Advanced machine learning and data analysis for the physical sciences

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Plans for the week of April 29- May 3, 2024

Deep generative models and summary of course.

1. Finalizing discussion of diffusion models
2. Generative Adversarial Networks (GANs)
3. Summary of course and plans for the lab sessions

Readings

1. Reading recommendation: Goodfellow et al, for GANs see sections 20.10-20.11

What is a GAN?

A GAN is a deep neural network which consists of two networks, a so-called generator network and a discriminating network, or just discriminator. Through several iterations of generation and discrimination, the idea is that these networks will train each other, while also trying to outsmart each other.

What is a generator network?

A generator network is often a deep network which uses existing data to generate new data (from for example simulations of physical systems, imagesm video, audio and more) from randomly generated inputs, the so-called latent space. Training the network allows us to generate say new data, images etc. As an example a generator network could for example be a Boltzmann machine as discussed earlier. This machine is trained to produce for example a quantum mechanical probability distribution.

It can a simple neural network with an input layer and an output layer and a given number of hidden layers.

And what is a discriminator network?

A discriminator tries to distinguish between real data and those generated by the abovementioned generator.

Appplications of GANs

There are exteremely many applications of GANs

1. Image generation
2. Text-to-image analysis
3. Face-aging
4. Image-to-image translation
5. Video synthesis
6. High-resolution image generation
7. Completing missing parts of images and much more

Generative Adversarial Networks

Generative Adversarial Networks are a type of unsupervised machine learning algorithm proposed by Goodfellow et. al, see https://arxiv.org/pdf/1406.2661.pdf in 2014 (Read the paper first it's only 6 pages). The simplest formulation of the model is based on a game theoretic approach, *zero sum game*, where we pit two neural networks against one another. We define two rival networks, one generator g, and one discriminator d. The generator directly produces samples

$$x = g(z; \theta^{(g)}).$$

Discriminator

The discriminator attempts to distinguish between samples drawn from the training data and samples drawn from the generator. In other words, it tries to tell the difference between the fake data produced by g and the actual data samples we want to do prediction on. The discriminator outputs a probability value given by

$$d(x; \theta^{(d)}).$$

indicating the probability that x is a real training example rather than a fake sample the generator has generated.

Zero-sum game

The simplest way to formulate the learning process in a generative adversarial network is a zero-sum game, in which a function

$$v(\theta^{(g)}, \theta^{(d)}),$$

determines the reward for the discriminator, while the generator gets the conjugate reward

$$-v(\theta^{(g)}, \theta^{(d)})$$

Maximizing reward

During learning both of the networks maximize their own reward function, so that the generator gets better and better at tricking the discriminator, while the discriminator gets better and better at telling the difference between the fake and real data. The generator and discriminator alternate on which one trains at one time (i.e. for one epoch). In other words, we keep the generator constant and train the discriminator, then we keep the discriminator constant to train the generator and repeat. It is this back and forth dynamic which lets GANs tackle otherwise intractable generative problems. As the generator improves with training, the discriminator's performance gets worse because it cannot easily tell the difference between real and fake. If the generator ends up succeeding perfectly, the the discriminator will do no better than random guessing i.e. 50%.

Progression in training

This progression in the training poses a problem for the convergence criteria for GANs. The discriminator feedback gets less meaningful over time, if we continue training after this point then the generator is effectively training on junk data which can undo the learning up to that point. Therefore, we stop training when the discriminator starts outputting 1/2 everywhere. At convergence we have

$$g^* = \underset{g}{\operatorname{argmin}} \max_{d} v(\theta^{(g)}, \theta^{(d)}),$$

Deafault choice

The default choice for v is

$$v(\theta^{(g)}, \theta^{(d)}) = \mathbb{E}_{x\sim p_{\text{data}}} \log d(x) + \mathbb{E}_{x\sim p_{\text{model}}} \log(1 - d(x)).$$

Design of GANs

The main motivation for the design of GANs is that the learning process requires neither approximate inference (variational autoencoders for example) nor approximation of a partition function. In the case where

$$\max_d v(\theta^{(g)}, \theta^{(d)})$$

is convex in $\theta^{(g)}$ then the procedure is guaranteed to converge and is asymptotically consistent (Seth Lloyd on QuGANs). This is in general not the case and it is possible to get situations where the training process never converges because the generator and discriminator chase one another around in the parameter space indefinitely.

