Statistical Models & Computing Methods

Lecture 19: Generative Adversarial Nets

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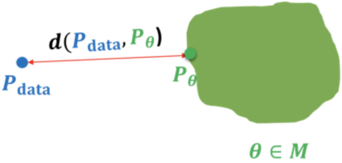
$\mathbf{x}_i \sim P_{\text{data}}$
$i = 1, 2, \ldots, n$



Model family

- Model families
  - Autoregressive Models: $p_\theta(x) = \prod_{i=1}^{n} p_\theta(x_i | x_{<i})$
  - Variational Autoencoders: $p_\theta(x) = \int_z p_\theta(x, z) dz$
  - Normalizing Flow Models:
    $$p_X(x;\theta) = p_Z(f_\theta^{-1}(x)) \left| \det \left(\frac{\partial f_\theta^{-1}(x)}{\partial x} \right) \right|$$
- All the above families are based on maximizing likelihoods (or approximations, e.g., lower bound)
- Is the likelihood a good indicator of the quality of samples generated by the model?

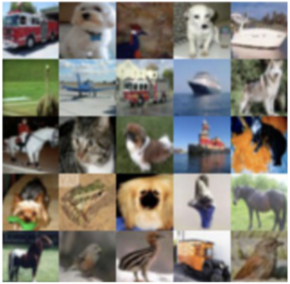
Sample Quality and Likelihood

- Optimal generative model will give best sample quality and highest test log-likelihood. However, in practice, high log-likelihoods $\neq$ good sample quality (Theis et al., 2016)
- Case 1: great test log-likelihoods, poor samples. Consider a mixture model $p_\theta(x) = 0.01 p_{\text{data}}(x) + 0.99 p_{\text{noise}}(x)$, we have

  $$\mathbb{E}_{p_{\text{data}}} \log p_{\text{data}}(x) \geq \mathbb{E}_{p_{\text{data}}} \log p_\theta(x) \geq \mathrm{E}_{p_{\text{data}}} \log p_{\text{data}}(x) - \log 100$$

  This means $\mathbb{E}_{p_{\text{data}}} \log p_\theta(x) \approx \mathrm{E}_{p_{\text{data}}} \log p_{\text{data}}(x)$ when the dimension of x is large.
- Case 2: great samples, poor test log-likelihoods. E.g., memorizing training set: samples look exactly like the training set; test set will have zero probability
- The above cases suggest that it might be useful to disentangle likelihoods and samples $\Rightarrow$ likelihood-free learning!

Comparing Distributions via Samples



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

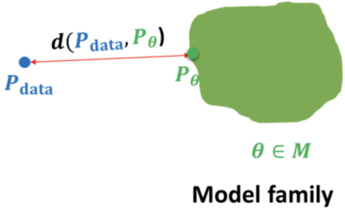
vs.

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

Given samples from two distributions $S_1 = \{x \sim P\}$ and $S_2 = \{x \sim Q\}$, how can we tell if these samples are from the same distribution? (i.e., $P = Q$?)

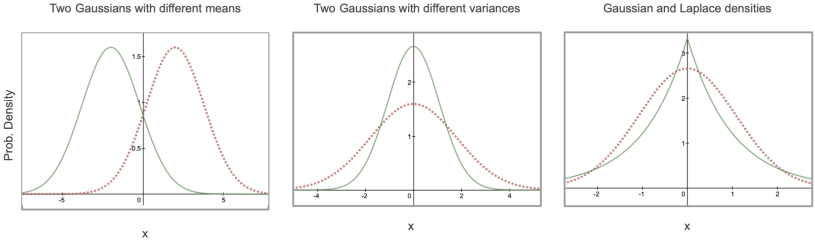
- Given $S_1 = \{x \sim P\}$ and $S_2 = \{x \sim Q\}$, a two-sample test considers the following hypotheses
  - Null hypothesis $H_0 : P = Q$
  - Alternative hypothesis $H_1 : p \neq Q$
- Test statistic T compares S_1 and S_2, e.g., difference in means, variances of the two sets of samples
- If T is less than a threshold α, the accept H_0 else reject it
- Key observation: Test statistics is likelihood-free since it does not involve the densities P or Q (only samples)

