Transpose Convolutions and Autoencoders

In our discussions of convolutional networks, we always started with an image, then reduced the "resolution" of the image until we made an image-level prediction. Specifically, we focused on image level classification problems: is the image of a cat or a dog? Which of the 10 digits does this image represent? We always went from a large image, to a lower-dimensional representation of the image.

Some tasks require us to go in the opposite direction. For example, we may wish to make pixel-wise predictions about the content of each pixel in an image. Is this pixel part of the foreground or the background? Is this pixel a part of a car or a pedestrian? Problems that require us to label each pixel is called a pixel-wise prediction problem. These problems require us to produce an high-resolution "image" from a low-dimensional representation of its contents.

A similar task is the task of *generating* an image given a low-dimensional *embedding* of the image. For example, we may wish to produce a neural network model that *generates* images of hand-written digits not in the MNIST data set. A neural network model that learns to generate new examples of data is called a **generative model**.

In both cases, we need a way to *increase* the resolution of our hidden units. We need something akin to convolution, but that goes in the *opposite* direction. We will use something called a **transpose convolution**. Transpose convolutions were first called *deconvolutions*, since it is the ``inverse" of a convolution operation. However, the terminology was confusing since it has nothing to do with the mathematical notion of deconvolution.

In [1]:

```
import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.optim as optim
import matplotlib.pyplot as plt
from torchvision import datasets, transforms

mnist_data = datasets.MNIST('data', train=True, download=True, transform=transforms.ToT
ensor())
mnist_data = list(mnist_data)[:4096]
```

Convolution Transpose

First, let's illustrate how convolution transposes can be `inverses'' of convolution layers.`
`We begin by creating a convolutional layer in PyTorch. This is the convolution that we will`
`try to find an`inverse" for.

In [2]:

```
conv = nn.Conv2d(in_channels=8,
                 out_channels=8,
                 kernel_size=5)
```

To illustrate how convolutional layers work, we'll create a random tensor and see how the convolution acts on that tensor:

In [3]:

```
x = torch.randn(2, 8, 64, 64)
y = conv(x)
y.shape
```

Out[3]:

```
torch.Size([2, 8, 60, 60])
```

A convolution transpose layer with the exact same specifications as above would have the ``reverse'' effect on the shape.

In [4]:

```
convt = nn.ConvTranspose2d(in_channels=8,
                           out_channels=8,
                           kernel_size=5)
convt(y).shape # should be same as x.shape
```

Out[4]:

```
torch.Size([2, 8, 64, 64])
```

And it does! Notice that the weights of this convolution transpose layer are all random, and are unrelated to the weights of the original `Conv2d`. So, the layer `convt` is not the mathematical inverse of the layer `conv`. However, with training, the convolution transpose has the potential to learn to act as an approximate inverse to `conv`.

Here is another example of `convt` in action:

In [5]:

```
x = torch.randn(32, 8, 64, 64)
y = convt(x)
y.shape
```

Out[5]:

```
torch.Size([32, 8, 68, 68])
```

Notice that the width and height of `y` is `68x68`, because the `kernel_size` is 5 and we have not added any padding. You can verify that if we start with a tensor with resolution `68x68` and applied a `5x5` convolution, we would end up with a tensor with resolution `64x64`.

```
In [6]:
```

```
conv = nn.Conv2d(in_channels=8,
                 out_channels=16,
                 kernel_size=5)
y = torch.randn(32, 8, 68, 68)
x = conv(y)
x.shape
```

```
Out[6]:

torch.Size([32, 16, 64, 64])
```

As before, we can add a padding to our convolution transpose, just like we added padding to our convolution operations:

```
In [7]:
```

```
convt = nn.ConvTranspose2d(in_channels=16,
                           out_channels=8,
                           kernel_size=5,
                           padding=2)
x = torch.randn(32, 16, 64, 64)
y = convt(x)
y.shape
```

```
Out[7]:

torch.Size([32, 8, 64, 64])
```

More interestingly, we can add a stride to the convolution to increase our resolution!

```
In [8]:
```

```
convt = nn.ConvTranspose2d(in_channels=16,
                           out_channels=8,
                           kernel_size=5,
                           stride=2,
                           output_padding=1, # needed because stride=2
                           padding=2)
x = torch.randn(32, 16, 64, 64)
y = convt(x)
y.shape
```

```
Out[8]:

torch.Size([32, 8, 128, 128])
```

Our resolution has doubled.

