Advanced machine learning and data analysis for the physical sciences

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February 20, 2025

Plans for February 20

1. Implementing Convolutional Neural Networks (CNNs), own codes, TensorFlow+Keras and PyTorch examples
2. Start discussion of Recurrent Neural Networks (RNNs).
3. Link to project examples from 2024 at `https://github.com/CompPhysics/AdvancedMachineLearning/tree/main/doc/Projects/ProjectExamples`

Reading recommendations

1. For CNNs, see Goodfellow et al chapter 9. See also chapter 11 and 12 on practicalities and applications
2. For RNNs, see Goodfellow et al chapter 10.
3. Reading suggestions for implementation of CNNs in PyTorch: See Rashcka et al.'s chapter 14 and GitHub site.
4. Reading suggestions for implementation of RNNs in PyTorch: See Rashcka et al.'s chapter 15 and GitHub site.

TensorFlow examples

For TensorFlow (using Keras) implementations, we recommend

1. David Foster Generative Learning, see chapters 2 and 3 from the GitHub link

2. Joseph Babcock and Raghav Bali Generative AI with Python and their GitHub link, chapter 3

CNNs in brief

In summary:

- A CNN architecture is in the simplest case a list of Layers that transform the image volume into an output volume (e.g. holding the class scores)
- There are a few distinct types of Layers (e.g. CONV/FC/RELU/POOL are by far the most popular)
- Each Layer accepts an input 3D volume and transforms it to an output 3D volume through a differentiable function
- Each Layer may or may not have parameters (e.g. CONV/FC do, RELU/POOL don't)
- Each Layer may or may not have additional hyperparameters (e.g. CONV/FC/POOL do, RELU doesn't)

A deep CNN model (From Raschka et al)

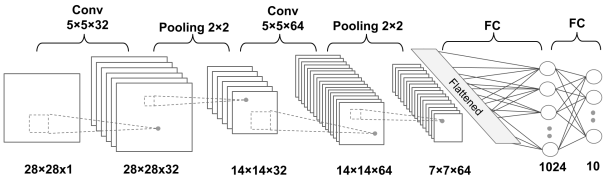


Figure 1: A deep CNN

Key Idea

A dense neural network is representd by an affine operation (like matrix-matrix multiplication) where all parameters are included.

The key idea in CNNs for say imaging is that in images neighbor pixels tend to be related! So we connect only neighboring neurons in the input instead of connecting all with the first hidden layer.

We say we perform a filtering (convolution is the mathematical operation).

How did we do image compression before the era of deep learning

The singular-value decomposition (SVD) algorithm has been for decades one of the standard ways of compressing images. The lectures on the SVD give many of the essential details concerning the SVD.

The orthogonal vectors which are obtained from the SVD, can be used to project down the dimensionality of a given image. In the example here we gray-scale an image and downsize it.

This recipe relies on us being able to actually perform the SVD. For large images, and in particular with many images to reconstruct, using the SVD may quickly become an overwhelming task. With the advent of efficient deep learning methods like CNNs and later generative methods, these methods have become in the last years the premier way of performing image analysis. In particular for classification problems with labelled images.

The SVD example

```python
from matplotlib.image import imread
import matplotlib.pyplot as plt
import scipy.linalg as ln
import numpy as np
import os
from PIL import Image
from math import log10, sqrt
plt.rcParams['figure.figsize'] = [16, 8]
# Import image
A = imread(os.path.join("figslides/photo1.jpg"))
X = A.dot([0.299, 0.5870, 0.114]) # Convert RGB to grayscale
img = plt.imshow(X)
# convert to gray
img.set_cmap('gray')
plt.axis('off')
plt.show()
# Call image size
print(': %s'%str(X.shape))


# split the matrix into U, S, VT
U, S, VT = np.linalg.svd(X,full_matrices=False)
S = np.diag(S)
m = 800 # Image's width
n = 1200 # Image's height
j = 0
# Try compression with different k vectors (these represent projections):
for k in (5,10, 20, 100,200,400,500):
    # Original size of the image
    originalSize = m * n
    # Size after compressed
    compressedSize = k * (1 + m + n)
    # The projection of the original image
    Xapprox = U[:,:k] @ S[0:k,:k] @ VT[:k,:]
    plt.figure(j+1)
    j += 1
    img = plt.imshow(Xapprox)
```

```
img.set_cmap('gray')

plt.axis('off')
plt.title('k = ' + str(k))
plt.show()
print('Original size of image:')
print(originalSize)
print('Compression rate as Compressed image / Original size:')
ratio = compressedSize * 1.0 / originalSize
print(ratio)
print('Compression rate is ' + str( round(ratio * 100 ,2)) + '%' )
# Estimate MQA
x= X.astype("float")
y=Xapprox.astype("float")
err = np.sum((x - y) ** 2)
err /= float(X.shape[0] * Xapprox.shape[1])
print('The mean-square deviation '+ str(round( err)))
max_pixel = 255.0
# Estimate Signal Noise Ratio
srv = 20 * (log10(max_pixel / sqrt(err)))
print('Signa to noise ratio '+ str(round(srv)) +'dB')
```

