Generative models for continuous random variables: GAN and GAIL

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Outline

Section 1

Introduction

Subsection 1

Why model of data distribution?

Why model of data distribution?

Analyzing data:

- Figure out the uncommon or rare elements
  - Anomalies, outliers, errors
- Find typical elements / prototypes

Prediction:

- How likely is something to happen?
- RL: If we can create model for environment, don't have to explore, but can just do planning.

Generalization: learning a familiy of conditional distributions.

- Recall classification: learned family of distributions $Y|X$ with shared parameters.

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Both knowing how likely something is and being able to generate samples can be useful depending on the situation.

Subsection 2

Fitting a probability distribution

Fitting a probability distribution

Given data points

$$-5.17, -1.01, -2.43, -6.01, -4.16, 0.3, -7.85, -3.86, -0.47 \ldots$$

- How do we fit a probability distribution?

Fitting a probability distribution

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$$-5.17, -1.01, -2.43, -6.01, -4.16, 0.3, -7.85, -3.86, -0.47 \ldots$$

- How do we fit a probability distribution?
- What do we mean by fitting a probability distribution?

Solution I

Define parametric family of functions, $p_\theta, \theta \in \Theta$, and then find the parameters that maximizes the *likelihood* of the data, or equivalently, the log-likelihood

$$\text{argmax}_\theta \sum_{i=1}^{N} \log p_\theta(x_i)$$

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$$\text{argmax}_\theta \sum_{i=1}^{N} \log p_\theta(x_i)$$

This minimizes the Kullback-Leibler divergence to the data distribution, i.e. $KL(p_{\text{data}} \parallel p_\theta)$.

Visualizing data distribution

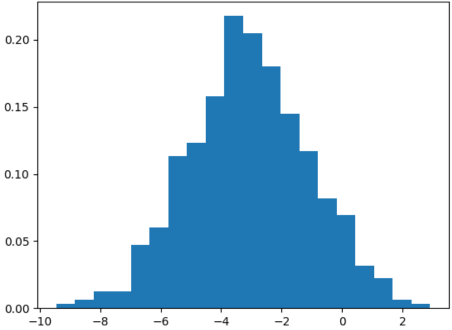

Figure: Histogram for data

Visualizing data distribution

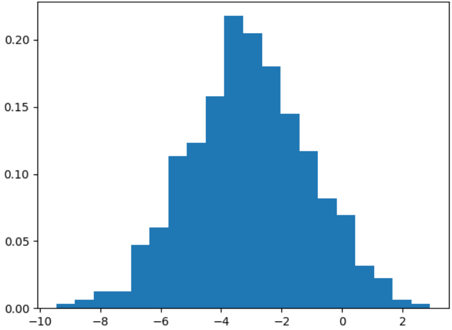

Figure: Histogram for data

- Normally distributed?

Fit distribution

Assuming normal distribution

$$\hat{\mu} = \frac{1}{N}\sum_{i=1}^{N} x_i, \qquad \hat{\sigma^2} = \frac{1}{N}\sum_{i=1}^{N}(x_i - \hat{\mu})^2$$

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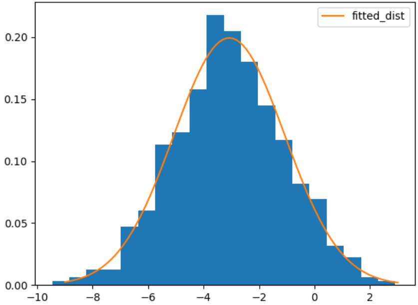

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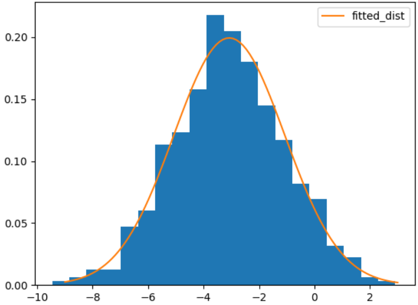

Generally may require iterative procedure to maximize likelihood.

Solution II

- Define a random variable Z on $\mathbb{R}^k$ for some k, e.g. $Z \sim \mathcal{N}(0, I)$. Let p_z denote distribution.
- Define $G : \mathbb{R}^k \to \mathbb{R}^d$
- Generate samples by
    1. Draw z from p_z.
    2. Map $z \to G(z)$.

