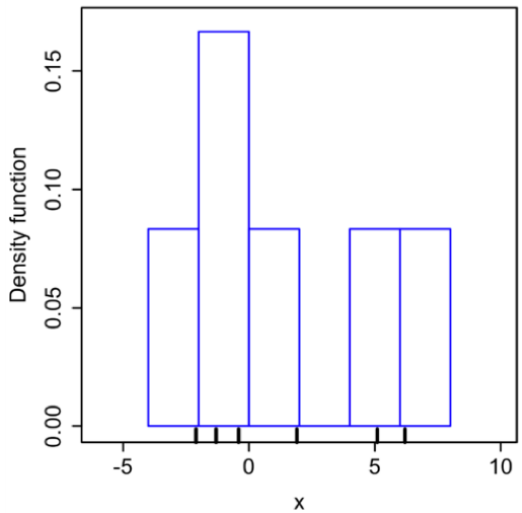
Note: These alternatives often make strong assumptions and don't always work easily and reliably in practice.

Kernel Density Estimation

- Given: A model $p_\theta(\mathbf{x})$ with an intractable/ill-defined density
- Let $\mathcal{S} = \{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \cdots, \mathbf{x}^{(6)}\}$ be 6 data points drawn from p_θ.

$\mathbf{x}^{(1)}$	$\mathbf{x}^{(2)}$	$\mathbf{x}^{(3)}$	$\mathbf{x}^{(4)}$	$\mathbf{x}^{(5)}$	$\mathbf{x}^{(6)}$
-2.1	-1.3	-0.4	1.9	5.1	6.2

- What is $p_\theta(-0.5)$?
- **Answer 1:** Since $-0.5 \notin \mathcal{S}$, $p_\theta(-0.5) = 0$
- **Answer 2:** Compute a histogram by binning the samples



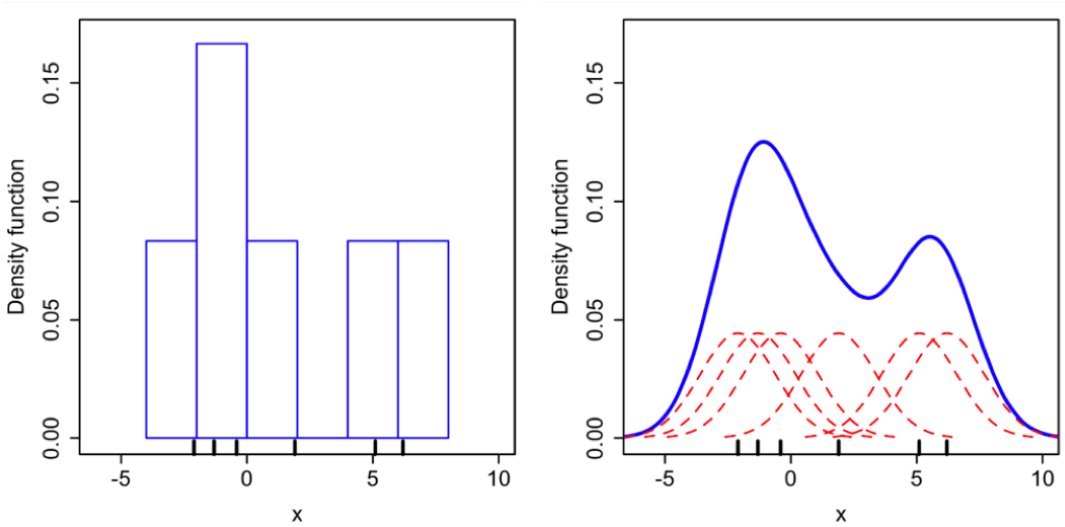
- Bin width= 2, min height= 1/12 (area under histogram should equal 1). What is $p_\theta(-0.5)$? 1/6 $p_\theta(-1.99)$? 1/6 $p_\theta(-2.01)$? 1/12

