Deep Generative models

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Interpretability of Neural Networks

Interpreting neural network with saliency map

why did neural network classify the image as a "dog"?



Saliency map of the image x and the NN model $f(\cdot)$ is defined as $\nabla_x f_{dog}(x)$



Saliency map

How much does this pixel contribute in classifying the image as a dog?

Segmenting those pixels with high saliency allows one to interpret NN decision

"Deep Inside Convolutional Networks: Visualising Image Classification Models and Saliency Maps" ³ Simonyan, Vedaldi, Zisserman, 2014

Interpreting neural networks with occlusion sensitivity







each occluded region is represented by $f_{dog}(x_{occluded})$ with a color map: blue is low confidence and red is high confidence

"Visualizing and Understanding Convolutional Networks", Zeiler, Fergus, 2013

Interpreting neural networks with occlusion sensitivity





Attacking Neural Networks with adversarial examples:

NNs are vulnerable

Attacking neural network with adversarial examples

 as an adversary, we want to generate an image that looks like a cat, but is classified as iguana (for a specific given NN classifier)



Attacking neural network with adversarial examples

 as an adversary, we want to generate an image that looks like a cat, but is classified as iguana (for a specific given NN classifier)





• the adversarial examples are misclassified as ostriches, and in the middle we show the perturbation times ten.



- In another experiment, you can start with a random noise and take one gradient step
- this often produces a confident classification
- the images outlined by yellow are classified as "airplane" with >50% confidence



Attacking neural network with adversarial examples

 as an adversary, we want an image to be misclassified (to anything but Panda)





$$\operatorname{sign}(\nabla_{\boldsymbol{x}} J(\boldsymbol{\theta}, \boldsymbol{x}, y))$$

"nematode" 8.2% confidence



 $m{x} + \epsilon \operatorname{sign}(
abla_{m{x}} J(m{ heta}, m{x}, y))$ "gibbon" 99.3 % confidence



"panda" 57.7% confidence

Attacking autoencoders

 Autoencoder: neural network that compresses the input, and recovers an example that is close to the input



 encoder and decoder are neural networks, jointly trained to minimize the squared loss between the input and output images

Adversarial examples

• one can create adversarial images that is reconstructed (after compression) as an entirely different image



Adversarial testing examples

- First reported in ["Intriguing properties of neural networks", 2013, by Christian Szegedy, Wojciech Zaremba, Ilya Sutskever, Joan Bruna, Dumitru Erhan, Ian Goodfellow, Rob Fergus]
- Led to serious concerns for security as, for example,
 - one can create road signs that fools a self-driving car to act in a certain way
- this is serious as
 - there is no reliable defense against adversarial examples
 - adversarial examples transfer to different networks, trained on disjoint subset of training data
 - you do not need the access to the model parameters; you can train your own model and create adversarial examples
 - you only need a black-box access via APIs (MetaMind, Amazon, Google)

Adversarial examples with bloack-box access to NN

- ["Practical Black-Box Attacks against Machine Learning", 2016, Nicolas Papernot, Patrick McDaniel, Ian Goodfellow, Somesh Jha, Z. Berkay Celik, Ananthram Swami]
- no access to the gradient of the NN classifier, but only allowed black-box access to the output



Physical-world adversarial examples

- ["Adversarial examples in the physical world", 2016, Alexey Kurakin, Ian Goodfellow, Samy Bengio]
- You can fool a classifier by taking picture of a print-out.
- one can potentially print over a stop sign to fool a selfdriving car



(a) Image from dataset

(b) Clean image

(c) Adv. image, $\epsilon = 4$

(d) Adv. image, $\epsilon = 8$

This 3-dimensional turtle is designed to be classified as "rifle"



Defense mechanism

Defense mechanism 1

• include adversarial testing examples (but with the correct classes) in the training data.



Adversarial perturbation intended to change the guess

label: bird

label: bird

Why are modern classifiers vulnerable

- small margin due to overfitting / high representation power
- there exists a direction from any example that can reach a boundary in a short distance





Defense mechanism 2

- **Defensive distillation:**
- Two models are trained
- model 1: trained on the training data in as standard manner
- model 2 (the robust model) : is trained on the same training data, but uses soft classes which is the probability provided by the first model
- This creates a model whose surface is smoothed in the directions an adversary will typically try to exploit, making it difficult for them to discover adversarial input tweaks that lead to incorrect categorization
- [Distilling the Knowledge in a Neural Network, 2015, Geoffrey Hinton, Oriol Vinyals, Jeff Dean]
- original idea came from model compression
- both are vulnerable against high-power adversary

Unsupervised Learning with Neural Networks

Deep generative model

- traditional parametric generative model
 - Gaussian:

$$f_{\mu,\sigma}(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

• Gaussian Mixture Models (GMM)

$$f_{\{\mu_i\},\{\sigma_i\},\{\pi_i\}}(x) = \sum_{i=1}^k \pi_i \frac{1}{\sqrt{2\pi\sigma_i^2}} e^{-\frac{(x-\mu_i)^2}{2\sigma_i^2}}$$

- deep generative model
 - easy to sample
 - high representation power
 - but no tractable evaluation of the density (i.e. p.d.f.)