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



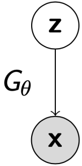
- Suppose we have direct access to the data set $S_1 = \mathcal{D} = \{x \sim p_{\text{data}}\}$
- Now assume that the model distribution p_θ permits efficient sampling (e.g., directed models). Let $S_2 = \{x \sim p_\theta\}$
- Use a two-sample test objective to measure the distance between distributions and train the generative model p_θ to minimize this distance between S_1 and S_2

Two-Sample Test via a Discriminator



- Finding a two-sample test objective in high dimensions is non-trivial
- In the generative model setup, we know that S_1 and S_2 come from different distributions p_{data} and p_θ respectively
- Key idea: Learn a statistic that maximizes a suitable notion of distance between the two sets of samples S_1 and S_2

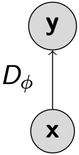
The **generator** and **discriminator** play a minimax game!



Generator

- Directed, latent variable model with a deterministic mapping between z and x given by G_θ
- Minimizes a two-sample test objective (in support of the null hypothesis $p_{\text{data}} = p_\theta$

The **generator** and **discriminator** play a minimax game!



Discriminator

- Any function (e.g., neural network) which tries to distinguish "real" samples from the dataset and "fake" sampels generated from the model
- Maximizes the two-sample test objectivee (in support of the alternative hypothesis $p_{\text{data}} \neq p_\theta$)

Discriminator Training Objective

- Training objective for discriminator:

$$\max_D V(G, D) = \mathbb{E}_{x \sim p_{\text{data}}} \log D(x) + \mathbb{E}_{x \sim p_G} \log(1 - D(x))$$

- For a fixed generator G, the discriminator is performing binary classification with the cross entropy objective
  - Assign probability 1 to true data points $x \sim p_{\text{data}}$
  - Assign probability 0 to fake samples $x \sim p_G$
- Optimal discriminator

$$D_G^*(x) = \frac{p_{\text{data}}(x)}{p_{\text{data}}(x) + p_G(x)}$$

- Training Objective for generator:

$$\min_G V(G, D) = \mathbb{E}_{x \sim p_{\text{data}}} \log D(x) + \mathbb{E}_{x \sim p_G} \log(1 - D(x))$$

- For the optimal discriminator $D_G^*(\cdot)$, we have

$$\begin{aligned}
V(G, D_G^*) &= \mathbb{E}_{x \sim p_{\text{data}}} \log \frac{p_{\text{data}}(x)}{p_{\text{data}}(x) + p_G(x)} + \mathbb{E}_{x \sim p_G} \log \frac{p_G(x)}{p_{\text{data}}(x) + p_G(x)} \\
&= \mathbb{E}_{x \sim p_{\text{data}}} \log \frac{p_{\text{data}}(x)}{\frac{p_{\text{data}}(x) + p_G(x)}{2}} + \mathbb{E}_{x \sim p_G} \log \frac{p_G(x)}{\frac{p_{\text{data}}(x) + p_G(x)}{2}} - \log 4 \\
&= \mathrm{KL}\left(p_{\text{data}} \middle\| \frac{p_{\text{data}} + p_G}{2}\right) + \mathrm{KL}\left(p_G \middle\| \frac{p_{\text{data}} + p_G}{2}\right) - \log 4
\end{aligned}$$

- The sum of KL in the above equation is known as Jensen-Shannon divergence (JSD)

Jensen-Shannon Divergence

$$\mathrm{JSD}(p,q) = \mathrm{KL}\left(p \middle\| \frac{p+q}{2}\right) + \mathrm{KL}\left(q \middle\| \frac{p+q}{2}\right)$$