Examples of CNN setups

Let us assume we have an input volume V given by an image of dimensionality $32 \times 32 \times 3$, that is three color channels and 32×32 pixels.

We apply a filter of dimension 5×5 ten times with stride $S = 1$ and padding $P = 0$.

The output volume is given by $(32 - 5)/1 + 1 = 28$, resulting in ten images of dimensionality $28 \times 28 \times 3$.

The total number of parameters to train for each filter is then $5 \times 5 \times 3 + 1$, where the last parameter is the bias. This gives us 76 parameters for each filter, leading to a total of 760 parameters for the ten filters.

How many parameters will a filter of dimensionality 3×3 (adding color channels) result in if we produce 32 new images? Use $S = 1$ and $P = 0$.

Note that strides constitute a form of **subsampling**. As an alternative to being interpreted as a measure of how much the kernel/filter is translated, strides can also be viewed as how much of the output is retained. For instance, moving the kernel by hops of two is equivalent to moving the kernel by hops of one but retaining only odd output elements.

Summarizing: Performing a general discrete convolution (From Raschka et al)

Pooling

In addition to discrete convolutions themselves, **pooling** operations make up another important building block in CNNs. Pooling operations reduce the size of feature maps by using some function to summarize subregions, such as taking the average or the maximum value.

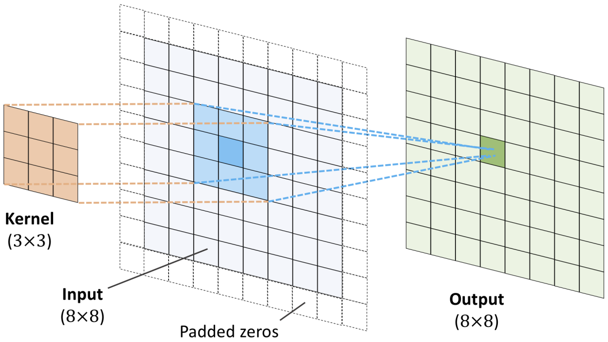


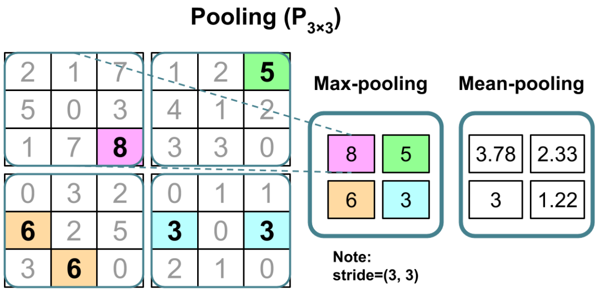
Figure 2: A deep CNN

Pooling works by sliding a window across the input and feeding the content of the window to a **pooling function**. In some sense, pooling works very much like a discrete convolution, but replaces the linear combination described by the kernel with some other function.

Pooling arithmetic

In a neural network, pooling layers provide invariance to small translations of the input. The most common kind of pooling is **max pooling**, which consists in splitting the input in (usually non-overlapping) patches and outputting the maximum value of each patch. Other kinds of pooling exist, e.g., mean or average pooling, which all share the same idea of aggregating the input locally by applying a non-linearity to the content of some patches.

