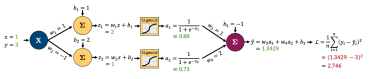
572 Quiz 2

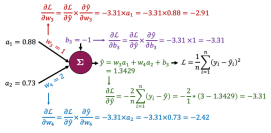
Backpropagation

Basic concept

- It is to calculate the gradient of the loss function with respect to the weights
- It is a special case of the chain rule of calculus
- **Process:**
  1. Do *forward pass* to calculate the output of the network (prediction and loss)



  2. Do *backward pass* to calculate the gradients of the loss function with respect to the weights. Below is an example of reverse-mode autmatic differentiation (backpropagation):



Torch: Autograd

- `torch.autograd` is PyTorch's automatic differentiation engine that powers neural network training

Vanishing and Exploding Gradients

- Backpropagation can suffer from two problems because of multiple chain rule applications:
  - **Vanishing gradients**: the gradients of the loss function with respect to the weights become very small
    - 0 gradients because of underflow
  - **Exploding gradients**: the gradients of the loss function with respect to the weights become very large
- Possible solutions:
  - Use **ReLU** activation function: but it can also suffer from the dying ReLU problem (gradients are 0)
  - **Weight initialization**: initialize the weights with small values
  - **Batch normalization**: normalize the input layer by adjusting and scaling the activations
  - **Skip connections**: add connections that skip one or more layers
  - **Gradient clipping**: clip the gradients during backpropagation

Training Neural Networks in PyTorch

Preventing Overfitting

- Add validation loss to the training loop
- **Early stopping**: if we see the validation loss is increasing, we stop training
  - Define a patience parameter: if the validation loss increases for `patience` epochs, we stop training
- **Regularization**: add a penalty term to the loss function to prevent overfitting
  - See 573 notes for more details
  - `weight_decay` parameter in the optimizer
- **Dropout**: randomly set some neurons to 0 during training
  - It prevents overfitting by reducing the complexity of the model
  - `torch.nn.Dropout(0.2)`

PyTorch Trainer Code

```
import torch
import torch.nn as nn

def trainer(model, criterion, optimizer, trainloader, validloader, epochs=5, patience=5):
    """Simple training wrapper for PyTorch network."""

    train_loss = []
    valid_loss = []

    for epoch in range(epochs):  # for each epoch
        train_batch_loss = 0
        valid_batch_loss = 0

        # Training
        for X, y in trainloader:
            optimizer.zero_grad()       # Zero all the gradients w.r.t. parameters
            y_hat = model(X).flatten()  # Forward pass to get output
            loss = criterion(y_hat, y)  # Calculate loss based on output
            loss.backward()             # Calculate gradients w.r.t. parameters
            optimizer.step()            # Update parameters

            train_batch_loss += loss.item()  # Add loss for this batch to running total
        train_loss.append(train_batch_loss / len(trainloader))

        # Validation
        with torch.no_grad():  # this stops pytorch doing computational graph stuff under

            for X_valid, y_valid in validloader:
                y_hat = model(X_valid).flatten()  # Forward pass to get output
                loss = criterion(y_hat, y_valid)  # Calculate loss based on output
                valid_batch_loss += loss.item()
        valid_loss.append(valid_batch_loss / len(validloader))

        # Early stopping
        if epoch > 0 and valid_loss[-1] > valid_loss[-2]:
            consec_increases += 1
        else:
            consec_increases = 0
        if consec_increases == patience:
            print(f"Stopped early at epoch {epoch + 1} - val loss increased for {consec_i
            break

    return train_loss, valid_loss
```

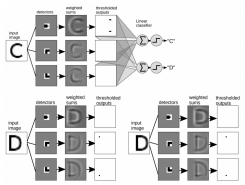
- Using the `trainer` function:

```
import torch
import torch.nn
import torch.optim

torch.manual_seed(1)

model = network(1, 6, 1)
criterion = torch.nn.MSELoss()
optimizer = torch.optim.Adam(model.parameters(), lr=0.05) # weight_decay=0.01 for L2 regu
train_loss, valid_loss = trainer(model, criterion, optimizer, trainloader, validloader, e

plot_loss(train_loss, valid_loss)
```