Solution II continued

Advantages:

- Easy to generate samples
- Works even if X does not have density on $\mathbb{R}^d$.
- Can use complex functions, e.g. neural networks to represent distribution

Disadvantages:

- Not straightforward to find likelihood of samples.

Solution II continued

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How do we fit G though?

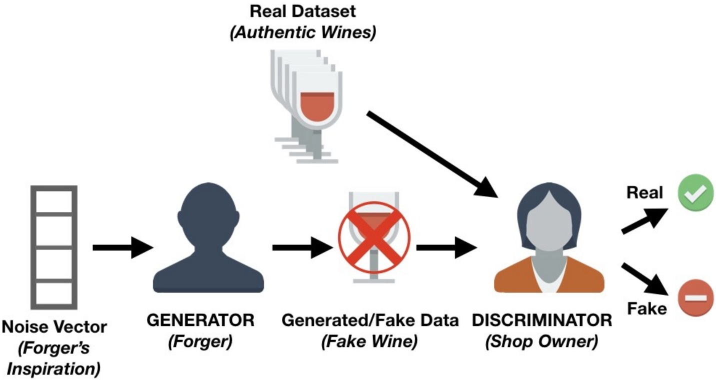
Section 2

Generative Adverserial Networks (GAN)

Subsection 1

Introduction

Analogy



https://towardsdatascience.com/demystifying-generative-adversarial-networks-c076d8db8f44

Adverserial networks

Generative Adversarial Nets (2014)

Adverserial networks

Generative Adversarial Nets (2014)

- Two networks: generator G and discriminator D.
- Discriminator: try to classify an input as real or fake (generated), outputs probability in $[0, 1]$, where 1 means real.
- Generator: try to fool discriminator
- Minimax game:

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

Minimax solutoin

Let p_g be the density function of the distribution induced by G and p_{data} be the density of data distribution[1]. Optimal D is given by

$$D^*(x) = \frac{p_{\text{data}}(x)}{p_{\text{data}}(x) + p_g(x)}$$

[1] We assume this exists here.

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$$D^*(x) = \frac{p_{\text{data}}(x)}{p_{\text{data}}(x) + p_g(x)}$$

Inserting D^* in minimax equation and rewriting leads to

$$\min_G 2 * JSD(p_{\text{data}} \parallel p_g) - \log(4)$$

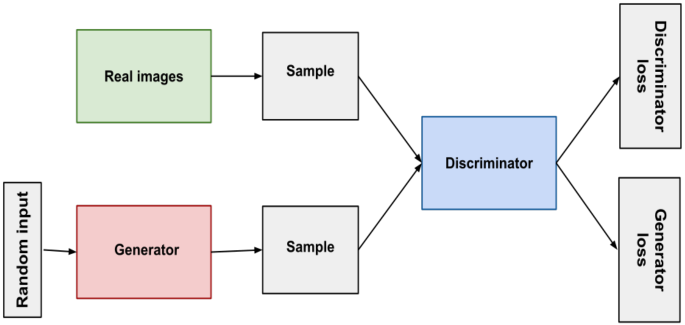
where JSD is the Jensen-Shannon divergence. The minimum value is achieved at $p_g = p_{\text{data}}$.

[1] We assume this exists here.

Subsection 2

Training

GAN overview



https://developers.google.com/machine-learning/gan/generator

Discriminator loss (minibatch)

Assume discriminator D parametrized by η.

$$-\Big(\frac{1}{m}\sum_{i=1}^{m}\log(D_\eta(x_i^{real})) + \frac{1}{m}\sum_{i=1}^{m}\log(1 - D_\eta(x_i^{fake}))\Big)$$

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which can also be written as

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Note: This is just the normal cross-entropy loss.

Generator loss (minibatch)

Negative of discriminator loss

$$\frac{1}{m}\sum_{i=1}^{m}\log(D_\eta(x_i)) + \frac{1}{m}\sum_{i=1}^{m}\log(1 - D_\eta(G_\theta(z_i)))$$

Generator loss (minibatch)

Negative of discriminator loss

$$\frac{1}{m}\sum_{i=1}^{m}\log(D_\eta(x_i)) + \frac{1}{m}\sum_{i=1}^{m}\log(1 - D_\eta(G_\theta(z_i)))$$

As generator cannot influence first term, we may simplify to

$$\frac{1}{m}\sum_{i=1}^{m}\log(1 - D_\eta(G_\theta(z_i)))$$

Algorithm

Algorithm 1 GAN training, k is a hyperparameter (e.g. 1).

for number of training iterations **do**

  for k steps **do**

    Sample minibatch of m noise samples $\{z_1, \ldots, z_m\}$ from noise prior p_z.