- Properties
  - $\mathrm{JSD}(p,q) \geq 0$
  - $\mathrm{JSD}(p,q) = 0$ iff $p = q$
  - $\mathrm{JSD}(p,q) = \mathrm{JSD}(q,p)$
  - $\sqrt{\mathrm{JSD}(p,q)}$ satisfies triangle inequality
- Optimal generator for the JSD GAN

$$p_G = p_{\text{data}}$$

- For the optimal discriminator $D^*_{G^*}(\cdot)$ and generator $G^*(\cdot)$, we have

$$V(G^*, D^*_{G^*}(x)) = -\log 4$$

Alternating Optimization in GAN

$$\min_\theta \max_\phi V(G_\theta, D_\phi) = \mathbb{E}_{x\sim p_{\text{data}}} \log D_\phi(x) + \mathbb{E}_{z\sim p(z)} \log(1 - D_\phi(G_\theta(z)))$$

- sample m training points $x^{(1)}, x^{(2)}, \ldots, x^{(m)}$ from $\mathcal{D}$
- sample m noise vectors $z^{(1)}, z^{(2)}, \ldots, z^{(m)}$ from p_z
- generator parameters θ update: stochastic gradient descent

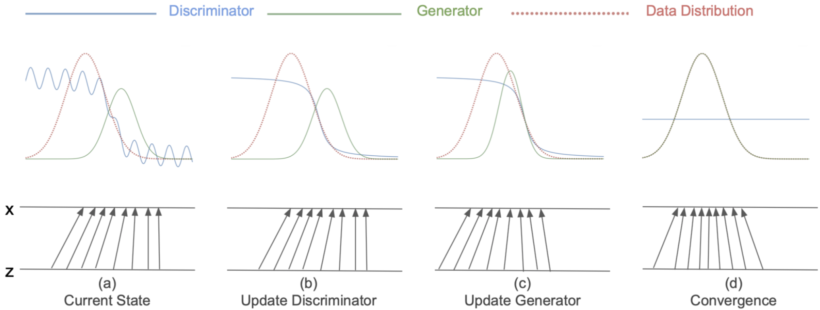
$$\nabla_\theta V(G_\theta, D_\phi) = \frac{1}{m} \nabla_\theta \sum_{i=1}^{m} \log(1 - D_\phi(G_\theta(z^{(i)})))$$

- discriminator parameters ϕ update: stochastic gradient ascent

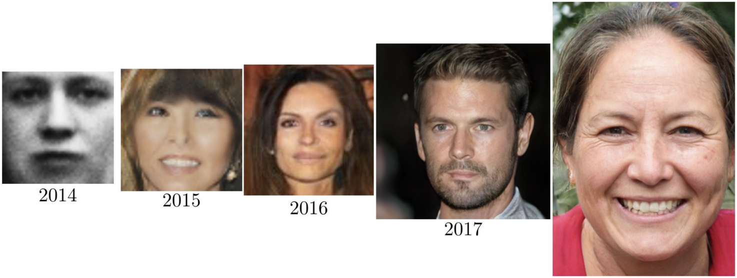
$$\nabla_\phi V(G_\theta, D_\phi) = \frac{1}{m} \nabla_\phi \sum_{i=1}^{m} \log D_\phi(x^{(i)}) + \log(1 - D_\phi(G_\theta(z^{(i)})))$$

- Repeat for fixed number of epochs

A Toy Example



Adapted from Goodfellow, 2014

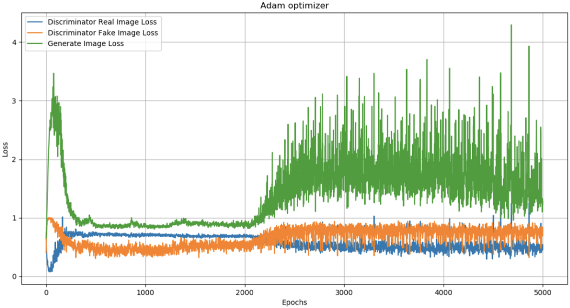


2014 2015 2016 2017 2018

- GANs have been successfully applied to several domains and tasks
- However, working with GANs can be very challenging in practice: unstable optimization/mode collapse/evaluation
- Many bag of tricks applied to train GANs successfully