Kernel Density Estimation

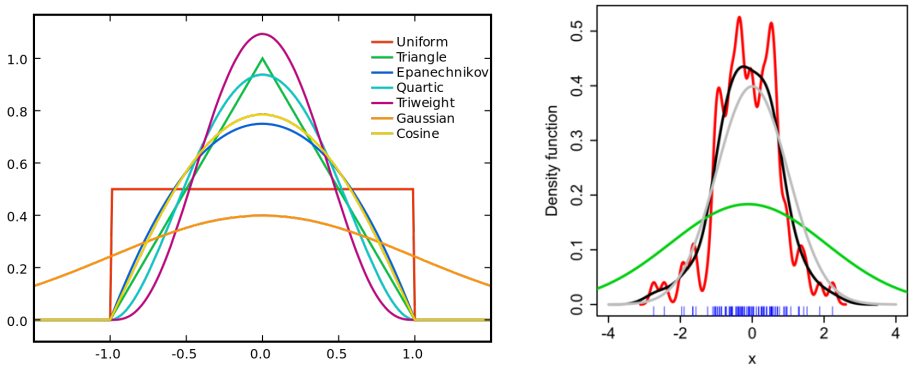
- **Answer 3:** Compute kernel density estimate (KDE) over $\mathcal{S}$

$$\hat{p}(\mathbf{x}) = \frac{1}{n} \sum_{\mathbf{x}^{(i)} \in \mathcal{S}} K\left(\frac{\mathbf{x} - \mathbf{x}^{(i)}}{\sigma}\right)$$

  where σ is called the bandwidth parameter and K is called the kernel function.
- Example: Gaussian kernel, $K(u) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}u^2\right)$
- Histogram density estimate vs. KDE estimate with Gaussian kernel



Kernel Density Estimation



- A **kernel** K is any non-negative function satisfying two properties
  - Normalization: $\int_{-\infty}^{\infty} K(u)\mathrm{d}u = 1$ (ensures KDE is also normalized)
  - Symmetric: $K(u) = K(-u)$ for all u
- Intuitively, a kernel is a measure of similarity between pairs of points (function is higher when the difference in points is close to 0)
- **Bandwidth** σ controls the smoothness (see right figure above)
  - Optimal sigma (black) is such that KDE is close to true density (grey)
  - Low sigma (red curve): undersmoothed
  - High sigma (green curve): oversmoothed
  - Tuned via crossvalidation
- **Con**: KDE is very unreliable in higher dimensions

Importance Sampling

Importance sampling is a clever way of applying Monte Carlo. First, we express $p_\theta(\mathbf{x})$ as a different kind of expectation:

$$p_\theta(\mathbf{x}) = \sum_{\mathbf{z}\in\mathcal{Z}} p_\theta(\mathbf{x},\mathbf{z}) = \sum_{\mathbf{z}\in\mathcal{Z}} \frac{q(\mathbf{z})}{q(\mathbf{z})} p_\theta(\mathbf{x},\mathbf{z}) = \mathbb{E}_{\mathbf{z}\sim q(\mathbf{z})}\left[\frac{p_\theta(\mathbf{x},\mathbf{z})}{q(\mathbf{z})}\right]$$

where q can be any distribution over $\mathbf{z}$. We then apply Monte Carlo:

1. Sample $\mathbf{z}^{(1)}, \cdots, \mathbf{z}^{(k)}$ from $q(\mathbf{z})$ (instead of uniformly at random!)
2. Approximate expectation with sample average

$$p_\theta(\mathbf{x}) \approx \frac{1}{k}\sum_{j=1}^{k} \frac{p_\theta(\mathbf{x},\mathbf{z}^{(j)})}{q(\mathbf{z}^{(j)})}$$

What is a good choice for $q(\mathbf{z})$? Using $p(\mathbf{z}|\mathbf{x})$ yields correct density in one sample. In practice we choose tractable $q(\mathbf{z}) \approx p(\mathbf{z}|\mathbf{x})$.

1. The same technique to any $f(\mathbf{z})$ such as $\log p_\theta(\mathbf{x},\mathbf{z})$ in VAEs.
2. *Annealed* importance sampling is an advanced extension that works for energy-based models.