Pooling types (From Raschka et al)



2	1	7	1	2	5
5	0	3	4	1	2
1	7	8	3	3	0
0	3	2	0	1	1
6	2	5	3	0	3
3	6	0	2	1	0

8	5
6	3

3.78	2.33
3	1.22

Figure 3: A deep CNN

Building convolutional neural networks in Tensorflow and Keras

As discussed above, CNNs are neural networks built from the assumption that the inputs to the network are 2D images. This is important because the number of features or pixels in images grows very fast with the image size, and an enormous number of weights and biases are needed in order to build an accurate network.

As before, we still have our input, a hidden layer and an output. What's novel about convolutional networks are the **convolutional** and **pooling** layers stacked in pairs between the input and the hidden layer. In addition, the data is no longer represented as a 2D feature matrix, instead each input is a number of 2D matrices, typically 1 for each color dimension (Red, Green, Blue).

Setting it up

It means that to represent the entire dataset of images, we require a 4D matrix or **tensor**. This tensor has the dimensions:

$$(n_{inputs}, n_{pixels,width}, n_{pixels,height}, depth).$$

The MNIST dataset again

The MNIST dataset consists of grayscale images with a pixel size of 28×28, meaning we require $28 \times 28 = 724$ weights to each neuron in the first hidden layer.

If we were to analyze images of size 128×128 we would require $128 \times 128 = 16384$ weights to each neuron. Even worse if we were dealing with color images, as most images are, we have an image matrix of size 128×128 for each color dimension (Red, Green, Blue), meaning 3 times the number of weights $= 49152$ are required for every single neuron in the first hidden layer.

Strong correlations

Images typically have strong local correlations, meaning that a small part of the image varies little from its neighboring regions. If for example we have an image of a blue car, we can roughly assume that a small blue part of the image is surrounded by other blue regions.

Therefore, instead of connecting every single pixel to a neuron in the first hidden layer, as we have previously done with deep neural networks, we can instead connect each neuron to a small part of the image (in all 3 RGB depth dimensions). The size of each small area is fixed, and known as a receptive.

Layers of a CNN

The layers of a convolutional neural network arrange neurons in 3D: width, height and depth. The input image is typically a square matrix of depth 3.

A **convolution** is performed on the image which outputs a 3D volume of neurons. The weights to the input are arranged in a number of 2D matrices, known as **filters**.

Each filter slides along the input image, taking the dot product between each small part of the image and the filter, in all depth dimensions. This is then passed through a non-linear function, typically the **Rectified Linear (ReLu)** function, which serves as the activation of the neurons in the first convolutional layer. This is further passed through a **pooling layer**, which reduces the size of the convolutional layer, e.g. by taking the maximum or average across some small regions, and this serves as input to the next convolutional layer.

Systematic reduction

By systematically reducing the size of the input volume, through convolution and pooling, the network should create representations of small parts of the input, and then from them assemble representations of larger areas. The final pooling layer is flattened to serve as input to a hidden layer, such that each neuron in the final pooling layer is connected to every single neuron in the hidden layer. This then serves as input to the output layer, e.g. a softmax output for classification.

Initialize TensorFlow

```
from tensorflow.keras import datasets, layers, models
from tensorflow.keras.layers import Input
from tensorflow.keras.models import Sequential      #This allows appending layers to existing mode
from tensorflow.keras.layers import Dense           #This allows defining the characteristics of
from tensorflow.keras import optimizers             #This allows using whichever optimiser we wan
from tensorflow.keras import regularizers           #This allows using whichever regularizer we w
from tensorflow.keras.utils import to_categorical   #This allows using categorical cross entropy
```

Example of how we can up a model (without a specific image)

The 6 lines of code below define the convolutional base using a common pattern: a stack of Conv2D and MaxPooling2D layers.