    Sample minibatch of m examples $\{x_1, \ldots, x_m\}$ from data generating distribution $p_{\text{data}}(x)$.

    Update the discriminator by ascending its stochastic gradient:

$$\nabla_\eta \frac{1}{m} \sum_{i=1}^{m} \left[\log D_\eta\left(x_i\right) + \log\left(1 - D_\eta\left(G_\theta\left(z_i\right)\right)\right)\right].$$

  end for

  Sample minibatch of m noise samples $\{z_1, \ldots, z_m\}$ from noise prior p_z.

  Update the generator by descending its stochastic gradient:

$$\nabla_\theta \frac{1}{m} \sum_{i=1}^{m} \log\left(1 - D_\eta\left(G_\theta\left(z_i\right)\right)\right)$$

end for

Training I

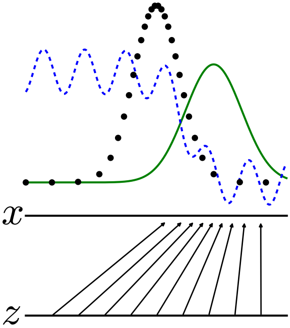
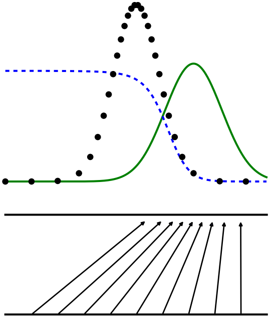
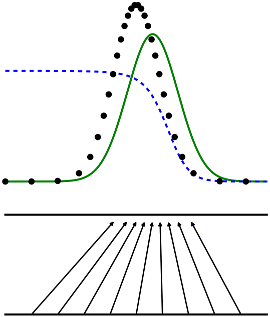


Figure: Green: p_g, black: p_{data}, blue: discriminator score.

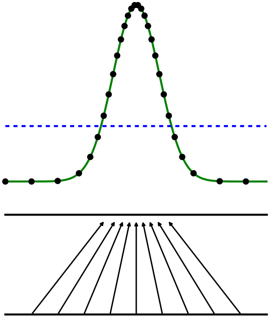
Training II



Training III



Training IV



Subsection 3

TensorFlow example

TensorFlow example I

```
import numpy as np
from scipy.stats import norm
import tensorflow as tf
from matplotlib import pyplot as plt
```

TensorFlow example II

```
class Generator(tf.keras.Model):
  def __init__(self):
    super(Generator, self).__init__()
    self.w = tf.Variable(1, dtype=tf.float32)
    self.b = tf.Variable(0, dtype=tf.float32)

  def call(self, z):
    x = self.w*z + self.b
    return x

class Discriminator(tf.keras.Model):
  def __init__(self, hidden_units=8):
    super(Discriminator, self).__init__()
    self.dense = tf.keras.layers.Dense(hidden_units)
    self.logits = tf.keras.layers.Dense(1,
    ↪  kernel_initializer=tf.keras.initializers.zeros())

  def call(self, x):
    x = tf.expand_dims(x, axis=-1)
    logits = self.logits(tf.nn.relu(self.dense(x)))
    logits = tf.squeeze(logits, axis=-1)
    p = 1 / (1 + tf.math.exp(-logits))
    return p
```

TensorFlow example III

```python
# parameters true distribution
mu = -4
sigma = 2

def visualize(G, D):
  interval = np.linspace(-10, 10, 100)
  d_values = D(interval)
  g_dist = norm.pdf(interval, loc=G.b.numpy(), scale=G.w.numpy())
  true_dist = norm.pdf(interval, loc=mu, scale=sigma)
  plt.plot(interval, true_dist, label="true_dist")
  plt.plot(interval, g_dist, label="G_dist")
  plt.plot(interval, d_values, label="D, p_true_data(x)")
  plt.legend()
  plt.show()
```

