

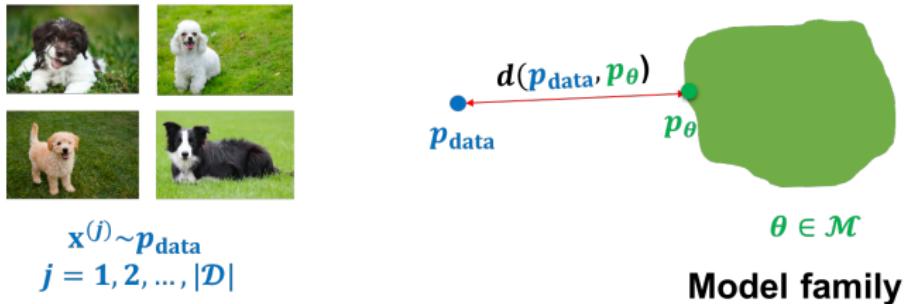
# Evaluating Generative Models

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Lecture 11

# Mid-quarter crisis



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?
  - Density estimation
  - Sampling/generation
  - Latent representation learning
  - More than one task? Custom downstream task? E.g., Semisupervised learning, image translation, compressive sensing etc.
- In any research field, evaluation drives progress. How do we evaluate generative models?

# Evaluation - Density Estimation

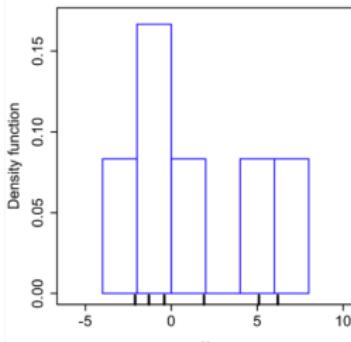
- Straightforward for models which have tractable likelihoods
  - Split dataset into train, validation, test sets
  - Evaluate gradients based on train set
  - Tune hyperparameters (e.g., learning rate, neural network architecture) based on validation set
  - Evaluate generalization by reporting likelihoods on test set
- **Caveat:** Not all models have tractable likelihoods e.g., VAEs, GANs
- For VAEs, we can compare evidence lower bounds (ELBO) to log-likelihoods
- In general, we can use kernel density estimates only via samples (non-parametric)

# Kernel Density Estimation

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

$\mathbf{x}^{(1)}$	$\mathbf{x}^{(2)}$	$\mathbf{x}^{(3)}$	$\mathbf{x}^{(4)}$	$\mathbf{x}^{(5)}$	$\mathbf{x}^{(6)}$
-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  $p_\theta(-0.5)$ ?  $1/6$   $p_\theta(-1.99)$ ?  $1/6$   $p_\theta(-2.01)$ ?  $1/12$

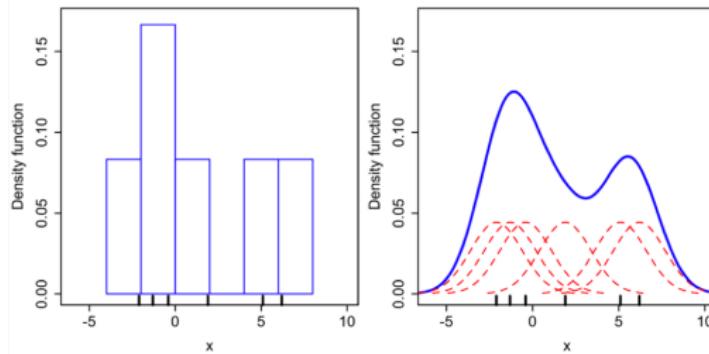
# Kernel Density Estimation

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

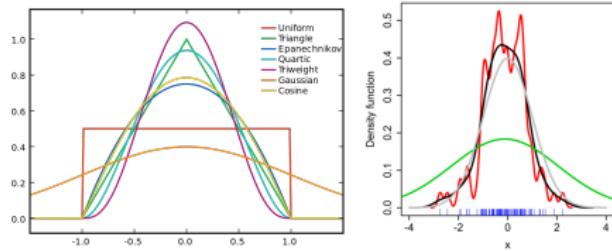
$$\hat{p}(\mathbf{x}) = \frac{1}{n} \sum_{\mathbf{x}^{(i)} \in \mathcal{S}} K\left(\frac{\mathbf{x} - \mathbf{x}^{(i)}}{\sigma}\right)$$

where  $\sigma$  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:  $\int_{-\infty}^{\infty} K(u)du = 1$  (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**  $\sigma$  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

- **Likelihood weighting:** Assume a Gaussian likelihood function  $p(\mathbf{x}|\mathbf{z})$

$$p(\mathbf{x}) = E_{p(\mathbf{z})}[p(\mathbf{x}|\mathbf{z})]$$

Can have high variance if  $p(\mathbf{z})$  is far from  $p(\mathbf{z}|\mathbf{x})$ !