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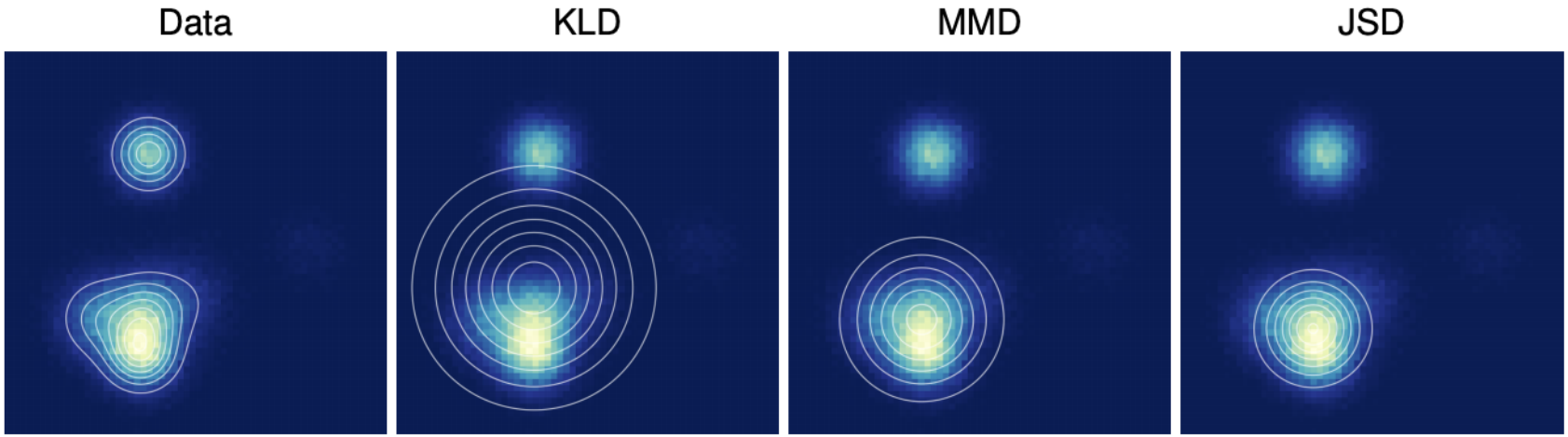
Log-Likelihood vs. Sample Quality

What are some pros and cons of using likelihood?

- Optimal generative model will give best **sample quality** and highest test **log-likelihood**
- For imperfect models, achieving high log-likelihoods might not always imply good sample quality, and vice-versa (Theis et al., 2016)
- Likelihood is only one possible metric to define the distance between two distributions



High Likelihood Does Not Imply Great Samples

Example: Great test log-likelihoods, poor samples. Consider a mixture model $p_\theta(\mathbf{x}) = 0.01 p_{\text{data}}(\mathbf{x}) + 0.99 p_{\text{noise}}(\mathbf{x})$ of data and noise.

- 99% of the samples are just noise
- Taking logs, we get a lower bound

$$\begin{aligned}\log p_\theta(\mathbf{x}) &= \log[0.01 p_{\text{data}}(\mathbf{x}) + 0.99 p_{\text{noise}}(\mathbf{x})] \\ &\geq \log 0.01 p_{\text{data}}(\mathbf{x}) = \log p_{\text{data}}(\mathbf{x}) - \log 100\end{aligned}$$

- For expected likelihoods, we know that
  - Lower bound

$$E_{p_{\text{data}}}[\log p_\theta(\mathbf{x})] \geq E_{p_{\text{data}}}[\log p_{\text{data}}(\mathbf{x})] - \log 100$$

  - Upper bound (via non-negativity of KL)

$$E_{p_{\text{data}}}[\log p_{\text{data}}(\mathbf{x}))] \geq E_{p_{\text{data}}}[\log p_\theta(\mathbf{x})]$$

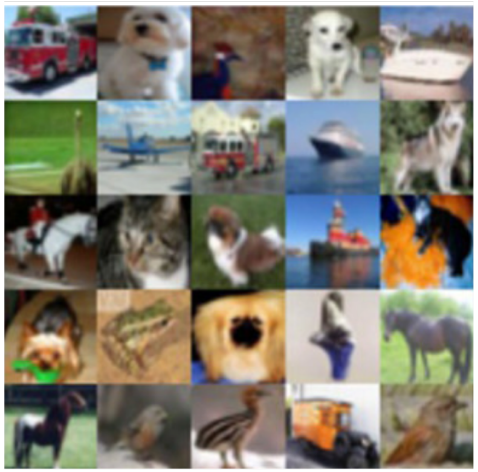
- As we increase the dimension of $\mathbf{x}$, absolute value of $\log p_{\text{data}}(\mathbf{x})$ increases proportionally but $\log 100$ remains constant. Hence, $E_{p_{\text{data}}}[\log p_\theta(\mathbf{x})] \approx E_{p_{\text{data}}}[\log p_{\text{data}}(\mathbf{x})]$ in very high dimensions

Great Samples Don't Imply High Likelihood

Example: Great samples, poor test log-likelihoods. Consider a model that simply memorizes the training set.