But what is actually happening? Essentially, we are adding a padding of zeros in between every row and every column of x. In the picture below, the blue image below represents the input x to the convolution transpose, and the green image above represents the output y.

You can check https://github.com/vdumoulin/conv_arithmetic (https://github.com/vdumoulin/conv_arithmetic) for more pictures and links to descriptions.

Autoencoder

To demonstrate the use of convolution transpose operations, we will build an **autoencoder**.

An autoencoder is not used for *supervised learning*. We will no longer try to *predict* something about our input. Instead, an autoencoder is considered a **generative model**: it learns a distributed *representation* of our training data, and can even be used to generate new instances of the training data.

An autoencoder model contains two components:

- An **encoder** that takes an image as input, and outputs a low-dimensional embedding (representation) of the image.
- A **decoder** that takes the low-dimensional embedding, and reconstructs the image.

An autoencoder is typically shown like below: (image from https://hackernoon.com/how-to-autoencode-your-pok%C3%A9mon-6b0f5c7b7d97 (https://hackernoon.com/how-to-autoencode-your-pok%C3%A9mon-6b0f5c7b7d97))

Here is an example of a *convolutional* autoencoder: an autoencoder that uses solely convolutional layers:

In [9]:

```
class Autoencoder(nn.Module):
    def __init__(self):
        super(Autoencoder, self).__init__()
        self.encoder = nn.Sequential( # like the Composition layer you built
            nn.Conv2d(1, 16, 3, stride=2, padding=1),
            nn.ReLU(),
            nn.Conv2d(16, 32, 3, stride=2, padding=1),
            nn.ReLU(),
            nn.Conv2d(32, 64, 7)
        )
        self.decoder = nn.Sequential(
            nn.ConvTranspose2d(64, 32, 7),
            nn.ReLU(),
            nn.ConvTranspose2d(32, 16, 3, stride=2, padding=1, output_padding=1),
            nn.ReLU(),
            nn.ConvTranspose2d(16, 1, 3, stride=2, padding=1, output_padding=1),
            nn.Sigmoid()
        )

    def forward(self, x):
        x = self.encoder(x)
        x = self.decoder(x)
        return x
```

Notice that the final activation on the decoder is a *sigmoid* activation. The reason is that all of our image pixels are in the range `[0, 1]`. A sigmoid gives us results in the same range.

Training an Autoencoder

How do we train an autoencoder? How do we know what kind of "encoder" and "decoder" we want?

One observation is that if we pass an image through the encoder, then pass the result through the decoder, we should get roughly the same image back. Ideally, reducing the dimensionality and then generating the image should give us the same result.

This observation provides us a training strategy: we will minimize the reconstruction error of the autoencoder across our training data. We use a loss function called `MSELoss`, which computes the square error at every pixel.

Beyond using a different loss function, the training scheme is roughly the same. Note that in the code below, we are using a new optimizer called `Adam`.

We switched to this optimizer not because it is specifically used for autoencoders, but because this is the optimizer that people tend to use in practice for convolutional neural networks. Feel free to use Adam for your other convolutional networks.

We are also saving the reconstructed images of the last iteration in every epoch. We want to look at these reconstructions at the end of training.

In [10]:

```
def train(model, num_epochs=5, batch_size=64, learning_rate=1e-3):
    torch.manual_seed(42)
    criterion = nn.MSELoss() # mean square error loss
    optimizer = torch.optim.Adam(model.parameters(),
                                 lr=learning_rate,
                                 weight_decay=1e-5) # <--
    train_loader = torch.utils.data.DataLoader(mnist_data,
                                               batch_size=batch_size,
                                               shuffle=True)
    outputs = []
    for epoch in range(num_epochs):
        for data in train_loader:
            img, _ = data
            recon = model(img)
            loss = criterion(recon, img)
            loss.backward()
            optimizer.step()
            optimizer.zero_grad()

        print('Epoch:{}, Loss:{:.4f}'.format(epoch+1, float(loss)))
        outputs.append((epoch, img, recon),)
    return outputs
```

Now, we can train this network.