Image source: Ian Goodfellow. Samples from Goodfellow et al., 2014, Radford et al., 2015, Liu et al., 2016, Karras et al., 2017, Karras et al., 2018

- Theorem: If the generator updates are made in function space and discriminator is optimal at every step, then the generator is guaranteed to converge to the data distribution
- Unrealistic assumptions! In practice, the generator and discriminator loss keeps oscillating during GAN training

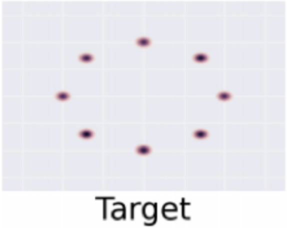


- No robust stopping criteria in practice (unlike MLE)

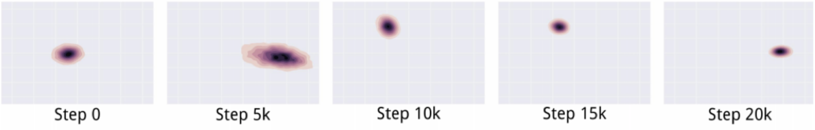
- GANs are notorious for suffering from mode collapse
- Intuitively, this refers to the phenomena where the generator of a GAN collapse to one or few samples (i.e., "modes")

Arjovsky et al., 2017

Mode Collapse



- True distribution is a mixture of Gaussians



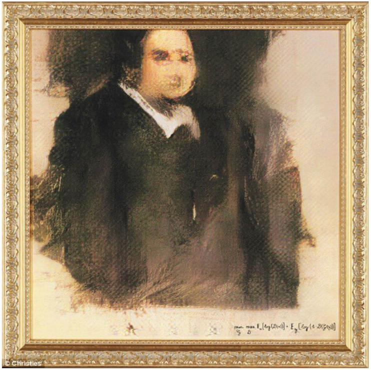
Source: Metz et al., 2017

- The generator distribution keeps oscillating between different models

Source: Metz et al., 2017

- Fixes to mode collapse are mostly empirically driven: alternate architectures, adding regularization terms, injecting small noise perturbations etc.
- Tips and tricks to make GAN work by Soumith Chintala: `https://github.com/soumith/ganhacks`

GAN Generated Artworks



Source: Robbie Barrat, Obvious

GAN generated art auctioned at Christie's.
Expected Price: \$7,000 – \$10,000
True Price: \$432,500

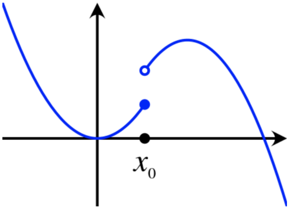
- The GAN Zoo:
  `https://github.com/hindupuravinash/the-gan-zoo`
- Examples
  - Rich class of likelihood-free objectives
  - Combination with latent representations
  - Application: Image-to-image translation, etc.

- Given two densities p and q, the $f-$ divergence is given by

$$D_f(p\|q) = \mathbb{E}_{x\sim q}\, f\left(\frac{p(x)}{q(x)}\right)$$

where f is any convex, lower-semicontinuous function with $f(1) = 0$

- Lower-semicontinuous: function value at any pint x_0 is close to $f(x_0)$ or greater than $f(x_0)$



- Example: KL divergence with $f(u) = u \log u$

f Divergence

Many more f-divergence!