Universal Approximation Theorem

- Any continuous function can be approximated arbitrarily well by a neural network with a single hidden layer
  - In other words, NN are universal function approximators

Convolutional Neural Networks (CNN)

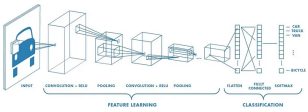


- Drastically reduces the number of params (compared to NN):
  - have activations depend on small number of inputs
  - same parameters (convolutional filter) are used for different parts of the image
- Can capture spatial information (preserves the structure of the image)

Convolution

- Idea: use a small filter/kernel to extract features from the image
  - Filter: a small matrix of weights (normally odd dimensioned -> for symmetry)
- Notice that the filter results in a smaller output image
  - This is because we are not padding the image
  - We can add padding to the image to keep the same size
    - Padding: add zeros around the image
  - Can also add stride to move the filter more than 1 pixel at a time

CNN Structure



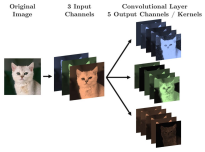
img src

CNN in PyTorch

1. Convolutional Layer

```
conv_1 = torch.nn.Conv2d(in_channels=1, out_channels=6, kernel_size=(3,3))
```

- Arguments:
  - `in_channels`: number of input channels (gray scale image has 1 channel, RGB has 3)
  - `out_channels`: number of output channels (similar to hidden nodes in NN)
  - `kernel_size`: size of the filter
  - `stride`: how many pixels to move the filter each time
  - `padding`: how many pixels to add around the image



- Size of input image (e.g. 256x256) doesn't matter, what matters is: `in_channels`, `out_channels`, `kernel_size`

$$\text{total params} = (\text{out channels} \times \text{in channels} \times \text{kernel size}^2) + \text{out channels}$$

$$\text{output size} = \frac{\text{input size} - \text{kernel size} + 2 \times \text{padding}}{\text{stride}} + 1$$

Dimensions of images and kernel tensors in PyTorch

- Images: `[batch_size, channels, height, width]`
- Kernel: `[out_channels, in_channels, kernel_height, kernel_width]`

2. Flattening

- `feature learning` -> `classification`
- Use `torch.nn.Flatten()` to flatten the image
- At the end need to either do regression or classification

3. Pooling

- Idea: reduce the size of the image
  - less params
  - less overfitting
- Common types:
  - **Max pooling**: take the max value in each region
    - Works well since it takes the sharpest features
  - **Average pooling**: take the average value in each region

Putting it all together

```
class CNN(torch.nn.Module):
    def __init__(self):
        super().__init__()
        self.main = torch.nn.Sequential(

            torch.nn.Conv2d(in_channels=1,
                out_channels=3,
                kernel_size=(3, 3),
                padding=1),
            torch.nn.ReLU(), # activation function
            torch.nn.MaxPool2d((2, 2)),

            torch.nn.Conv2d(in_channels=3,
                out_channels=2,
                kernel_size=(3, 3),
                padding=1),
            torch.nn.ReLU(),
            torch.nn.MaxPool2d((2, 2)),

            torch.nn.Flatten(),
            torch.nn.Linear(1250, 1)
        )

    def forward(self, x):
        out = self.main(x)
        return out
```

- Trainer code is the same as before

Using torchsummary

- To get a summary of the model
  - No need to manually calculate the output size of each layer

```
from torchsummary import summary

model = CNN()
summary(model, (1, 256, 256))
```

Preparing Data

Turning images to tensors

- Normally there are 2 steps:
  1. create a `dataset` object: the raw data
  2. create a `dataloader` object: batches the data, shuffles, etc.
- Use `torchvision` to load the data
  - `torchvision.datasets.ImageFolder`: loads images from folders
  - Assumes structure: `root/class_1/xxx.png`, `root/class_2/xxx.png`, ...

```
import torch
from torchvision import datasets, transforms

IMAGE_SIZE = (256, 256)
BATCH_SIZE = 32

# create transform object
data_transforms = transforms.Compose([
    transforms.Resize(IMAGE_SIZE),
    transforms.ToTensor()
])

# create dataset object
train_dataset = datasets.ImageFolder(root='path/to/data', transform=data_transforms)

# check out the data
train_dataset.classes # list of classes
train_dataset.targets # list of labels
train_dataset.samples # list of (path, label) tuples

# create dataloader object
train_loader = torch.utils.data.DataLoader(
    train_dataset,          # our raw data
    batch_size=BATCH_SIZE,  # the size of batches we want the dataloader to return
    shuffle=True,           # shuffle our data before batching
    drop_last=False         # don't drop the last batch even if it's smaller than batch_s
)

# get a batch of data
images, labels = next(iter(train_loader))
```