- Samples look exactly like the training set (cannot do better!)
- Test set will have zero probability assigned (cannot do worse!)
- The above cases suggest that it might be useful to disentangle likelihoods and samples.

Evaluation of Sample Quality



vs.

$S_1 = \{\mathbf{x} \sim P\}$ $S_2 = \{\mathbf{x} \sim Q\}$

- Which of these two sets of generated samples "look" better?
- Human evaluations (e.g., Mechanical Turk) are expensive, biased, hard to reproduce
- Generalization is hard to define and assess: memorizing the training set would give excellent samples but clearly undesirable
- Quantitative evaluation of a qualitative task can have many answers
- Popular metrics: Inception Scores, Frechet Inception Distance, Kernel Inception Distance

Inception Scores

- **Assumption 1:** We are evaluating sample quality for generative models trained on labelled datasets
- **Assumption 2:** We have a good probabilistic classifier $c(y|\mathbf{x})$ for predicting the label y for any point $\mathbf{x}$
- We want samples from a good generative model to satisfy two criteria: sharpness and diversity
- **Sharpness (S)**

Low sharpness

High sharpness

$$S = \exp\left(E_{\mathbf{x}\sim p}\left[\int c(y|\mathbf{x}) \log c(y|\mathbf{x}) \mathrm{d}y\right]\right)$$

- High sharpness implies classifier is confident in making predictions for generated images
- That is, classifier's predictive distribution $c(y|\mathbf{x})$ has low entropy

Inception Scores

- **Diversity (D)**

Low diversity

High diversity

$$D = \exp\left(-E_{\mathbf{x}\sim p}\left[\int c(y|\mathbf{x})\log c(y)\mathrm{d}y\right]\right)$$

where $c(y) = E_{\mathbf{x}\sim p}[c(y|\mathbf{x})]$ is the classifier's marginal predictive distribution

- High diversity implies $c(y)$ has high entropy
- Inception scores (IS) combine the two criteria of sharpness and diversity into a simple metric

$$IS = D \times S = \mathbb{E}_{x\sim p}\left[KL\left(c(y|x)||c(y)\right)\right]$$

- Correlates well with human judgement in practice
- If classifier is not available, a classifier trained on a large dataset, e.g., Inception Net trained on the ImageNet dataset

Frechet Inception Distance

- Inception Scores only require samples from p_θ and do not take into account the desired data distribution p_{data} directly (only implicitly via a classifier)
- **Frechet Inception Distance (FID)** measures similarities in the feature representations (e.g., those learned by a pretrained classifier) for datapoints sampled from p_θ and the test dataset
- Computing FID:
  - Let $\mathcal{G}$ denote the generated samples and $\mathcal{T}$ denote the test dataset
  - Compute feature representations $F_{\mathcal{G}}$ and $F_{\mathcal{T}}$ for $\mathcal{G}$ and $\mathcal{T}$ respectively (e.g., prefinal layer of Inception Net)
  - Fit a multivariate Gaussian to each of $F_{\mathcal{G}}$ and $F_{\mathcal{T}}$. Let $(\mu_{\mathcal{G}}, \Sigma_{\mathcal{G}})$ and $(\mu_{\mathcal{T}}, \Sigma_{\mathcal{T}})$ denote the mean and covariances of the two Gaussians
  - FID is defined as

$$\text{FID} = \|\mu_{\mathcal{T}} - \mu_{\mathcal{G}}\|^2 + \text{Tr}(\Sigma_{\mathcal{T}} + \Sigma_{\mathcal{G}} - 2(\Sigma_{\mathcal{T}}\Sigma_{\mathcal{G}})^{1/2})$$

- Lower FID implies better sample quality

Kernel Inception Distance

- **Maximum Mean Discrepancy (MMD)** is a two-sample test statistic that compares samples from two distributions p and q by computing differences in their moments (mean, variances etc.)
- Key idea: Use a suitable kernel e.g., Gaussian to measure similarity between points

$$MMD(p, q) = E_{\mathbf{x},\mathbf{x}' \sim p}[K(\mathbf{x}, \mathbf{x}')] + E_{\mathbf{x},\mathbf{x}' \sim q}[K(\mathbf{x}, \mathbf{x}')] - 2E_{\mathbf{x} \sim p, \mathbf{x}' \sim q}[K(\mathbf{x}, \mathbf{x}')]$$