As input, a CNN takes tensors of shape (image_height, image_width, color_channels), ignoring the batch size. If you are new to these dimensions, color_channels refers to (R,G,B). In this example, you will configure the CNN to process inputs of shape (32, 32, 3) as an example. You can do this by passing the argument input_shape to our first layer.

```
model = models.Sequential()
model.add(layers.Conv2D(32, (3, 3), activation='relu', input_shape=(32, 32, 3)))
model.add(layers.MaxPooling2D((2, 2)))
model.add(layers.Conv2D(64, (3, 3), activation='relu'))
model.add(layers.MaxPooling2D((2, 2)))
model.add(layers.Conv2D(64, (3, 3), activation='relu'))
# Here we  display the architecture of our model so far.
model.summary()
```

You can see that the output of every Conv2D and MaxPooling2D layer is a 3D tensor of shape (height, width, channels). The width and height dimensions tend to shrink as you go deeper in the network. The number of output channels for each Conv2D layer is controlled by the first argument (e.g., 32 or 64). Typically, as the width and height shrink, you can afford (computationally) to add more output channels in each Conv2D layer.

Add Dense layers on top

To complete this model, you will feed the last output tensor from the convolutional base (of shape (4, 4, 64)) into one or more Dense layers to perform classification. Dense layers take vectors as input (which are 1D), while the current output is a 3D tensor. First, you will flatten (or unroll) the 3D output to 1D, then add one or more dense layers on top. The MNIST data discussed below has 10 output classes, so we would use a final dense layer with 10 outputs and a softmax activation.

```
model.add(layers.Flatten())
model.add(layers.Dense(64, activation='relu'))
model.add(layers.Dense(10))
# Now we list  the complete architecture of our model.
model.summary()
```

As you can see, our (4, 4, 64) outputs were flattened into vectors of shape (1024) before going through two Dense layers.

Prerequisites: Collect and pre-process data

Now we switch to the MNIST data set.

```
# import necessary packages
import numpy as np
import matplotlib.pyplot as plt
from sklearn import datasets


# ensure the same random numbers appear every time
np.random.seed(0)

# display images in notebook
%matplotlib inline
plt.rcParams['figure.figsize'] = (12,12)


# download MNIST dataset
digits = datasets.load_digits()

# define inputs and labels
inputs = digits.images
labels = digits.target

# RGB images have a depth of 3
# our images are grayscale so they should have a depth of 1
```

```
inputs = inputs[:,:,:,np.newaxis]

print("inputs = (n_inputs, pixel_width, pixel_height, depth) = " + str(inputs.shape))
print("labels = (n_inputs) = " + str(labels.shape))


# choose some random images to display
n_inputs = len(inputs)
indices = np.arange(n_inputs)
random_indices = np.random.choice(indices, size=5)

for i, image in enumerate(digits.images[random_indices]):
    plt.subplot(1, 5, i+1)
    plt.axis('off')
    plt.imshow(image, cmap=plt.cm.gray_r, interpolation='nearest')
    plt.title("Label: %d" % digits.target[random_indices[i]])
plt.show()
```

Importing Keras and Tensorflow

```
from tensorflow.keras import datasets, layers, models
from tensorflow.keras.layers import Input
from tensorflow.keras.models import Sequential      #This allows appending layers to existing mode
from tensorflow.keras.layers import Dense           #This allows defining the characteristics of
from tensorflow.keras import optimizers             #This allows using whichever optimiser we wan
from tensorflow.keras import regularizers           #This allows using whichever regularizer we w
from tensorflow.keras.utils import to_categorical   #This allows using categorical cross entropy
from sklearn.model_selection import train_test_split

# representation of labels
labels = to_categorical(labels)

# split into train and test data
# one-liner from scikit-learn library
train_size = 0.8
test_size = 1 - train_size
X_train, X_test, Y_train, Y_test = train_test_split(inputs, labels, train_size=train_size,
                                                    test_size=test_size)
```

Running with Keras and setting up the model

```
def create_convolutional_neural_network_keras(input_shape, receptive_field,
                                              n_filters, n_neurons_connected, n_categories,
                                              eta, lmbd):
    model = Sequential()
    model.add(layers.Conv2D(n_filters, (receptive_field, receptive_field), input_shape=input_shape
              activation='relu', kernel_regularizer=regularizers.l2(lmbd)))
    model.add(layers.MaxPooling2D(pool_size=(2, 2)))
    model.add(layers.Flatten())
    model.add(layers.Dense(n_neurons_connected, activation='relu', kernel_regularizer=regularizers
    model.add(layers.Dense(n_categories, activation='softmax', kernel_regularizer=regularizers.l2

    sgd = optimizers.SGD(learning_rate=eta)
    model.compile(loss='categorical_crossentropy', optimizer=sgd, metrics=['accuracy'])

    return model
#model.summary()
```

```
epochs = 100
batch_size = 100
input_shape = X_train.shape[1:4]
receptive_field = 3
n_filters = 10
n_neurons_connected = 50
n_categories = 10

eta_vals = np.logspace(-5, 1, 7)
lmbd_vals = np.logspace(-5, 1, 7)
```