In [11]:

```
model = Autoencoder()
max_epochs = 20
outputs = train(model, num_epochs=max_epochs)
```

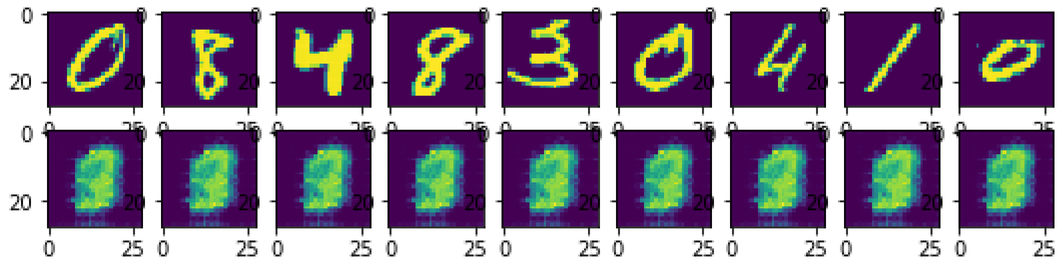
```
Epoch:1, Loss:0.0740
Epoch:2, Loss:0.0659
Epoch:3, Loss:0.0689
Epoch:4, Loss:0.0638
Epoch:5, Loss:0.0613
Epoch:6, Loss:0.0545
Epoch:7, Loss:0.0411
Epoch:8, Loss:0.0320
Epoch:9, Loss:0.0244
Epoch:10, Loss:0.0194
Epoch:11, Loss:0.0197
Epoch:12, Loss:0.0157
Epoch:13, Loss:0.0125
Epoch:14, Loss:0.0124
Epoch:15, Loss:0.0101
Epoch:16, Loss:0.0100
Epoch:17, Loss:0.0086
Epoch:18, Loss:0.0085
Epoch:19, Loss:0.0078
Epoch:20, Loss:0.0077
```

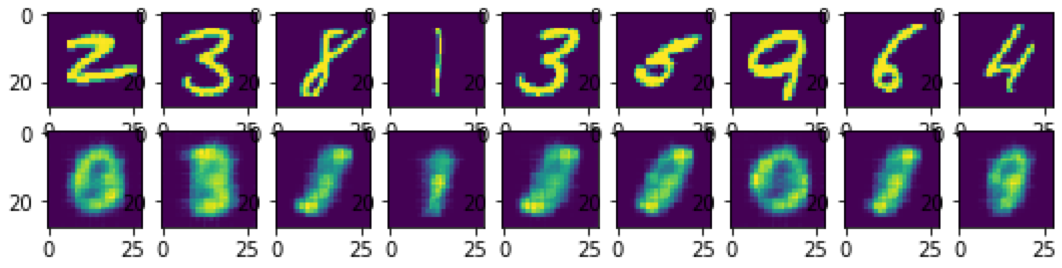
The loss goes down as we train, meaning that our reconstructed images look more and more like the actual images!

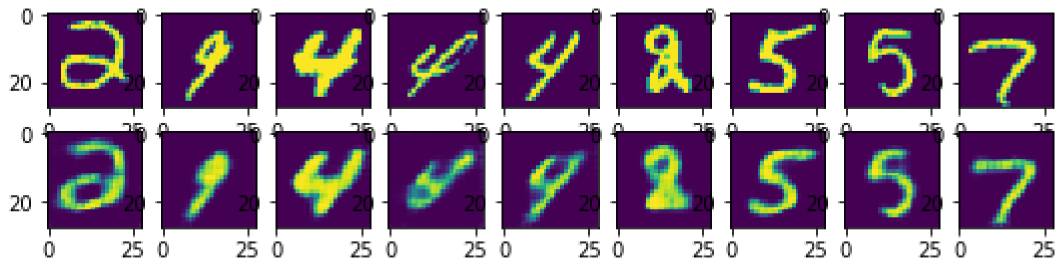
Let's look at the training progression: that is, the reconstructed images at various points of training:

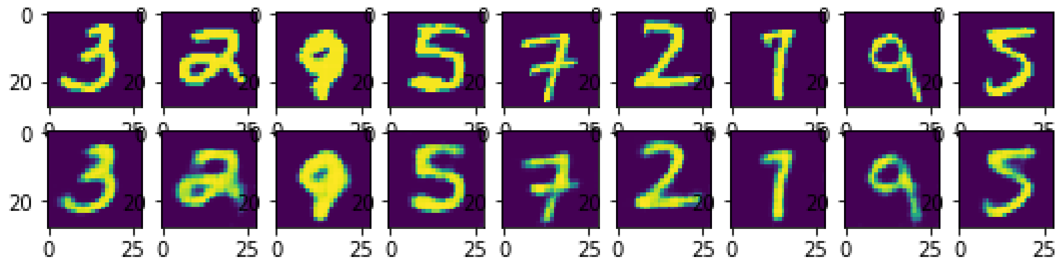
In [12]:

```
for k in range(0, max_epochs, 5):
    plt.figure(figsize=(9, 2))
    imgs = outputs[k][1].detach().numpy()
    recon = outputs[k][2].detach().numpy()
    for i, item in enumerate(imgs):
        if i >= 9: break
        plt.subplot(2, 9, i+1)
        plt.imshow(item[0])

    for i, item in enumerate(recon):
        if i >= 9: break
        plt.subplot(2, 9, 9+i+1)
        plt.imshow(item[0])
```









At first, the reconstructed images look nothing like the originals. Rather, the reconstructions look more like the average of some training images. As training progresses, our reconstructions are clearer.