- Intuitively, MMD is comparing the "similarity" between samples within p and q individually to the samples from the mixture of p and q
- **Kernel Inception Distance (KID):** compute the MMD in the feature space of a classifier (e.g., Inception Network)
- FID vs. KID
  - FID is biased (can only be positive), KID is unbiased
  - FID can be evaluated in $O(n)$ time, KID evaluation requires $O(n^2)$ time

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Evaluating Latent Representations on Downstream Tasks

- What does it mean to learn "good" latent representations?
- For a downstream task, the representations can be evaluated based on the corresponding performance metrics e.g., accuracy for semi-supervised learning, reconstruction quality for denoising
- Example: Improved GANs by Salimans et al.

Model	Number of incorrectly predicted test examples for a given number of labeled samples			
	20	50	100	200
DGN [22]			333 ± 14	
Virtual Adversarial [23]			212	
CatGAN [14]			191 ± 10	
Skip Deep Generative Model [24]			132 ± 7	
Ladder network [25]			106 ± 37	
Auxiliary Deep Generative Model [24]			96 ± 2	
Our model	1677 ± 452	221 ± 136	93 ± 6.5	90 ± 4.2
Ensemble of 10 of our models	1134 ± 445	142 ± 96	86 ± 5.6	81 ± 4.3

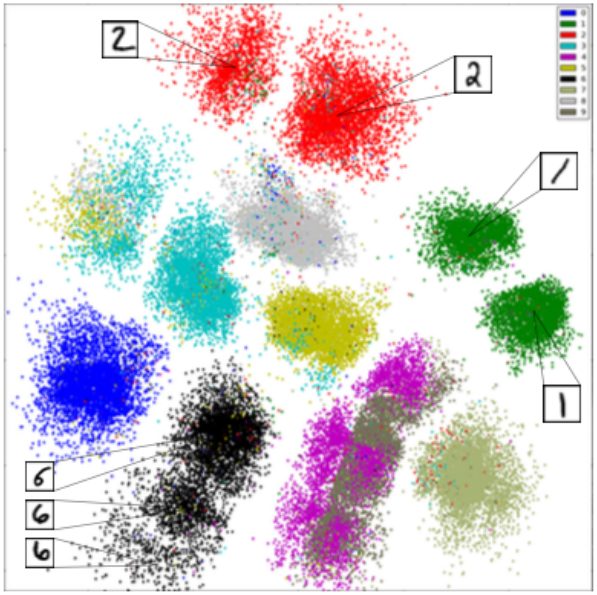
Table 1: Number of incorrectly classified test examples for the semi-supervised setting on permutation invariant MNIST. Results are averaged over 10 seeds.

Evaluating Latents Without Downstream Tasks

- What does it mean to learn "good" latent representations?
- For unsupervised tasks, there is no one-size-fits-all
- Three commonly used notions for evaluating unsupervised latent representations
  - Clustering
  - Compression
  - Disentanglement

Clustering in Latent Space

- Clusters in latent space often reveal useful structure about the data:



- These clusters can be computed automatically by applying k-means or any other algorithm in the latent space of generative model
- When labels are available (e.g., MNIST digits), we can evaluate clusters quantitatively using standard clustering metrics e.g., completeness score, homogeneity score, v-measure.

Evaluating Clustering When Labels Are Available

- For labelled datasets, there exists many quantitative evaluation metrics
- Note labels are only used for evaluation, not obtaining clusters itself (i.e., clustering is unsupervised)
- `from sklearn.metrics.cluster import completeness_score, homogeneity_score, v_measure_score`
- **Completeness score** (between [0, 1]): maximized when all the data points that are members of a given class are elements of the same cluster
  `completeness_score(labels_true=[0, 0, 1, 1], labels_pred=[0, 1, 0, 1]) % 0`
- **Homogeneity score** (between [0, 1]): maximized when all of its clusters contain only data points which are members of a single class
  `homogeneity_score(labels_true=[0, 0, 1, 1], labels_pred=[1, 1, 0, 0]) % 1`
- **V measure score** (also called normalized mutual information, between [0, 1]): harmonic mean of completeness and homogeneity score
  `v_measure_score(labels_true=[0, 0, 1, 1], labels_pred=[1, 1, 0, 0]) % 1`