Name	$D_f(P\|Q)$	Generator $f(u)$
Total variation	$\frac{1}{2}\int \lvert p(x)-q(x)\rvert \,\mathrm{d}x$	$\frac{1}{2}\lvert u-1\rvert$
Kullback-Leibler	$\int p(x)\log\frac{p(x)}{q(x)}\,\mathrm{d}x$	$u\log u$
Reverse Kullback-Leibler	$\int q(x)\log\frac{q(x)}{p(x)}\,\mathrm{d}x$	$-\log u$
Pearson χ^2	$\int \frac{(q(x)-p(x))^2}{p(x)}\,\mathrm{d}x$	$(u-1)^2$
Neyman χ^2	$\int \frac{(p(x)-q(x))^2}{q(x)}\,\mathrm{d}x$	$\frac{(1-u)^2}{u}$
Squared Hellinger	$\int \left(\sqrt{p(x)}-\sqrt{q(x)}\right)^2\,\mathrm{d}x$	$(\sqrt{u}-1)^2$
Jeffrey	$\int (p(x)-q(x))\log\left(\frac{p(x)}{q(x)}\right)\,\mathrm{d}x$	$(u-1)\log u$
Jensen-Shannon	$\frac{1}{2}\int p(x)\log\frac{2p(x)}{p(x)+q(x)}+q(x)\log\frac{2q(x)}{p(x)+q(x)}\,\mathrm{d}x$	$-(u+1)\log\frac{1+u}{2}+u\log u$
Jensen-Shannon-weighted	$\int p(x)\pi\log\frac{p(x)}{\pi p(x)+(1-\pi)q(x)}+(1-\pi)q(x)\log\frac{q(x)}{\pi p(x)+(1-\pi)q(x)}\,\mathrm{d}x$	$\pi u\log u-(1-\pi+\pi u)\log(1-\pi+\pi u)$
GAN	$\int p(x)\log\frac{2p(x)}{p(x)+q(x)}+q(x)\log\frac{2q(x)}{p(x)+q(x)}\,\mathrm{d}x-\log(4)$	$u\log u-(u+1)\log(u+1)$
α-divergence ($\alpha\notin\{0,1\}$)	$\frac{1}{\alpha(\alpha-1)}\int\left(p(x)\left[\left(\frac{q(x)}{p(x)}\right)^\alpha-1\right]-\alpha(q(x)-p(x))\right)\mathrm{d}x$	$\frac{1}{\alpha(\alpha-1)}\left(u^\alpha-1-\alpha(u-1)\right)$

Source: Nowozin et al., 2016

- To use f-divergences as a two-sample test objective for likelihood-free learning, we need to be able to estimate it only via samples
- Fenchel conjugate: For any function $f(\cdot)$, its convex conjugate is defined as

$$f^*(t) = \sup_{u \in \mathrm{dom}_f} ut - f(u)$$

- Duallity: $f^{**} = f$. When $f(\cdot)$ is convex, lower semicontinuous, so is $f^*(\cdot)$

$$f(u) = \sup_{t \in \mathrm{dom}_{f^*}} tu - f^*(t)$$

- We can obtain a lower bound to any f-divergence via its Fenchel conjugate

$$
\begin{aligned}
D_f(p\|q) &= \mathbb{E}_{x\sim q}\, f\left(\frac{p(x)}{q(x)}\right) \\
&= \mathbb{E}_{x\sim q} \sup_{t\in \mathrm{dom}_{f^*}} \left(t\frac{p(x)}{q(x)} - f^*(t)\right) \\
&\geq \mathbb{E}_{x\sim q}\, t(x)\frac{p(x)}{q(x)} - f^*(t(x)) \\
&= \int_{\mathcal{X}} t(x)p(x) - f^*(t(x))q(x)dx \\
&= \mathbb{E}_{x\sim p}\, t(x) - \mathbb{E}_{x\sim q}\, f^*(t(x))
\end{aligned}
$$

for any function $t : \mathcal{X} \mapsto \mathrm{dom}_{f^*}$

f-GAN

- Variational lower bound

$$D_f(p\|q) \geq \sup_{t\in\mathcal{T}}(\mathbb{E}_{x\sim p}\, t(x) - \mathbb{E}_{x\sim q}\, f^*(t(x)))$$