Deep generative model

- sampling from a deep generative model, parametrized by w
 - first sample a **latent code** $z \in \mathbb{R}^k$ of small dimension $k \ll d$, from a simple distribution like standard Gaussian $N(0, \mathbf{I}_{k \times k})$
 - pass the code through a neural network of your choice, with parameter w
 - the output sample $x \in \mathbb{R}^d$ is the sample of this deep generative model



Deep generative model



Generative model

- a task of importance in unsupervised learning is fitting a generative model
- classically, if we fit a parametric model like mixture of Gaussians, we write the likelihood function explicitly in terms of the model parameters, and maximize it using some algorithms

maximize_w
$$\sum_{i=1}^{n} \log \left(P_{w}(x_{i}) \right)$$

 $P.J.f.$

 deep generative models use neural networks, but the likelihood of deep generative models cannot be evaluated easily, so we use alternative methods

Goal

• Given examples $\{x_i\}_{i=1}^n$ coming i.i.d from an unknown distribution P(x), train a generative model that can generate samples from a distribution close to P(x)

These are computer generated images from the "bigGAN".



- Classification
 - Consider the example of SPAM detection
 - Each sample x_i is an email
 - Distribution of **true email** is P(x)
 - Suppose spammers generate **spams** with distribution Q(x)
 - Spam detection: Typical classification task
 - Generate samples from true emails and label them $y_i = 1$
 - Generate samples from spams and label them $y_i = 0$
 - Using these as training data, train a classifier that outputs

$$\mathbb{P}(y_i = 1 \mid x_i) \simeq \frac{1}{1 + e^{-f_{\theta}(x)}}$$

for some neural network $f_{\theta}(\cdot)$ with parameter θ (this is the **logistic model** for binary classification)

• Applying logistic regression, we want to solve

$$\max_{\theta} \sum_{i:y_i=1} \log\left(\frac{1}{1+e^{-f_{\theta}(x_i)}}\right) + \sum_{i:y_i=0} \log\left(1-\frac{1}{1+e^{-f_{\theta}(x_i)}}\right)$$

• in adversarial training, it is customary to write

$$D_{\theta}(x) = \frac{1}{1 + e^{-f_{\theta}(x)}}$$

which is called a **discriminator**

and find the "best" discriminator by solving for

$$\max_{\theta} \mathscr{L}(\theta) = \sum_{x_i \sim P(\cdot)} \log D_{\theta}(x_i) + \sum_{x_i \sim Q(\cdot)} \log(1 - D_{\theta}(x_i))$$

as 1 labelled examples come from real distribution $P(\cdot)$
and 0 labelled examples come from spam distribution $Q(\cdot)$

• Suppose now that the **spam detector (i.e. the discriminator)** is fixed, then the spammer's job is to generate spams that can fool the detector by making the likelihood of the spams being classified as spams **small**:

$$\min_{Q(\cdot)} \mathscr{L}(\theta) = \sum_{\substack{x_i \sim P(\cdot) \\ \text{does not depend on } Q(\cdot)}} \log D_{\theta}(x_i) + \sum_{\substack{x_i \sim Q(\cdot) \\ x_i \sim Q(\cdot)}} \log(1 - D_{\theta}(x_i))$$

- where 0 labelled examples are coming from the distribution $Q(\cdot)$, which is modeled by a **deep neural network generative model,** i.e. $x_i = G_w(z_i)$ where $z_i \sim N(0, \mathbf{I}_{k \times k})$.
- The minimization can be solved by finding. The "best" generative model that can fool the discriminator

$$\min_{w} \mathscr{L}(w, \theta) = \sum_{\substack{x_i \sim P(\cdot) \\ \text{does not depend on } Q(\cdot)}} \log \left(1 - D_{\theta} \left(G_w(z_i) \right) \right)$$

Now we have a game between the spammer and the spam detector:

$$\min_{w} \max_{\theta} \sum_{x_i \sim P(\cdot)} \log D_{\theta}(x_i) + \sum_{z_i \sim N(0,\mathbf{I})} \log(1 - D_{\theta}(G_W(z_i)))$$

- Where $P(\cdot)$ is the distribution of real data (true emails), and $Q(\cdot)$ is the distribution of the generated data (spams) that we want to train with a **deep generative model**
- jointly training the discriminator and the generator is called adversarial training
- Alternating method is used to find the solution