Structure in the Embeddings

Since we are drastically reducing the dimensionality of the image, there has to be some kind of structure in the embedding space. That is, the network should be able to "save" space by mapping similar images to similar embeddings.

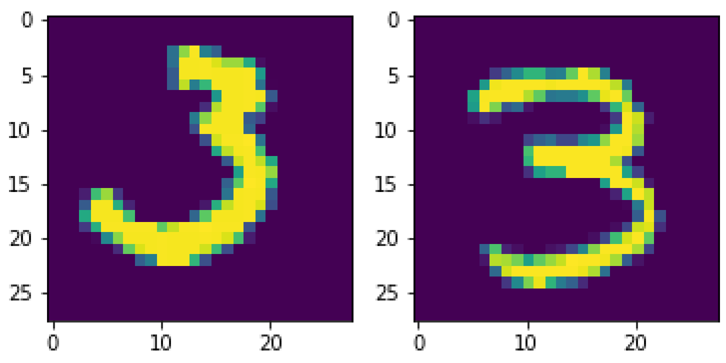
We will demonstrate the structure of the embedding space by hving some fun with our autoencoders. Let's begin with two images in our training set. For now, we'll choose images of the same digit.

In [13]:

```
imgs = outputs[max_epochs-1][1].detach().numpy()
plt.subplot(1, 2, 1)
plt.imshow(imgs[0][0])
plt.subplot(1, 2, 2)
plt.imshow(imgs[8][0])
```

Out[13]:

```
<matplotlib.image.AxesImage at 0x11da3c5c0>
```



We will then compute the **low-dimensional embeddings** of both images, by applying the **encoder**:

In [14]:

```
x1 = outputs[max_epochs-1][1][0,:,:,:] # first image
x2 = outputs[max_epochs-1][1][8,:,:,:] # second image
x = torch.stack([x1,x2])     # stack them together so we only call `encoder` once
embedding = model.encoder(x)
e1 = embedding[0] # embedding of first image
e2 = embedding[1] # embedding of second image
```

Now we will do something interesting. Not only are we goign to run the decoder on those two embeddings e1 and e2, we are also going to **interpolate** between the two embeddings and decode those as well!

In [15]:

```
embedding_values = []
for i in range(0, 10):
    e = e1 * (i/10) + e2 * (10-i)/10
    embedding_values.append(e)
embedding_values = torch.stack(embedding_values)

recons = model.decoder(embedding_values)
```

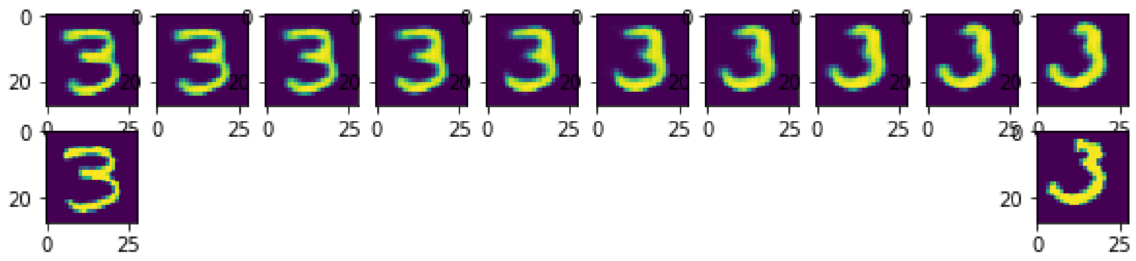
Let's plot the reconstructions of each interpolated values. The original images are shown below too:

In [16]:

```
plt.figure(figsize=(10, 2))
for i, recon in enumerate(recons.detach().numpy()):
    plt.subplot(2,10,i+1)
    plt.imshow(recon[0])
plt.subplot(2,10,11)
plt.imshow(imgs[8][0])
plt.subplot(2,10,20)
plt.imshow(imgs[0][0])
```