Final part

```
CNN_keras = np.zeros((len(eta_vals), len(lmbd_vals)), dtype=object)

for i, eta in enumerate(eta_vals):
    for j, lmbd in enumerate(lmbd_vals):
        CNN = create_convolutional_neural_network_keras(input_shape, receptive_field,
                                              n_filters, n_neurons_connected, n_categories,
                                              eta, lmbd)
        CNN.fit(X_train, Y_train, epochs=epochs, batch_size=batch_size, verbose=0)
        scores = CNN.evaluate(X_test, Y_test)

        CNN_keras[i][j] = CNN

        print("Learning rate = ", eta)
        print("Lambda = ", lmbd)
        print("Test accuracy: %.3f" % scores[1])
        print()
```

Final visualization

```
# visual representation of grid search
# uses seaborn heatmap, could probably do this in matplotlib
import seaborn as sns

sns.set()

train_accuracy = np.zeros((len(eta_vals), len(lmbd_vals)))
test_accuracy = np.zeros((len(eta_vals), len(lmbd_vals)))

for i in range(len(eta_vals)):
    for j in range(len(lmbd_vals)):
        CNN = CNN_keras[i][j]

        train_accuracy[i][j] = CNN.evaluate(X_train, Y_train)[1]
        test_accuracy[i][j] = CNN.evaluate(X_test, Y_test)[1]


fig, ax = plt.subplots(figsize = (10, 10))
sns.heatmap(train_accuracy, annot=True, ax=ax, cmap="viridis")
ax.set_title("Training Accuracy")
ax.set_ylabel("$\eta$")
ax.set_xlabel("$\lambda$")
plt.show()

fig, ax = plt.subplots(figsize = (10, 10))
```

```
sns.heatmap(test_accuracy, annot=True, ax=ax, cmap="viridis")
ax.set_title("Test Accuracy")
ax.set_ylabel("$\eta$")
ax.set_xlabel("$\lambda$")
plt.show()
```

Finally, evaluate the model

```
plt.plot(history.history['accuracy'], label='accuracy')
plt.plot(history.history['val_accuracy'], label = 'val_accuracy')
plt.xlabel('Epoch')
plt.ylabel('Accuracy')
plt.ylim([0.5, 1])
plt.legend(loc='lower right')

test_loss, test_acc = model.evaluate(test_images,  test_labels, verbose=2)

print(test_acc)
```

Building code using Pytorch

This code loads and normalizes the MNIST dataset. Thereafter it defines a CNN architecture using PyTorch with:

1. Two convolutional layers
2. Max pooling
3. Dropout for regularization
4. Two fully connected layers

It uses the Adam optimizer and for cost function it employs the Cross-Entropy function. It trains for 10 epochs. You can modify the architecture (number of layers, channels, dropout rate) or training parameters (learning rate, batch size, epochs) to experiment with different configurations.

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

# Set device
device = torch.device("cuda" if torch.cuda.is_available() else "cpu")

# Define transforms
transform = transforms.Compose([
   transforms.ToTensor(),
   transforms.Normalize((0.1307,), (0.3081,))
])

# Load datasets
```

```
train_dataset = datasets.MNIST(root='./data', train=True, download=True, transform=transform)
test_dataset = datasets.MNIST(root='./data', train=False, download=True, transform=transform)

# Create data loaders
train_loader = torch.utils.data.DataLoader(train_dataset, batch_size=64, shuffle=True)
test_loader = torch.utils.data.DataLoader(test_dataset, batch_size=64, shuffle=False)