Saving and loading PyTorch models

- PyTorch documentation
- Convention: `.pt` or `.pth` file extension

```
PATH = "models/my_cnn.pt"

# load model
model = bitmoji_CNN() # must have defined the model class
model.load_state_dict(torch.load(PATH))
model.eval() # set model to evaluation mode (not training mode)

# save model
torch.save(model.state_dict(), PATH)
```

Data augmentation

- To make CNN more robust to different images + increase the size of the dataset
- Common augmentations:
  - Crop
  - Rotate
  - Flip
  - Color jitter

```
data_transforms = transforms.Compose([
    transforms.Resize(IMAGE_SIZE),
    transforms.RandomVerticalFlip(p=0.5), # p=0.5 means 50% chance of applying this augme
    transforms.RandomHorizontalFlip(p=0.5),
    transforms.ToTensor()
])
```

Hyperparameter Tuning

- NN has a lot of hyperparameters
  - Grid search will take a long time
  - Need a smarter approach: **Optimization Algorithms**
- Examples: Ax (we will use this), Raytune, Neptune, skorch.

Transfer Learning

- Idea: use a pre-trained model and fine-tune it to our specific task
- Install from `torchvision.models`
  - All models have been trained on ImageNet dataset (224x224 images)
- See here for code

Approach 1: Adding layers to pre-trained model

```
densenet = models.densenet121(weights='DenseNet121_Weights.DEFAULT')

for param in densenet.parameters():  # Freeze parameters so we don't update them
    param.requires_grad = False
# can fine-tune to freeze only some layers

list(densenet.named_children())[-1] # check the last layer

# update the last layer
new_layers = nn.Sequential(
    nn.Linear(1024, 500),
    nn.ReLU(),
    nn.Linear(500, 1)
)
densenet.classifier = new_layers
```

Then train the model as usual.

```
densenet.to(device)
criterion = nn.BCEWithLogitsLoss()
optimizer = torch.optim.Adam(densenet.parameters(), lr=2e-3)
results = trainer(densenet, criterion, optimizer, train_loader, valid_loader, device, epo
```

Approach 2: Use Extracted Features in a New Model

- Idea:
  1. Take output from pre-trained model
  2. Feed output to a new model

```
def get_features(model, train_loader, valid_loader):
    """
    Extract features from both training and validation datasets using the provided model.

    This function passes data through a given neural network model to extract features. I
    to work with datasets loaded using PyTorch's DataLoader. The function operates under
    that gradients are not required, optimizing memory and computation for inference task
    """

    # Disable gradient computation for efficiency during inference
    with torch.no_grad():
        # Initialize empty tensors for training features and labels
        Z_train = torch.empty((0, 1024))  # Assuming each feature vector has 1024 element
        y_train = torch.empty((0))

        # Initialize empty tensors for validation features and labels
        Z_valid = torch.empty((0, 1024))
        y_valid = torch.empty((0))

        # Process training data
        for X, y in train_loader:
            # Extract features and concatenate them to the corresponding tensors
            Z_train = torch.cat((Z_train, model(X)), dim=0)
            y_train = torch.cat((y_train, y))

        # Process validation data
        for X, y in valid_loader:
            # Extract features and concatenate them to the corresponding tensors
```

```
            Z_valid = torch.cat((Z_valid, model(X)), dim=0)
            y_valid = torch.cat((y_valid, y))

    # Return the feature and label tensors
    return Z_train, y_train, Z_valid, y_valid
```

Now we can use the extracted features to train a new model.