TensorFlow example IV

```
N = 32
x = np.random.normal(loc=mu, scale=sigma, size=N)
indices = np.array(range(N))

G = Generator()
D = Discriminator()

D_learning_rate = 0.1
G_learning_rate = 0.1
D_optimizer = tf.keras.optimizers.Adam(D_learning_rate)
G_optimizer = tf.keras.optimizers.Adam(G_learning_rate)

batch_size = 16
critic_iters = 1
iterations = 100
plot_interval = 1
```

TensorFlow example V

```
for iteration in range(iterations):
  if iteration % plot_interval == 0: visualize(G, D)

  # discriminator update
  for _ in range(critic_iters):
    # sample real data (from data distribution)
    np.random.shuffle(indices)
    real = x[indices[:batch_size]]
    z = tf.random.normal(shape=[batch_size])
    fake = G(z)
    with tf.GradientTape() as tape:
      loss_real = tf.reduce_mean(-tf.math.log(D(real)))
      loss_fake = tf.reduce_mean(-tf.math.log(1-D(fake)))
      D_loss = loss_real + loss_fake
    grads = tape.gradient(D_loss, D.trainable_variables)
    D_optimizer.apply_gradients(zip(grads, D.trainable_variables))

  # generator update
  z = tf.random.normal(shape=[batch_size])
  with tf.GradientTape() as tape:
    G_loss = tf.reduce_mean(tf.math.log(1-D(G(z))))
  grads = tape.gradient(G_loss, G.trainable_variables)
  G_optimizer.apply_gradients(zip(grads, G.trainable_variables))
```

Subsection 4

Does it work?

4 years of GAN progress

The Malicious Use of Artificial Intelligence: Forecasting, Prevention, and Mitigation

Does it end there?

Does it end there?

A Style-Based Generator Architecture for Generative Adversarial Networks

Subsection 5

Conditional GANs

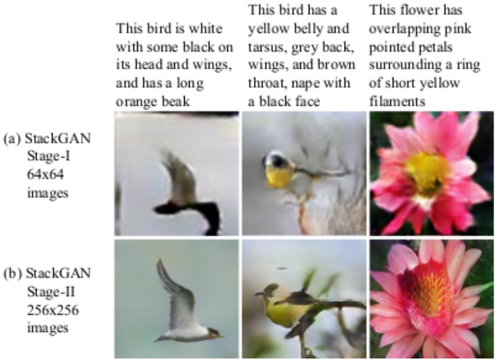
Conditional GANs

- Before: data were samples $x_1, x_2, \ldots, x_N$
- Now: data are sample pairs $(x_1, c_1), (x_2, c_2), \ldots, (x_N, c_N)$
- Generator and discriminator get c as extra input:
  - $G(z, c)$
  - $D(x, c)$

Subsection 6

Applications

Text-to-image



StackGAN: Text to Photo-realistic Image Synthesis with Stacked Generative Adversarial Networks

- (x, c) = (image, corresponding sentence)

Text-to-image II

StackGAN: Text to Photo-realistic Image Synthesis with Stacked Generative Adversarial Networks

Image impainting

Figure: Conditional image

Figure: L2 loss

Figure: Sample with GAN loss

Context Encoders: Feature Learning by Inpainting

- (x, c) = (image, image with missing data)

Super-resolution

Figure: Bicubic

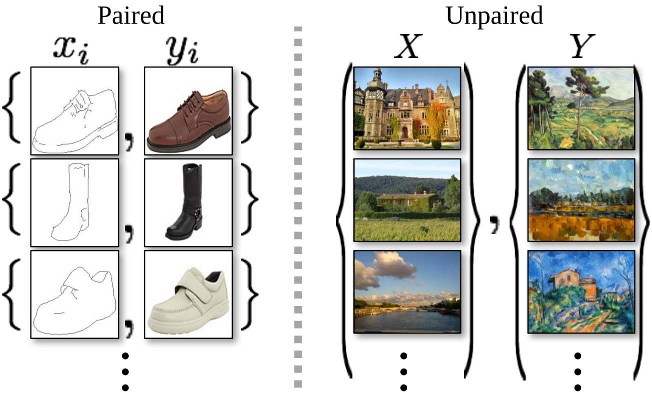
Figure: SRGAN

Figure: original

Photo-Realistic Single Image Super-Resolution Using a Generative Adversarial Network

- (x, c) = (image, lower resolution image)