More references

A much deeper discussion on the currently open research problem of GAN convergence is available from `https://www.deeplearningbook.org/contents/generative_models.html`. To anyone interested in learning more about GANs it is a highly recommended read. Direct quote: **In this best-performing formulation, the generator aims to increase the log probability that the discriminator makes a mistake, rather than aiming to decrease the log probability that the discriminator makes the correct prediction.** Another interesting read can be found at `https://arxiv.org/abs/1701.00160`.

Writing Our First Generative Adversarial Network

This part is best seen using the jupyter-notebook.

Let us implement a GAN in tensorflow. We will study the performance of our GAN on the MNIST dataset. This code is based on and adapted from the Google tutorial at `https://www.tensorflow.org/tutorials/generative/dcgan`

First we import our libraries

```
import os
import time
import numpy as np
import tensorflow as tf
import matplotlib.pyplot as plt
from tensorflow.keras import layers
from tensorflow.keras.utils import plot_model
```

Next we define our hyperparameters and import our data the usual way

```
BUFFER_SIZE = 60000
BATCH_SIZE = 256
EPOCHS = 30

data = tf.keras.datasets.mnist.load_data()
(train_images, train_labels), (test_images, test_labels) = data
train_images = np.reshape(train_images, (train_images.shape[0],
                                         28,
                                         28,
                                         1)).astype('float32')

# we normalize between -1 and 1
train_images = (train_images - 127.5) / 127.5
training_dataset = tf.data.Dataset.from_tensor_slices(
                      train_images).shuffle(BUFFER_SIZE).batch(BATCH_SIZE)
```

Let's have a quick look

```
plt.imshow(train_images[0], cmap='Greys')
plt.show()
```

Now we define our two models. This is where the 'magic' happens. There are a huge amount of possible formulations for both models. A lot of engineering and trial and error can be done here to try to produce better performing models. For more advanced GANs this is by far the step where you can 'make or break' a model.

We start with the generator. As stated in the introductory text the generator g upsamples from a random sample to the shape of what we want to predict. In our case we are trying to predict MNIST images (28×28 pixels).

```
def generator_model():
    """
    The generator uses upsampling layers tf.keras.layers.Conv2DTranspose() to
    produce an image from a random seed. We start with a Dense layer taking this
    random sample as an input and subsequently upsample through multiple
    convolutional layers.
    """

    # we define our model
    model = tf.keras.Sequential()


    # adding our input layer. Dense means that every neuron is connected and
    # the input shape is the shape of our random noise. The units need to match
    # in some sense the upsampling strides to reach our desired output shape.
    # we are using 100 random numbers as our seed
    model.add(layers.Dense(units=7*7*BATCH_SIZE,
                           use_bias=False,
                           input_shape=(100, )))
    # we normalize the output form the Dense layer
    model.add(layers.BatchNormalization())
    # and add an activation function to our 'layer'. LeakyReLU avoids vanishing
    # gradient problem
    model.add(layers.LeakyReLU())
    model.add(layers.Reshape((7, 7, BATCH_SIZE)))
    assert model.output_shape == (None, 7, 7, BATCH_SIZE)
    # even though we just added four keras layers we think of everything above
    # as 'one' layer

    # next we add our upscaling convolutional layers
    model.add(layers.Conv2DTranspose(filters=128,
                                     kernel_size=(5, 5),
                                     strides=(1, 1),
                                     padding='same',
                                     use_bias=False))
    model.add(layers.BatchNormalization())
    model.add(layers.LeakyReLU())
    assert model.output_shape == (None, 7, 7, 128)

    model.add(layers.Conv2DTranspose(filters=64,
                                     kernel_size=(5, 5),
                                     strides=(2, 2),
                                     padding='same',
                                     use_bias=False))
    model.add(layers.BatchNormalization())
    model.add(layers.LeakyReLU())
    assert model.output_shape == (None, 14, 14, 64)

    model.add(layers.Conv2DTranspose(filters=1,
                                     kernel_size=(5, 5),
                                     strides=(2, 2),
                                     padding='same',
                                     use_bias=False,
                                     activation='tanh'))
    assert model.output_shape == (None, 28, 28, 1)

    return model
```