- Choose any f-divergence
- Let $p = p_{\text{data}}$ and $q = p_G$
- Parameterize t by ϕ and G by θ
- Consider the following f-GAN objective

$$\min_\theta \max_\phi F(\theta, \phi) = \mathbb{E}_{x\sim p_{\text{data}}}\, t_\phi(x) - \mathbb{E}_{x\sim p_{G_\theta}} f^*(t_\phi(x))$$

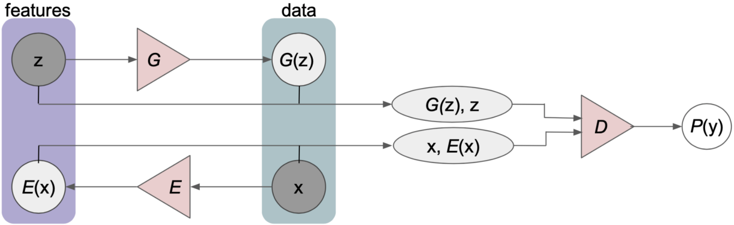
- Generator G_θ tries to minimize the divergence estimate and discriminator t_ϕ tries to tighten the lower bound

Inferring Latent Representation in GANs

- The generator of a GAN is typically a directed, latent variable model with latent variable z and observed variables x. How can we infer the latent feature representations in a GAN?
- Unlike a normalizing flow model, the mapping $G : z \mapsto x$ need not to be invertible
- Unlike a variational autoencoder, there is no inference network $q(\cdot)$ which can learn a variational posterior over latent variables
- Solution 1: For any point x, use the activations of the prefinal layer of a discriminator as a feature representation
- Intuition: similar to supervised deep neural networks, the discriminator would have learned useful representations for x while distinguishing real and fake x

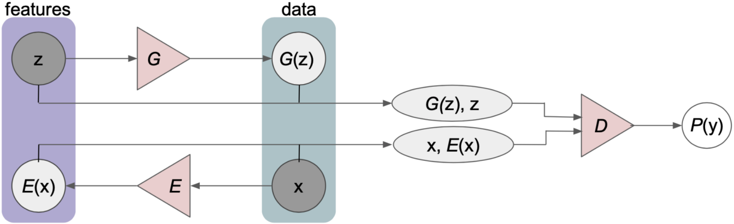
- If we want to directly learn the latent representation of x, we need a different learning algorithm
- A regular GAN optimizes a two-sample test objective that compares samples of x from the generator and the data distribution
- Solution 2: To infer latent representations, we will compare samples of x, z from joint distributions of observed and latent variables as per the model and the data distribution
- For any x generated via the model, we have access to z (sampled from a simple prior $p(z)$)
- For any x from the data distribution, the z is however unobserved (latent)

Bidirectional GAN



- In a BiGAN, we have an encoder network E in addtion to the generator network G
- The encoder network only observes $x \sim p_{\text{data}}(x)$ during training to learn a mapping $E : x \mapsto z$
- As before, the generator network only observes the samples from the prior $z \sim p(z)$ during training to learn a mapping $G : z \mapsto x$

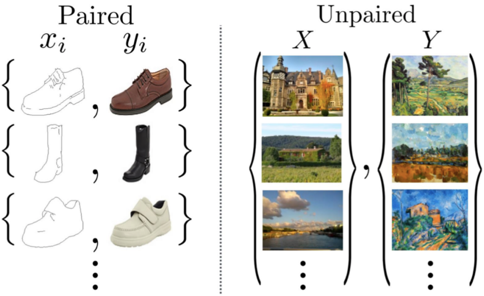
Bidirectional GAN



- The discriminator D observes samples from the generative model $z, G(z)$ and encoding distribution $E(x), x$
- The goal of the discriminator is the maximize the two-sample test objective between $z, G(z)$ and $E(x), x$
- After training is complete, new samples are generated via G and latent representations are inferred via E

Translating Across Domains

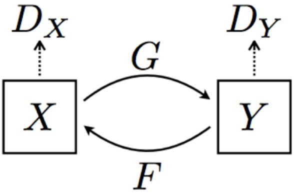
- Image-to-image translation: we are given image from two domains, $\mathcal{X}$ and $\mathcal{Y}$
- Paired vs. unpaired examples



Source: Zhu et al., 2016

- Paired examples can be expensive to obtain. Can we translate from $\mathcal{X} \Leftrightarrow \mathcal{Y}$ in an unsupervised manner?