Out[16]:

```
<matplotlib.image.AxesImage at 0x11dd127f0>
```

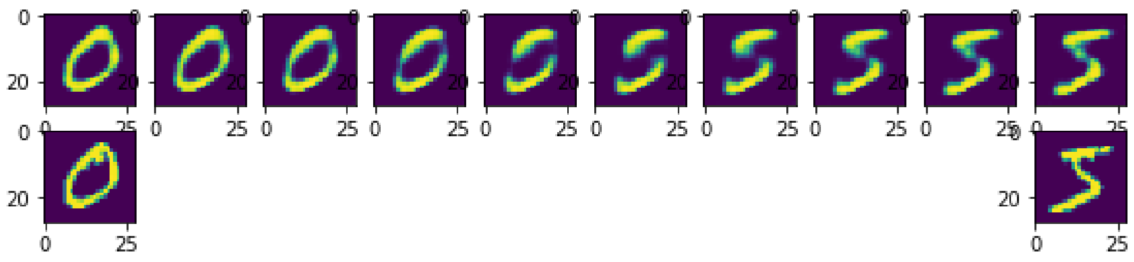


Notice that there is a smooth transition between the two images! The middle images are likely new, in that there are no training images that are exactly like any of the generated images.

As promised, we can do the same thing with two images containing different digits. There should be a smooth transition between the two digits.

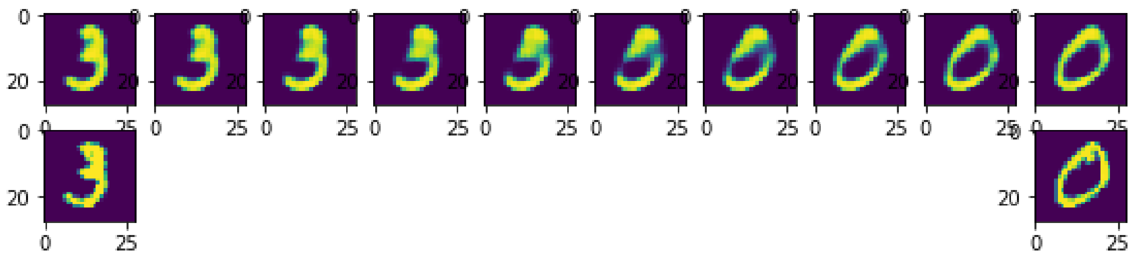
In [17]:

```
def interpolate(index1, index2):
    x1 = mnist_data[index1][0]
    x2 = mnist_data[index2][0]
    x = torch.stack([x1,x2])
    embedding = model.encoder(x)
    e1 = embedding[0] # embedding of first image
    e2 = embedding[1] # embedding of second image


    embedding_values = []
    for i in range(0, 10):
        e = e1 * (i/10) + e2 * (10-i)/10
        embedding_values.append(e)
    embedding_values = torch.stack(embedding_values)

    recons = model.decoder(embedding_values)

    plt.figure(figsize=(10, 2))
    for i, recon in enumerate(recons.detach().numpy()):
        plt.subplot(2,10,i+1)
        plt.imshow(recon[0])
    plt.subplot(2,10,11)
    plt.imshow(x2[0])
    plt.subplot(2,10,20)
    plt.imshow(x1[0])

interpolate(0, 1)
```



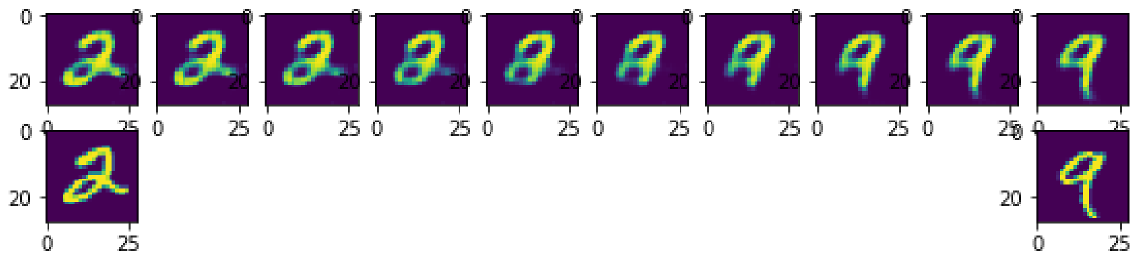
In [18]:

```
interpolate(1, 10)
```



In [19]:

```
interpolate(4, 5)
```



In [20]:

```
interpolate(20, 30)
```