And there we have our 'simple' generator model. Now we move on to defining our discriminator model d, which is a convolutional neural network based image classifier.

```
def discriminator_model():
    """
    The discriminator is a convolutional neural network based image classifier
    """

    # we define our model
    model = tf.keras.Sequential()
    model.add(layers.Conv2D(filters=64,
                            kernel_size=(5, 5),
                            strides=(2, 2),
                            padding='same',
                            input_shape=[28, 28, 1]))
    model.add(layers.LeakyReLU())
    # adding a dropout layer as you do in conv-nets
    model.add(layers.Dropout(0.3))


    model.add(layers.Conv2D(filters=128,
                            kernel_size=(5, 5),
                            strides=(2, 2),
                            padding='same'))
    model.add(layers.LeakyReLU())
    # adding a dropout layer as you do in conv-nets
    model.add(layers.Dropout(0.3))

    model.add(layers.Flatten())
    model.add(layers.Dense(1))

    return model
```

Let us take a look at our models. **Note**: double click images for bigger view.

```
generator = generator_model()
plot_model(generator, show_shapes=True, rankdir='LR')


discriminator = discriminator_model()
plot_model(discriminator, show_shapes=True, rankdir='LR')
```

Next we need a few helper objects we will use in training

```
cross_entropy = tf.keras.losses.BinaryCrossentropy(from_logits=True)
generator_optimizer = tf.keras.optimizers.Adam(1e-4)
discriminator_optimizer = tf.keras.optimizers.Adam(1e-4)
```

The first object, *cross_entropy* is our loss function and the two others are our optimizers. Notice we use the same learning rate for both g and d. This is because they need to improve their accuracy at approximately equal speeds to get convergence (not necessarily exactly equal). Now we define our loss functions

```
def generator_loss(fake_output):
    loss = cross_entropy(tf.ones_like(fake_output), fake_output)

    return loss


def discriminator_loss(real_output, fake_output):
    real_loss = cross_entropy(tf.ones_like(real_output), real_output)
    fake_loss = cross_entropy(tf.zeros_liks(fake_output), fake_output)
    total_loss = real_loss + fake_loss

    return total_loss
```

Next we define a kind of seed to help us compare the learning process over multiple training epochs.

```
noise_dimension = 100
n_examples_to_generate = 16
seed_images = tf.random.normal([n_examples_to_generate, noise_dimension])
```

Now we have everything we need to define our training step, which we will apply for every step in our training loop. Notice the @tf.function flag signifying that the function is tensorflow 'compiled'. Removing this flag doubles the computation time.

```python
@tf.function
def train_step(images):
    noise = tf.random.normal([BATCH_SIZE, noise_dimension])

    with tf.GradientTape() as gen_tape, tf.GradientTape() as disc_tape:
        generated_images = generator(noise, training=True)

        real_output = discriminator(images, training=True)
        fake_output = discriminator(generated_images, training=True)

        gen_loss = generator_loss(fake_output)
        disc_loss = discriminator_loss(real_output, fake_output)

    gradients_of_generator = gen_tape.gradient(gen_loss,
                                        generator.trainable_variables)
    gradients_of_discriminator = disc_tape.gradient(disc_loss,
                                        discriminator.trainable_variables)
    generator_optimizer.apply_gradients(zip(gradients_of_generator,
                                        generator.trainable_variables))
    discriminator_optimizer.apply_gradients(zip(gradients_of_discriminator,
                                        discriminator.trainable_variables))

    return gen_loss, disc_loss
```

Next we define a helper function to produce an output over our training epochs to see the predictive progression of our generator model. **Note**: I am including this code here, but comment it out in the training loop.

```python
def generate_and_save_images(model, epoch, test_input):
    # we're making inferences here
    predictions = model(test_input, training=False)

    fig = plt.figure(figsize=(4, 4))

    for i in range(predictions.shape[0]):
        plt.subplot(4, 4, i+1)
        plt.imshow(predictions[i, :, :, 0] * 127.5 + 127.5, cmap='gray')
        plt.axis('off')

    plt.savefig(f'./images_from_seed_images/image_at_epoch_{str(epoch).zfill(3)}.png')
    plt.close()
    #plt.show()
```

Setting up checkpoints to periodically save our model during training so that everything is not lost even if the program were to somehow terminate while training.

```python
# Setting up checkpoints to save model during training
checkpoint_dir = './training_checkpoints'
checkpoint_prefix = os.path.join(checkpoint_dir, 'ckpt')
checkpoint = tf.train.Checkpoint(generator_optimizer=generator_optimizer,
                            discriminator_optimizer=discriminator_optimizer,
                            generator=generator,
                            discriminator=discriminator)
```