- **Annealed importance sampling:** General purpose technique to estimate ratios of normalizing constants  $\mathcal{N}_2/\mathcal{N}_1$  of any two distributions via importance sampling
- For estimating  $p(\mathbf{x})$ , first distribution is  $p(\mathbf{z})$  (with  $\mathcal{N}_1 = 1$ ) and second distribution is  $p(\mathbf{x}|\mathbf{z})$  (with  $\mathcal{N}_2 = p(\mathbf{x}) = \int_{\mathbf{x}} p(\mathbf{x}, \mathbf{z}) d\mathbf{z}$ )
- A good implementation available in Tensorflow probability  
`tfp.mcmc.sample_annealed_importance_chain`

# Evaluation - Sample quality



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

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

- 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)**



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

- 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)**



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

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

$$IS = D \times S$$

- 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  $p_\theta$  and do not take into account the desired data distribution  $p_{\text{data}}$  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  $p_\theta$  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

# Evaluating sample quality - Best practices

## Are GANs Created Equal? A Large-Scale Study

Mario Lucic, Karol Kurach, Marcin Michalski, Sylvain Gelly, Olivier Bousquet

(Submitted on 28 Nov 2017 (v1), last revised 29 Oct 2018 (this version, v4))

Generative adversarial networks (GAN) are a powerful subclass of generative models. Despite a very rich research activity leading to numerous interesting GAN algorithms, it is still very hard to assess which algorithm(s) perform better than others. We conduct a neutral, multi-faceted large-scale empirical study on state-of-the art models and evaluation measures. We find that most models can reach similar scores with enough hyperparameter optimization and random restarts. This suggests that improvements can arise from a higher computational budget and tuning more than fundamental algorithmic changes. To overcome some limitations of the current metrics, we also propose several data sets on which precision and recall can be computed. Our experimental results suggest that future GAN research should be based on more systematic and objective evaluation procedures.

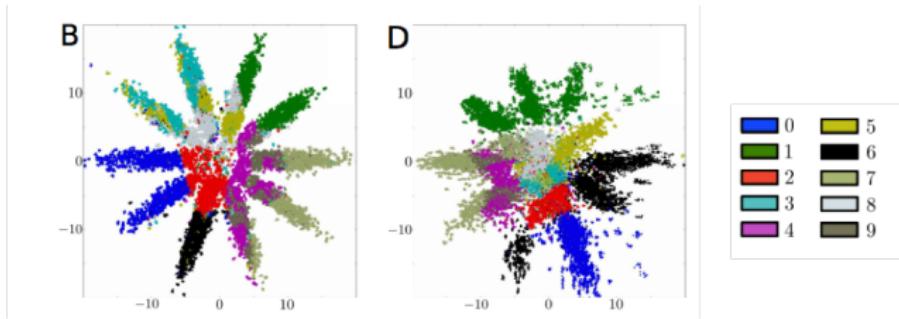
- Spend time tuning your baselines (architecture, learning rate, optimizer etc.). Be amazed (rather than dejected) at how well they can perform
- Use random seeds for reproducibility
- Report results averaged over multiple random seeds along with confidence intervals

# Evaluating latent representations

- 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
- For unsupervised tasks, there is no one-size-fits-all
- Three commonly used notions for evaluating unsupervised latent representations
  - Clustering
  - Compression
  - Disentanglement

# Clustering

- Representations that can group together points based on some semantic attribute are potentially useful (e.g., for semi-supervised classification)



Source: Makhzani et al., 2018

- 2D representations learned by two generative models for MNIST digits with colors denoting true labels. Which is better? B or D?
- Quantitative evaluation based on standard clustering metrics E.g., completeness score, homogeneity score, v measure score

# Compression

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



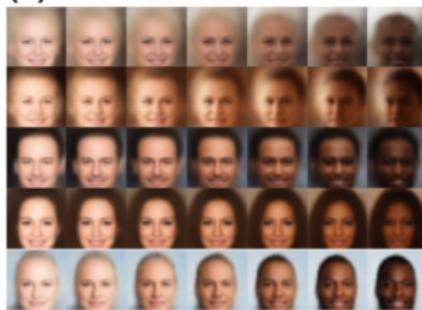
Source: Santurkar et al., 2018

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

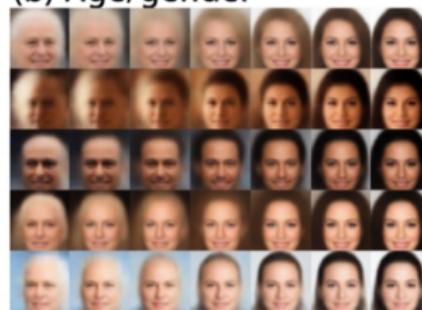
# Disentanglement

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

(a) Skin colour



(b) Age/gender

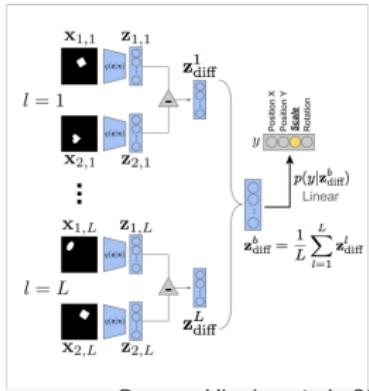


Source: Higgins et al., 2018

- Provide user control over the attributes of the generated data

# Disentanglement

- Quantitative evaluation via disentanglement metric score



Source: Higgins et al., 2018

- Over a batch of  $L$  samples, each pair of images has a fixed value for one target generative factor  $y$  (here  $y = \text{scale}$ ) and differs on all others
- A linear classifier is then trained to identify the target factor using the average pairwise difference  $z_{\text{diff}}^b$  in the latent space over  $L$  samples

# 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