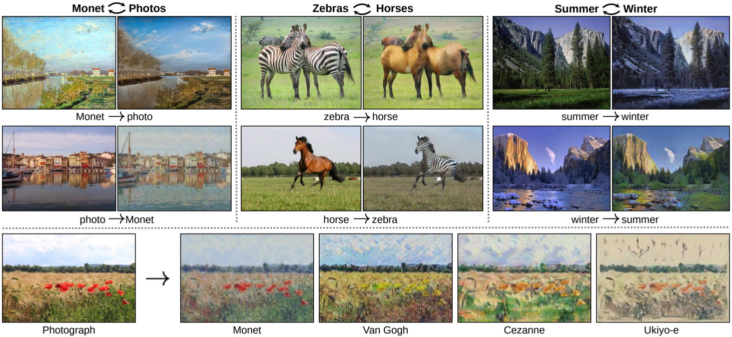
CycleGAN: unpaired image-to-image translation



Unpaired Image-to-Image Translation using Cycle-Consistent Adversarial Networks

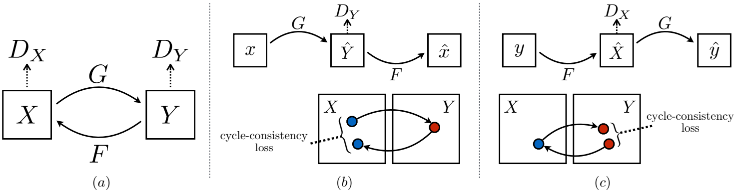
- TensorFlow tutorial on CycleGan

CycleGAN



Unpaired Image-to-Image Translation using Cycle-Consistent Adversarial Networks

CycleGAN: how?



- Where is z?

Unpaired Image-to-Image Translation using Cycle-Consistent Adversarial Networks

CycleGAN: how?

- Two generators F and G, each with their own discriminator.
  - Takes samples from other distribution as input, not z!
- Learn F such that $x \sim X$, $F(x)$ should be distributed as Y.
- Learn G such that $y \sim Y$, $G(y)$ should be distributed as X.
- Need additional constraints to get *pairing* that we need for translation. Propose cycle-consistency:
  - Losses on $G(F(x)) - x$ and $F(G(y)) - y$
  - In order to reconstruct the information must be retained in the target domain, so should perhaps be a similar image?
    - Likely some conflict between the different goals. . .

Unpaired Image-to-Image Translation using Cycle-Consistent Adversarial Networks

Subsection 7

Evaluation (not curriculum)

Challenges in evaluation

- No likelihood to evaluate

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- Look at discriminator?
  - Optimal discriminator loss is $2 * JSD(p_{\text{data}}, p_g) - log(4)$ where JSD is the Jensen-Shannon divergence.

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Challenges in evaluation

- No likelihood to evaluate
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  - Optimal discriminator loss is $2 * JSD(p_{\text{data}}, p_g) - log(4)$ where JSD is the Jensen-Shannon divergence.
- Discriminator likely imperfect
- A single number not enough? Quality vs diversity

Visual inspection

For image data we may look at images...

- Quality may be eaiser to evaluate then diversity

FID

- Extract *features* and estimate difference in distributions in these.
- Assuming features are normally distributed (quite strong assumption!), can measure Fréchet distance (also known as Wasserstein-2 distance), which is given by

$$d^2((m, C), (m_g, C_g)) = \|m - m_g\|_2^2 + trace(C + C_g - 2(CC_g)^{1/2})$$

where (m, C) and (m_g, C_g) are the mean and covariance of the features of the real and generated data respectively, and the *trace* of a matrix is the sum of its diagonal elements.

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where (m, C) and (m_g, C_g) are the mean and covariance of the features of the real and generated data respectively, and the *trace* of a matrix is the sum of its diagonal elements.