Now we define our training loop

```
def train(dataset, epochs):
    generator_loss_list = []
    discriminator_loss_list = []

    for epoch in range(epochs):
        start = time.time()

        for image_batch in dataset:
            gen_loss, disc_loss = train_step(image_batch)
            generator_loss_list.append(gen_loss.numpy())
            discriminator_loss_list.append(disc_loss.numpy())

        #generate_and_save_images(generator, epoch + 1, seed_images)

        if (epoch + 1) % 15 == 0:
            checkpoint.save(file_prefix=checkpoint_prefix)

        print(f'Time for epoch {epoch} is {time.time() - start}')

    #generate_and_save_images(generator, epochs, seed_images)

    loss_file = './data/lossfile.txt'
    with open(loss_file, 'w') as outfile:
        outfile.write(str(generator_loss_list))
        outfile.write('\n')
        outfile.write('\n')
        outfile.write(str(discriminator_loss_list))
        outfile.write('\n')
        outfile.write('\n')
```

To train simply call this function. **Warning**: this might take a long time so there is a folder of a pretrained network already included in the repository.

```
train(train_dataset, EPOCHS)
```

And here is the result of training our model for 100 epochs

Movie 1: `images_from_seed_images/generation.gif`

Now to avoid having to train and everything, which will take a while depending on your computer setup we now load in the model which produced the above gif.

```
checkpoint.restore(tf.train.latest_checkpoint(checkpoint_dir))
restored_generator = checkpoint.generator
restored_discriminator = checkpoint.discriminator

print(restored_generator)
print(restored_discriminator)
```

Exploring the Latent Space

So we have successfully loaded in our latest model. Let us now play around a bit and see what kind of things we can learn about this model. Our generator takes an array of 100 numbers. One idea can be to try to systematically change our input. Let us try and see what we get

```
def generate_latent_points(number=100, scale_means=1, scale_stds=1):
    latent_dim = 100
    means = scale_means * tf.linspace(-1, 1, num=latent_dim)
    stds = scale_stds * tf.linspace(-1, 1, num=latent_dim)
    latent_space_value_range = tf.random.normal([number, number],
                                                 means,
                                                 stds,
                                                 dtype=tf.float64)

    return latent_space_value_range

def generate_images(latent_points):
    # notice we set training to false because we are making inferences
    generated_images = restored_generator(latent_space_value_range,
                                          training=False)

    return generated_images


def plot_result(generated_images, number):
    # obviously this assumes sqrt number is an int
    fig, axs = plt.subplots(int(np.sqrt(number)), int(np.sqrt(number)),
                            figsize=(10, 10))

    for i in range(int(np.sqrt(number))):
        for j in range(int(np.sqrt(number))):
            axs[i, j].imshow(generated_images[i*j], cmap='Greys')
            axs[i, j].axis('off')

    plt.show()


generated_images = generate_images(generate_latent_points())
plot_result(generated_images, number)
```

Interesting! We see that the generator generates images that look like MNIST numbers: $1, 4, 7, 9$. Let's try to tweak it a bit more to see if we are able to generate a similar plot where we generate every MNIST number. Let us now try to 'move' a bit around in the latent space. **Note**: decrease the plot number if these following cells take too long to run on your computer.

```
plot_number = 225

generated_images = generate_images(generate_latent_points(number=plot_number,
                                                          scale_means=5,
                                                          scale_stds=1))
plot_result(generated_images, plot_number)

generated_images = generate_images(generate_latent_points(number=plot_number,
                                                          scale_means=-5,
                                                          scale_stds=1))
plot_result(generated_images, plot_number)

generated_images = generate_images(generate_latent_points(number=plot_number,
                                                          scale_means=1,
                                                          scale_stds=5))
plot_result(generated_images, plot_number)
```

Again, we have found something interesting. *Moving* around using our means takes us from digit to digit, while *moving* around using our standard deviations seem to increase the number of different digits! In the last image above, we can barely make out every MNIST digit. Let us make on last plot using this information by upping the standard deviation of our Gaussian noises.

```
plot_number = 400
generated_images = generate_images(generate_latent_points(number=plot_number,
                                                          scale_means=1,
                                                          scale_stds=10))
```

A pretty cool result! We see that our generator indeed has learned a distribution which qualitatively looks a whole lot like the MNIST dataset.