Compression

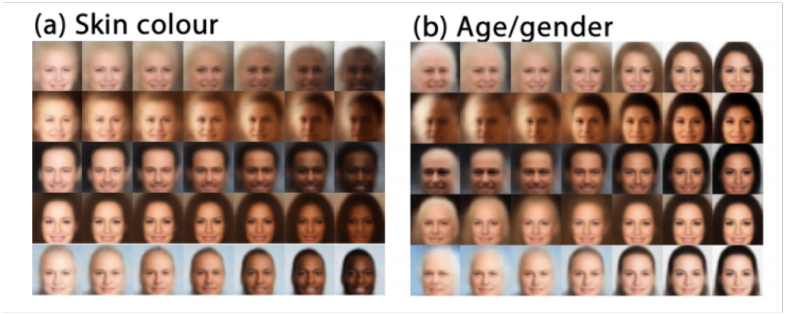
- Latent representations can be evaluated based on the maximum compression they can achieve without significant loss in reconstruction accuracy

Source: Santurkar et al., 2018

- Standard metrics such as Mean Squared Error (MSE), Peak Signal to Noise Ratio (PSNR), Structure Similarity Index (SSIM)

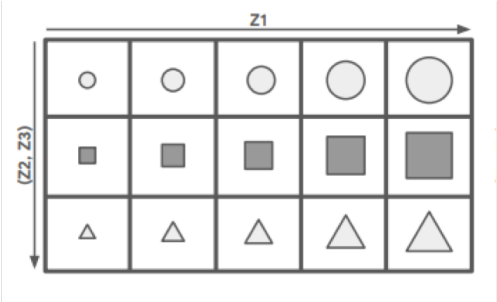
Disentanglement

- Intuitively, we want representations that disentangle **independent and interpretable** attributes of the observed data



Source: Higgins et al., 2018

- Provide user control over the attributes of the generated data



Source: Shu et al., 2019

  - When Z_1 is fixed, size of the generated object never changes
  - When Z_1 is changed, the change is restricted to the size of the generated object

Recall: InfoVAE and InfoGAN

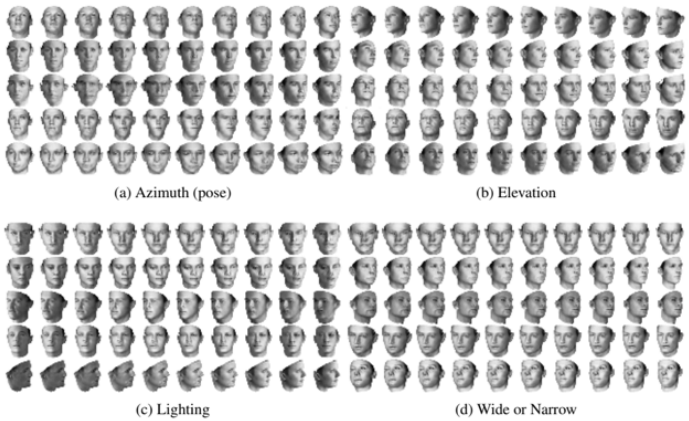
- Explicitly add a mutual information term to the objective

$$-D_{KL}(\underbrace{p_{data}(\mathbf{x})q(\mathbf{z} \mid \mathbf{x};\phi)}_{q(\mathbf{z},\mathbf{x};\phi)} \| \underbrace{p(\mathbf{x};\theta)p(\mathbf{z}|\mathbf{x};\theta)}_{p(\mathbf{z},\mathbf{x};\theta)}) + \alpha MI(\mathbf{x},\mathbf{z})$$

- MI intuitively measures how far $\mathbf{x}$ and $\mathbf{z}$ are from being independent

$$MI(\mathbf{x},\mathbf{z}) = D_{KL}\left(p(\mathbf{z},\mathbf{x};\theta)\|p(\mathbf{z})p(\mathbf{x};\theta)\right)$$

- InfoGAN (Chen et al, 2016) learns disentangled representations of the data



- Many quantiative metrics: Beta-VAE metric (Higgins et al., 2017), Factor-VAE metric, Mutual Information Gap, SAP score, DCI disentanglement, Modularity. None is perfect yet.

Summary

- Quantitative evaluation of generative models is a challenging task
- For downstream applications, one can rely on application-specific metrics
- For unsupervised evaluation, metrics can significantly vary based on end goal: density estimation, sampling, latent representations