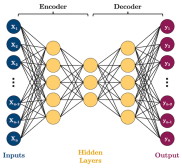
```
# Extract features from the pre-trained model
densenet = models.densenet121(weights='DenseNet121_Weights.DEFAULT')
densenet.classifier = nn.Identity()  # remove that last "classification" layer
Z_train, y_train, Z_valid, y_valid = get_features(densenet, train_loader, valid_loader)

# Train a new model using the extracted features
# Let's scale our data
scaler = StandardScaler()
Z_train = scaler.fit_transform(Z_train)
Z_valid = scaler.transform(Z_valid)

# Fit a model
model = LogisticRegression(max_iter=1000)
model.fit(Z_train, y_train)
```

Advanced CNN

Generative vs Discriminative Models

Generative Models	Discriminative Models
Directly model the joint probability distribution of the input and output	Model the conditional probability of the output given the input
Directly model $P(y\|x)$	Estimate $P(x\|y)$ to then deduce $P(y\|x)$
Build model for each class	Make boundary between classes
"Generate or draw a cat"	"Distinguish between cats and dogs"
Examples: Naïbe bayes, ChatGPT	Examples: Logistic Regression, SVM, Tree based models, CNN

Autoencoders



- Designed to reconstruct the input
- Encoder and a decoder
- Why do we need autoencoders?
  - Dimensionality reduction
  - Denoising

Dimensionality Reduction

- Maybe the z axis is unimportant in the input space for classification

```
from torch import nn

class autoencoder(torch.nn.Module):
    def __init__(self, input_size, hidden_size):
        super().__init__()
        self.encoder = nn.Sequential(
            nn.Linear(input_size, 2),
            nn.Sigmoid()
        )
        self.decoder = nn.Sequential(
            nn.Linear(2, input_size),
            nn.Sigmoid()
        )

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

```
# Set up the training
BATCH_SIZE = 100
torch.manual_seed(1)
X_tensor = torch.tensor(X, dtype=torch.float32)
dataloader = DataLoader(X_tensor,
                        batch_size=BATCH_SIZE)
model = autoencoder(3, 2)
criterion = nn.MSELoss()
optimizer = optim.Adam(model.parameters())

# Train the model
EPOCHS = 5

for epoch in range(EPOCHS):
    for batch in dataloader:
        optimizer.zero_grad()           # Clear gradients w.r.t. parameters
        y_hat = model(batch)            # Forward pass to get output
        loss = criterion(y_hat, batch)  # Calculate loss
        loss.backward()                 # Getting gradients w.r.t. parameters
        optimizer.step()                # Update parameters

# Use encoder
model.eval()
X_encoded = model.encoder(X_tensor)
```

Denoising

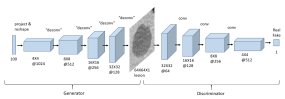
- Remove noise from the input
- Use *Transposed Convolution Layers* to upsample the input
  - Normal convolution: downsample (output is smaller than input)
  - Transposed convolution: upsample (output is larger than input)

```
def conv_block(input_channels, output_channels):
    return nn.Sequential(
        nn.Conv2d(input_channels, output_channels, 3, padding=1),
        nn.ReLU(),
        nn.MaxPool2d(2)  # reduce x-y dims by two; window and stride of 2
    )

def deconv_block(input_channels, output_channels, kernel_size):
    return nn.Sequential(
        nn.ConvTranspose2d(input_channels, output_channels, kernel_size, stride=2),
        nn.ReLU()
    )

class autoencoder(torch.nn.Module):
    def __init__(self):
        super().__init__()
        self.encoder = nn.Sequential(
            conv_block(1, 32),
            conv_block(32, 16),
            conv_block(16, 8)
        )
        self.decoder = nn.Sequential(
            deconv_block(8, 8, 3),
            deconv_block(8, 16, 2),
            deconv_block(16, 32, 2),
            nn.Conv2d(32, 1, 3, padding=1)  # final conv layer to decrease channel back t
        )

    def forward(self, x):
        x = self.encoder(x)
        x = self.decoder(x)
        x = torch.sigmoid(x)  # get pixels between 0 and 1
        return x
```