- To make comparable: Use Inception architecture with weights from `http://download.tensorflow.org/models/image/imagenet/inception-2015-12-05.tgz`.
  - Known as Fréchet Inception Distance (FID)

GANs Trained by a Two Time-Scale Update Rule Converge to a Local Nash Equilibrium

FID example

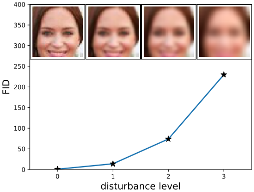

Figure: Blur

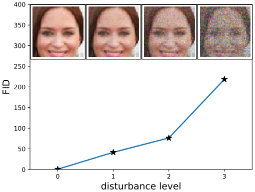

Figure: Gaussian noise

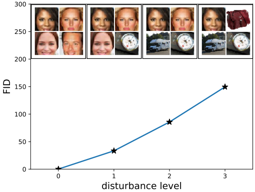

Figure: Mixed in ImageNet images

- Empirically proved to correlate well(?) with visual inspection.

GANs Trained by a Two Time-Scale Update Rule Converge to a Local Nash Equilibrium

Subsection 8

Challenges (not curriculum)

Challenges

- Not obvous how to track progress or measure performance
- Training can be unstable due to interactions between G and D
  - Input distribution of D changes over time
  - Loss function of G changes over time
- Choice of optimizer is important
  - Standard SGD not normally used, Adam popular
- Mode collapse - G only able to capture some of modes in data

Generator loss I

Let D_l denote the logits of D, i.e. $D(x) = \sigma(D_l(x))$ where σ is the sigmoid function.

$$\nabla_\theta \frac{1}{m} \sum_{i=1}^{m} \log(1 - D(G_\theta(z_i))) = \frac{1}{m} \sum_{i=1}^{m} D(G_\theta(z_i)) \nabla_\theta D_l(G_\theta(z_i))$$

When generator is poor, may have $D(G_\theta(z_i)) \approx 0$, and thus gradients ≈ 0.

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$$-\frac{1}{m} \sum_{i=1}^{m} \log(D_\eta(G_\theta(z_i)))$$

to mitigate vanishing gradients issue.

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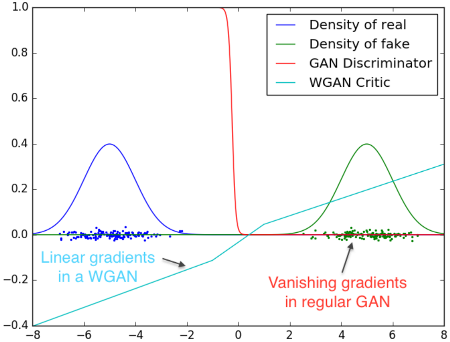
to mitigate vanishing gradients issue. This does however introduce other potential problems: Sample weighting as an explanation for mode collapse in generative adversarial networks

Loss function II

Original GAN loss have some theoretical (and practical?) issues



Wasserstein GAN

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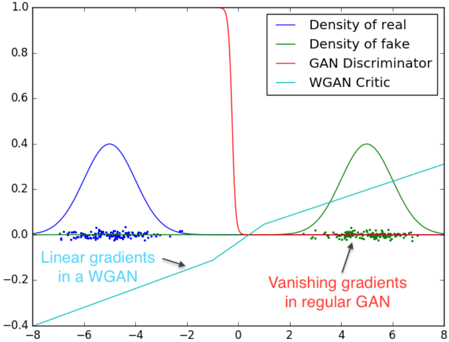

Wasserstein GAN

Note: regularizing discriminator can also mitigate problem.

Wasserstein loss

Wasserstein GAN discriminator loss:

$$-(\frac{1}{m}\sum_{i=1}^{m} D_\eta(x_i) - D_\eta(G_\theta(z_i))$$

- Note that D_η no longer outputs a probability, but any real number is valid.

Wasserstein GAN generator loss:

$$-\frac{1}{m}\sum_{i=1}^{m} D_\eta(G_\theta(z_i))$$

- Assumes some Lipschitz-constraints on D_η.

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$$-\frac{1}{m}\sum_{i=1}^{m} D_\eta(G_\theta(z_i))$$

- Assumes some Lipschitz-constraints on D_η.
- G now tries to minimize Wasserstein distance between generated distribution and data distribution.

Wasserstein GAN

Section 3

Generative Adverserial Imitation Learning (GAIL)

Subsection 1

Introduction

Why imitation learning?