Alternating gradient descent for adversarial training

• Gradient update for the **discriminator** (for fixed w)

$$\max_{\theta} \sum_{x_i \sim P(\cdot)} \log D_{\theta}(x_i) + \sum_{x_i \sim Q(\cdot)} \log(1 - D_{\theta}(x_i))$$

- First sample *n* examples from real data (in the training set) and the generator data $x_i \sim G_w(z_i)$ (for the current iterate of the generator weight *w*)
- compute the gradient for those 2n samples using back-propagation
- Update the discriminator weight θ by subtracting the gradient with a choice of a step size

Alternating gradient descent for adversarial training

• gradient update for the generator (for fixed θ)

$$\min_{w} \sum_{x_i \sim P(\cdot)} \log D_{\theta}(x_i) + \sum_{z_i \sim N(0,\mathbf{I})} \log(1 - D_{\theta}(G_w(z_i)))$$

• Consider the gradient update on a single sample

$$\min_{w} \mathscr{L}(w, z_i) = \log(1 - D_{\theta}(G_w(z_i)))$$

for a single $z_i \sim N(0, \mathbf{I})$ sampled from a Gaussian

• The gradient update is

$$w = w - \eta \nabla_{w} \mathscr{L}(w, z_{i})$$

= $w - \eta \nabla_{w} G_{w}(z_{i}) \nabla_{x} D_{\theta}(x) \frac{-1}{1 - D_{\theta}(x)}$

with $x = G_w(z_i)$

This gives a new way to train a deep generative model



Generator G(Z)

 $\min_{G} \max_{D} V(G,D)$

Not only is GAN amazing in generating realistic samples

http://whichfaceisreal.com



It opens new doors to exciting applications

Cvcle-GAN





orange \rightarrow apple


Figure 3: Street scene image translation results. For each pair, left is input and right is the translated image.



Style transfer with generative model

- If we have paired training data,
- And want to train a generative model G(x,z)=y,
- This can be posed as a regression problem



How do we do style transfer without paired data? Cycle-GAN















40

How do we do style transfer without paired data? Cycle-GAN



Super resolution



https://www.youtube.com/watch?v=PCBTZh41Ris

The learned latent space is important



How do we check if we found the right manifold (of faces)?

latent traversal



Can we make the relation between the latent space and the image space more meaningful?

- Disentangling
 - GANs learn arbitrary mapping from z to x
 - As the loss only depends on the marginal distribution of x and not the conditional distribution of x given z (how z is mapped to x)













Disentangling seeks meaningful mapping from z to x

 there is no formal (mathematical) universally agreed upon definition of disentangling



informally, we seek latent codes that

- are "informative" or make "noticeable" changes
- are "uncorrelated" or make "distinct" changes

Decompose data into a set of underlying **human-interpretable** factors of variation



Explainable models

What is in the scene?

Controllable generation

Generate a red ball instead

Fully-supervised case

Strategy: Label everything



C₁ C₂ C₃ {dark blue wall, green floor, green oval}

{green wall, red floor, green cylinder}

{red wall, green floor, pink ball}

Controllable generation as **label-conditional** generative modeling

green wall, red floor, blue cylinder





Train a conditional GAN, where

 (c_1, c_2, c_3) is a numerical representation of the **labels** given in the training data, and *z* is drawn from Gaussian

However, some properties are hard to represent numerically



What kind of hairstyle?

What kind of glasses?



Unsupervised training of Disentangled GAN









Disentangled GAN training: InfoGAN-CR, 2019

• 1. As in standard GAN training, we want $G_w(z)$ to look like training data (which is achieved by adversarial loss provided by a discriminator)

- 2. We also want the controllable latent code c to be predictable from the image
 - add a NN regressor that predicts $\hat{c}(x)$, and train the generator that makes the prediction accuracy high (note that both this predictor and the generator works to make the prediction accurate, unlike adversarial loss)

minimize $\|\hat{c}(\boldsymbol{O}) - c\|^2$

- 3. We also want each code to control distinct properties
 - add a NN that predicts which code was changed

Disentangling with contrastive regularizer

• To train a disentangled GAN, we use contrastive regularizer

But is still challenging

Synthetic training data (with planted disentangled representation)

Synthetic data with two attributes (angle, radius)

• Trained Disentangled GAN (latent traversal)

Challenges in training GANs

- GAN training suffers from **mode collapse**
- this refers to the phenomenon where the generated samples are not as diverse as the training samples

Arjovsky et al., 2017

Mode collapse

Mode collapse

• True distribution is a mixture of Gaussians

• The generator distribution keeps oscillating between different modes

Mode collapse

• "A man in a orange jacket with sunglasses and a hat ski down a hill."

• "This guy is in black trunks and swimming underwater."

 "A tennis player in a blue polo shirt is looking down at the green court."