```
# Set up the training
EPOCHS = 20
criterion = nn.MSELoss()
optimizer = torch.optim.Adam(model.parameters())
img_list = []

for epoch in range(EPOCHS):
    losses = 0
    for batch, _ in trainloader:
        noisy_batch = batch + noise * torch.randn(*batch.shape)
        noisy_batch = torch.clip(noisy_batch, 0.0, 1.0)
        optimizer.zero_grad()
        y_hat = model(noisy_batch)
        loss = criterion(y_hat, batch)
        loss.backward()
        optimizer.step()
        losses += loss.item()
    print(f"epoch: {epoch + 1}, loss: {losses / len(trainloader):.4f}")
    # Save example results each epoch so we can see what's going on
    with torch.no_grad():
        noisy_8 = noisy_batch[:1, :1, :, :]
        model_8 = model(input_8)
        real_8 = batch[:1, :1, :, :]
    img_list.append(utils.make_grid([noisy_8[0], model_8[0], real_8[0]], padding=1))```
```

Generative Adversarial Networks (GANs)

- Model used to generate new data (indistinguishable from real data)
- No need for labels (unsupervised learning)
- See here



- Two networks:
  - Generator: creates new data
  - Discriminator: tries to distinguish between real and fake data
- Both are battling each other:
  - Generator tries to create data that the discriminator can't distinguish from real data
  - Discriminator tries to distinguish between real and fake data

Training GANs

1. Train the discriminator (simple binary classification)
   - Train the discriminator on real data
   - Train the discriminator on fake data (generated by the generator)
2. Train the generator
   - Generate fake images with the generator and label them as real
   - Pass to discriminator and ask it to classify them (real or fake)
   - Pass judgement to a loss function (see how far it is from the ideal output)
     - ideal output: all fake images are classified as real
   - Do backpropagation and update the generator
3. Repeat

Pytorch Implementation

1. Creating the data loader

```
DATA_DIR = "../input/face-recognition-dataset/Extracted Faces"

BATCH_SIZE = 64
IMAGE_SIZE = (128, 128)

data_transforms = transforms.Compose([
    transforms.Resize(IMAGE_SIZE), # uses CPU (bottleneck)
    transforms.ToTensor(),
    transforms.Normalize((0.5, 0.5, 0.5), (0.5, 0.5, 0.5))
])

dataset = datasets.ImageFolder(root=DATA_DIR, transform=data_transforms)
data_loader = torch.utils.data.DataLoader(dataset, batch_size=BATCH_SIZE, shuffle=Tru
```

2. Creating the generator

```
class Generator(nn.Module):

 def __init__(self, LATENT_SIZE):
     super(Generator, self).__init__()

     self.main = nn.Sequential(
         nn.ConvTranspose2d(LATENT_SIZE, 1024, kernel_size=4, stride=1, padding=0, bi
         nn.BatchNorm2d(1024),
         nn.LeakyReLU(0.2, inplace=True),

     ...

         nn.ConvTranspose2d(128, 3, kernel_size=4, stride=2, padding=1, bias=False),
         nn.BatchNorm2d(3),

         nn.Tanh()
     )

 def forward(self, input):
     return self.main(input)
```

3. Creating the discriminator

```
class Discriminator(nn.Module):

 def __init__(self):
     super(Discriminator, self).__init__()

     self.main = nn.Sequential(
         nn.Conv2d(3, 128, kernel_size=4, stride=2, padding=1, bias=False),
         nn.BatchNorm2d(128),
         nn.LeakyReLU(0.2, inplace=True),

         ...

         nn.Conv2d(512, 1, kernel_size=4, stride=1, padding=0, bias=False),
         nn.Flatten(),
         nn.Sigmoid()
     )

 def forward(self, input):
     return self.main(input)
```

4. Instantiating the models

```
device = torch.device('mps' if torch.backends.mps.is_available() else 'cpu')