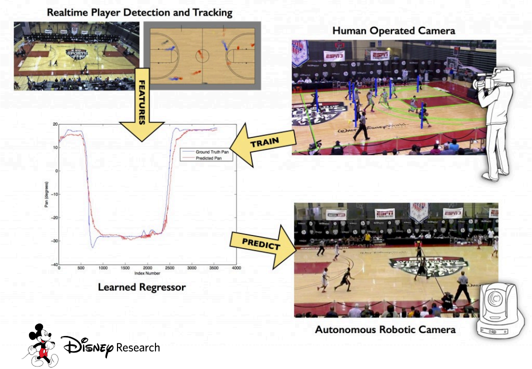

Figure: Source: New Frontiers in Imitation Learning.

Smooth Imitation Learning for Online Sequence Prediction

Imitation learning by behaviour cloning

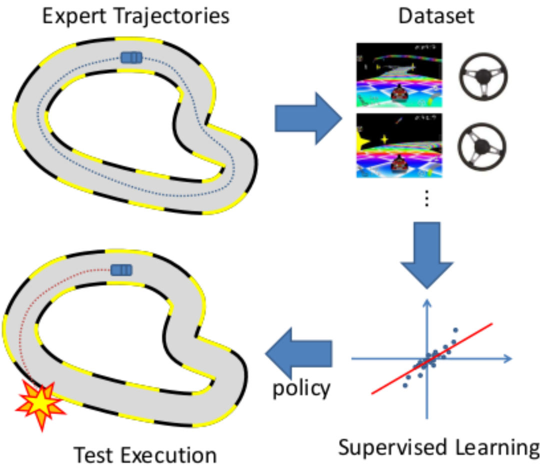

Figure: Source: Interactive Learning for Sequential Decisions and Predictions

Equivalence of policy and occupancy measure

Previously defined ρ_π as the unnormalized discounted visitation frequencies

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It turns out that if we have a policy π' with the same occupancy measure as for π, i.e. $\rho_{\pi'} = \rho_\pi$, then $\pi' = \pi$.

GAIL

Generative Adversarial Imitation Learning (2016)

- To imitate a policy we may imitate state-action frequencies
- Data samples are (state, action) pairs from expert policy
  - $(s_1, a_1), (s_2, a_2), ..., (s_N, a_N)$
  - Note: not conditional GAN, $x_i = (s_i, a_i)$

GAIL

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  - Note: not conditional GAN, $x_i = (s_i, a_i)$
- Generator is here a deterministic policy $\pi(s) \rightarrow a$. By interacting with the environment we get generated/"fake" state-action pairs $(s_1, a_1)_g, (s_2, a_2)_g, \ldots, (s_N, a_N)_g$.
- Discriminator takes state, action pairs and try to classify them as real or fake.

GAIL vs GAN

Differences from standard GAN:

- Sequential process
- Policy network don't have directly control over samples, interaction with (possibly stochastic) environment.
- Can't train "generator" by backpropagating through discriminator, instead trained with reinforcement learning with discriminator feedback as reward signal. E.g. generator gets high reward for samples the discriminator finds more real.
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Discriminator update is unchanged.

GAIL algorithm

Algorithm 2 Generative adversarial imitation learning

1: **Input:** Expert trajectories $\tau_E \sim \pi_E$, initial policy and discriminator parameters θ_0, η_0
2: **for** $i = 0, 1, 2, \ldots$ **do**
3: Sample trajectories $\tau_i \sim \pi_{\theta_i}$
4: Update the discriminator parameters from η_i to η_{i+1} with the gradient

$$\hat{\mathbb{E}}_{\tau_i}[\nabla_\eta \log(D_\eta(s,a))] + \hat{\mathbb{E}}_{\tau_E}[\nabla_\eta \log(1 - D_\eta(s,a))] \tag{1}$$

5: Take a policy step from θ_i to θ_{i+1}, using the TRPO rule with cost function $\log(D_{\eta_{i+1}}(s,a))$. Specifically, take a KL-constrained natural gradient step with

$$\begin{aligned} &\hat{\mathbb{E}}_{\tau_i}\left[\nabla_\theta \log \pi_\theta(a|s) Q(s,a)\right] - \lambda \nabla_\theta H(\pi_\theta), \\ &\text{where } Q(\bar{s},\bar{a}) = \hat{\mathbb{E}}_{\tau_i}[\log(D_{\eta_{i+1}}(s,a)) \,|\, s_0 = \bar{s}, a_0 = \bar{a}] \end{aligned} \tag{2}$$

6: **end for**

Note: TRPO is an RL algorithm, you may switch this out with e.g. a PPO iteration (recall second RL lecture).