# Define CNN model
class CNN(nn.Module):
   def __init__(self):
       super(CNN, self).__init__()
       self.conv1 = nn.Conv2d(1, 32, 3, padding=1)
       self.conv2 = nn.Conv2d(32, 64, 3, padding=1)
       self.pool = nn.MaxPool2d(2, 2)
       self.fc1 = nn.Linear(64*7*7, 1024)
       self.fc2 = nn.Linear(1024, 10)
       self.dropout = nn.Dropout(0.5)

   def forward(self, x):
       x = self.pool(F.relu(self.conv1(x)))
       x = self.pool(F.relu(self.conv2(x)))
       x = x.view(-1, 64*7*7)
       x = self.dropout(F.relu(self.fc1(x)))
       x = self.fc2(x)
       return x

# Initialize model, loss function, and optimizer
model = CNN().to(device)
criterion = nn.CrossEntropyLoss()
optimizer = optim.Adam(model.parameters(), lr=0.001)

# Training loop
num_epochs = 10
for epoch in range(num_epochs):
   model.train()
   running_loss = 0.0
   for batch_idx, (data, target) in enumerate(train_loader):
       data, target = data.to(device), target.to(device)
       optimizer.zero_grad()
       outputs = model(data)
       loss = criterion(outputs, target)
       loss.backward()
       optimizer.step()
       running_loss += loss.item()

   print(f'Epoch [{epoch+1}/{num_epochs}], Loss: {running_loss/len(train_loader):.4f}')

# Testing the model
model.eval()
correct = 0
total = 0
with torch.no_grad():
   for data, target in test_loader:
       data, target = data.to(device), target.to(device)
       outputs = model(data)
       _, predicted = torch.max(outputs.data, 1)
       total += target.size(0)
       correct += (predicted == target).sum().item()

print(f'Test Accuracy: {100 * correct / total:.2f}%')
```

What is dropout?

Dropout is a regularization technique used to prevent overfitting in neural networks. During training, a randomly selected fraction (typically 20-50%) of neurons in each layer are temporarily deactivated (dropped out). This compels the network to distribute feature representation across multiple neurons instead of relying on a small subset.

Key benefits of Dropout:

1. Random Neuron Deactivation: Neurons are randomly ignored during each forward pass.
2. Overfitting Reduction: Encourages the learning of more robust data representations by preventing reliance on specific neurons.
3. Improved Robustness: At test time, all neurons are active, with weights scaled down to account for the training phase dropout rate.

Dropout is commonly applied after fully connected layers in CNNs, but can also be used after convolutional layers.

1. Application after convolutional layers: While less frequent, dropout can be applied between convolutional and pooling layers. The inherent regularization provided by shared weights and pooling in convolutional layers already mitigates overfitting.
2. Application after fully connected Layers: Dropout is typically applied to fully connected layers due to the increased risk of overfitting caused by the large number of parameters.

Building our own CNN code

Here we present a flexible and readable python code for a CNN implemented with NumPy. We will present the code, showcase how to use the codebase and fit a CNN that yields a 99% accuracy on the 28x28 MNIST dataset within reasonable time.

The codes here were developed by Eric Reber and Gregor Kajda during spring 2023.

The CNN is compatible with all schedulers, cost functions and activation functions discussed in constructing our neural network codes.

The CNN code consists of different types of Layer classes, including Convolution2DLayer, Pooling2DLayer, FlattenLayer, FullyConnectedLayer and OutputLayer, which can be added to the CNN object using the interface of the CNN class. This allows you to easily construct your own CNN, as well as allowing you to get used to an interface similar to that of TensorFlow which is used for real world applications.

Another important feature of this code is that it throws errors if unreasonable decisions are made (for example using a kernel that is larger than the image, not using a FlattenLayer, etc), and provides the user with an informative error message.

List of contents:

1. Schedulers
2. Activation Functions
3. Cost Functions
4. Convolution
5. Layers
6. CNN
7. Some final remarks

Schedulers. The code below shows object oriented implementations of the Constant, Momentum, Adagrad, AdagradMomentum, RMS prop and Adam schedulers. All of the classes belong to the shared abstract Scheduler class, and share the update_change() and reset() methods allowing for any of the schedulers to be seamlessly used during the training stage, as will later be shown in the fit() method of the neural network. The function Update_change() only has one parameter, the gradient $(\delta_j^l a_k^{l-1})$, and returns the change which will be subtracted from the weights. The reset() function takes no parameters, and resets the desired variables. For Constant and Momentum, reset does nothing.