LATENT_SIZE = 100
generator = Generator(LATENT_SIZE).to(device)
discriminator = Discriminator().to(device)

criterion = nn.BCELoss()

optimizerG = optim.Adam(generator.parameters(), lr=0.001, betas=(0.5, 0.999))
optimizerD = optim.Adam(discriminator.parameters(), lr=0.001, betas=(0.5, 0.999))

 def weights_init(m):
     if isinstance(m, (nn.Conv2d, nn.ConvTranspose2d)):
         nn.init.normal_(m.weight.data, 0.0, 0.02)
     elif isinstance(m, nn.BatchNorm2d):
         nn.init.normal_(m.weight.data, 1.0, 0.02)
         nn.init.constant_(m.bias.data, 0)


 generator.apply(weights_init)
 discriminator.apply(weights_init);
```

5. Training the GAN

```
 img_list = []
fixed_noise = torch.randn(BATCH_SIZE, LATENT_SIZE, 1, 1).to(device)

 NUM_EPOCHS = 50
from statistics import mean
print('Training started:\n')

 D_real_epoch, D_fake_epoch, loss_dis_epoch, loss_gen_epoch = [], [], [], []

 for epoch in range(NUM_EPOCHS):
     D_real_iter, D_fake_iter, loss_dis_iter, loss_gen_iter = [], [], [], []

     for real_batch, _ in data_loader:

         # STEP 1: train discriminator
         # ================================
         optimizerD.zero_grad()

         real_batch = real_batch.to(device)
         real_labels = torch.ones((real_batch.shape[0],), dtype=torch.float).to(devic

         output = discriminator(real_batch).view(-1)
         loss_real = criterion(output, real_labels)

         # Iteration book-keeping
         D_real_iter.append(output.mean().item())

         # Train with fake data
         noise = torch.randn(real_batch.shape[0], LATENT_SIZE, 1, 1).to(device)

         fake_batch = generator(noise)
         fake_labels = torch.zeros_like(real_labels)

         output = discriminator(fake_batch.detach()).view(-1)
         loss_fake = criterion(output, fake_labels)

         # Update discriminator weights
         loss_dis = loss_real + loss_fake
         loss_dis.backward()
         optimizerD.step()

         # Iteration book-keeping
         loss_dis_iter.append(loss_dis.mean().item())
         D_fake_iter.append(output.mean().item())

         # STEP 2: train generator
         # ================================
         optimizerG.zero_grad()

         # Calculate the output with the updated weights of the discriminator
         output = discriminator(fake_batch).view(-1)
         loss_gen = criterion(output, real_labels)
         loss_gen.backward()

         # Book-keeping
         loss_gen_iter.append(loss_gen.mean().item())

         # Update generator weights and store loss
         optimizerG.step()

     print(f"Epoch ({epoch + 1}/{NUM_EPOCHS})\t",
         f"Loss_G: {mean(loss_gen_iter):.4f}",
         f"Loss_D: {mean(loss_dis_iter):.4f}\t",
         f"D_real: {mean(D_real_iter):.4f}",
         f"D_fake: {mean(D_fake_iter):.4f}")

     # Epoch book-keeping
     loss_gen_epoch.append(mean(loss_gen_iter))
     loss_dis_epoch.append(mean(loss_dis_iter))
     D_real_epoch.append(mean(D_real_iter))
     D_fake_epoch.append(mean(D_fake_iter))

     # Keeping track of the evolution of a fixed noise latent vector
     with torch.no_grad():
         fake_images = generator(fixed_noise).detach().cpu()
         #img_list.append(utils.make_grid(fake_images, normalize=True, nrows=10))

 print("\nTraining ended.")
```

6. Visualize training process

```
plt.plot(np.array(loss_gen_epoch), label='loss_gen')
plt.plot(np.array(loss_dis_epoch), label='loss_dis')
plt.xlabel("Epoch")
plt.ylabel("Loss")
plt.legend();
```

```
plt.plot(np.array(D_real_epoch), label='D_real')
plt.plot(np.array(D_fake_epoch), label='D_fake')
plt.xlabel("Epoch")
plt.ylabel("Probability")
plt.legend();
```

Multi-Input Networks

```
class multiModel(nn.Module):
    def __init__(self):
        super().__init__()
        ...

    def forward(self, image, data):
        x_cnn = self.cnn(image) # 1st model: CNN
        x_fc = self.fc(data) # 2nd model: Fully connected
        return torch.cat((x_cnn, x_fc), dim=1) # concatenate the two outputs
```