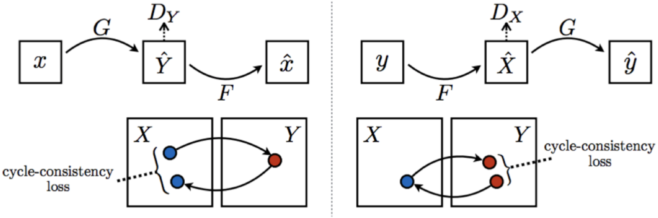
- To match the two distributions, we learn two parameterized conditional generative models $G : \mathcal{X} \mapsto \mathcal{Y}$ and $F : \mathcal{Y} \mapsto \mathcal{X}$
- G maps an element of $\mathcal{X}$ to an element of $\mathcal{Y}$. A discriminator $D_{\mathcal{Y}}$ compares the observed dataset Y and the generated samples $\hat{Y} = G(X)$
- Similarly, F maps an element of $\mathcal{Y}$ to an element of $\mathcal{X}$. A discriminator $D_{\mathcal{X}}$ compares the observed dataset X and the generated samples $\hat{X} = F(Y)$



Source: Zhu et al., 2016

CycleGAN

- Cycle consistency: If we can go from X to $\hat{Y}$ via G, then it should also be possible to go from $\hat{Y}$ back to X via F
  - $F(G(X)) \approx X$
  - Similarly, vice versa: $G(F(Y)) \approx Y$

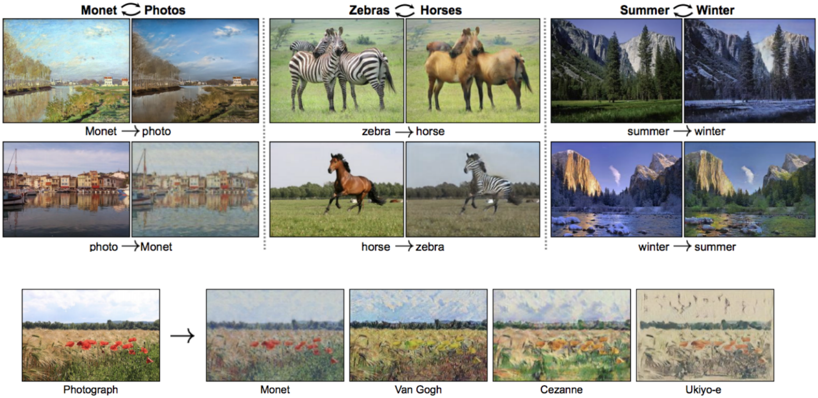


Source: Zhu et al., 2016

- Overall loss function

$$\mathcal{L}_{\mathrm{GAN}}(G, D_{\mathcal{Y}}, X, Y) + \mathcal{L}_{\mathrm{GAN}}(F, D_{\mathcal{X}}, X, Y)$$
$$+\lambda(\mathbb{E}_X\|F(G(X)) - X\|_1 + \mathbb{E}_Y\|G(F(Y)) - Y\|_1)$$

CycleGAN in Practice



Source: Zhu et al., 2016

- Key observation: Samples and likelihoods are not correlated in practice
- Two-sample test objectives allow for learning generative mdoels only via samples (likelihood-free)
- Wide range of two-sample test objectives covering f-divergences (and more)
- Latent representations can be inferred via BiGAN (and other GANs with similar autoencoder structures)
- Cycle-consistent domain translations via CycleGAN and other variants

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