^{[&}quot;Generating interpretable images with controllable structure", by Reed et al., 2016]

- Lack of diversity is easier to detect if we see multiple samples
- Consider MNIST hand-written digits
 - If we have a generator that generates 1,3,5,7 perfectly, it is hard to tell from a single sample that mode collapse has happened
 - But easier to tell from a collection of, say, 5 samples all from wither training data or all from generated data

• Turning this intuition into a training algorithm:

Principled approach to mode collapse: PacGAN, 2018

• Turning this intuition into a training algorithm:

Х

	Modes
	(Max 25)
GAN	17.3
PacGAN2	23.8
PacGAN3	24.6
PacGAN4	24.8

	Modes (Max 1000)
DCGAN	99.0
ALI	16.0
Unrolled GAN	48.7
VEEGAN	150.0
PacDCGAN2	1000.0
PacDCGAN3	1000.0
PacDCGAN4	1000.0

- Could PacGAN be cheating, as it is a larger discriminator network?
- 1. Discriminator size

GAN

- Could PacGAN be cheating, as it is a larger discriminator network?
- 1. Discriminator size

of parameters in $D(\cdot)$

- Could PacGAN be cheating, as it uses more samples at each mini-batch?
- 1. Discriminator size

GAN

PacGAN2

Could PacGAN be cheating, as it uses more samples at each mini-batch?

2. Minibatch size

- Could PacGAN be cheating, as it uses more samples at each mini-batch?
 - 2. Minibatch size

ModesDCGAN99.0PacDCGAN21000.0

• Typical Gan training loss is

$$\min_{w} \max_{\theta} \sum_{x_i \sim P(\cdot)} \log D_{\theta}(x_i) + \sum_{z_i \sim N(0,\mathbf{I})} \log(1 - D_{\theta}(G_W(z_i)))$$

• We will consider

$$\begin{split} \min_{w} \max_{\theta} & \sum_{x_i \sim P(\cdot)} D_{\theta}(x_i) + \sum_{z_i \sim N(0,\mathbf{I})} (1 - D_{\theta}(G_W(z_i))) \\ \text{subject to} & |D_{\theta}(x)| \leq 1 , \quad \text{for all } x \end{split}$$

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• this is a finite sample approximation of the following expectation

$$\min_{w} \max_{\theta} \mathbb{E}_{x \sim P(\cdot)} \left[D_{\theta}(x) \right] + \mathbb{E}_{z \sim N(0,\mathbf{I})} \left[1 - D_{\theta}(G_{W}(z)) \right]$$

• let $Q(\cdot)$ denote the distribution of the generator $G_w(z_i)$

 $\min_{\substack{Q(\cdot) \quad \theta}} \max_{\substack{x \sim P(\cdot)}} \left[D_{\theta}(x) \right] + \mathbb{E}_{x \sim Q(\cdot)} \left[1 - D_{\theta}(x) \right]$ subject to $|D_{\theta}(x)| \le 1$, for all x

- at this point, we can solve the maximization w.r.t. D_{θ} assuming it can represent any functions (for the purpose of theoretical analysis)
 - the optimal solution is

$$D_{\theta}(x) = \begin{cases} +1 & \text{if } P(x) \ge Q(x) \\ -1 & \text{if } P(x) < Q(x) \end{cases}$$

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• Plugging this back in to the loss, we get

0.8 Target distribution P0.7 0.6 0.5 $d_{\rm TV}(P^2, Q_1^2)$ 0.4 $P \times P$ 0.3 1 0.2 $d_{\mathrm{TV}}(P^2,Q_2^2)$ 0.1 0 5 2 3 4 6 Generator Q_2 Generator Q_1 without mode collapse with mode collapse 1.4^{2} 1.25^{2} $Q_2 \times Q_2$ $Q_1 \times Q$ 1.4×0.6 0.6^{2} 0.20.51 0.2 $d_{\rm TV}(P \times P, Q_1 \times Q_1) = 0.36$ $d_{\rm TV}(P \times P, Q_2 \times Q_2) = 0.24$

Theoretical intuition behind PacGAN
Theoretical intuition behind PacGAN



Deep Image prior

 in standard de-noising/inpainting with trained GAN we want to recover original image from some distortion



 if we have a GAN trained on similar class of images, then we can use the latent space and the manifold of natural images to recover the image as follows



Deep Image prior

• Given a trained generator *w* that knows the manifold of natural images, find the latent vector *z* that

minimize_z $\ell(G_w(z),$



• let $G_w(z)$ be the recovered image



Deep image prior

• deep image prior does amazing recovery, without training



Deep image prior

Deep image prior

Deep image prior

Deep image prior

Deep image prior

• fix *z* to be something random and find *w* that



and let $G_w(z)$ be the recovered image

https://www.youtube.com/watch?v=kSLJriaOumA&feature=youtu.be