```
import autograd.numpy as np

class Scheduler:
    """
    Abstract class for Schedulers
    """

    def __init__(self, eta):
        self.eta = eta

    # should be overwritten
    def update_change(self, gradient):
        raise NotImplementedError

    # overwritten if needed
    def reset(self):
        pass


class Constant(Scheduler):
    def __init__(self, eta):
        super().__init__(eta)
    def update_change(self, gradient):
        return self.eta * gradient

    def reset(self):
        pass


class Momentum(Scheduler):
    def __init__(self, eta: float, momentum: float):
        super().__init__(eta)
        self.momentum = momentum
        self.change = 0

    def update_change(self, gradient):
        self.change = self.momentum * self.change + self.eta * gradient
        return self.change

    def reset(self):
        pass


class Adagrad(Scheduler):
    def __init__(self, eta):
        super().__init__(eta)
        self.G_t = None

    def update_change(self, gradient):
        delta = 1e-8  # avoid division ny zero

        if self.G_t is None:
            self.G_t = np.zeros((gradient.shape[0], gradient.shape[0]))

        self.G_t += gradient @ gradient.T

        G_t_inverse = 1 / (
            delta + np.sqrt(np.reshape(np.diagonal(self.G_t), (self.G_t.shape[0], 1)))
        )
        return self.eta * gradient * G_t_inverse

    def reset(self):
        self.G_t = None


class AdagradMomentum(Scheduler):
    def __init__(self, eta, momentum):
        super().__init__(eta)
        self.G_t = None
        self.momentum = momentum
        self.change = 0

    def update_change(self, gradient):
        delta = 1e-8  # avoid division ny zero

        if self.G_t is None:
            self.G_t = np.zeros((gradient.shape[0], gradient.shape[0]))

        self.G_t += gradient @ gradient.T

        G_t_inverse = 1 / (
            delta + np.sqrt(np.reshape(np.diagonal(self.G_t), (self.G_t.shape[0], 1)))
        )
        self.change = self.change * self.momentum + self.eta * gradient * G_t_inverse
        return self.change

    def reset(self):
        self.G_t = None


class RMS_prop(Scheduler):
    def __init__(self, eta, rho):
        super().__init__(eta)
        self.rho = rho
        self.second = 0.0

    def update_change(self, gradient):
        delta = 1e-8  # avoid division ny zero
        self.second = self.rho * self.second + (1 - self.rho) * gradient * gradient
        return self.eta * gradient / (np.sqrt(self.second + delta))

    def reset(self):
        self.second = 0.0


class Adam(Scheduler):
    def __init__(self, eta, rho, rho2):
        super().__init__(eta)
        self.rho = rho
        self.rho2 = rho2
        self.moment = 0
        self.second = 0
        self.n_epochs = 1

    def update_change(self, gradient):
        delta = 1e-8  # avoid division ny zero

        self.moment = self.rho * self.moment + (1 - self.rho) * gradient
        self.second = self.rho2 * self.second + (1 - self.rho2) * gradient * gradient

        moment_corrected = self.moment / (1 - self.rho**self.n_epochs)
        second_corrected = self.second / (1 - self.rho2**self.n_epochs)

        return self.eta * moment_corrected / (np.sqrt(second_corrected + delta))

    def reset(self):
        self.n_epochs += 1
        self.moment = 0
        self.second = 0
```

Usage of schedulers. To initalize a scheduler, simply create the object and pass in the necessary parameters such as the learning rate and the momentum as shown below. As the Scheduler class is an abstract class it should not called directly, and will raise an error upon usage.

```
momentum_scheduler = Momentum(eta=1e-3, momentum=0.9)
adam_scheduler = Adam(eta=1e-3, rho=0.9, rho2=0.999)
```

Here is a small example for how a segment of code using schedulers could look. Switching out the schedulers is simple.

```
weights = np.ones((3,3))
print(f"Before scheduler:\n{weights=}")

epochs = 10
for e in range(epochs):
    gradient = np.random.rand(3, 3)
    change = adam_scheduler.update_change(gradient)
    weights = weights - change
    adam_scheduler.reset()

print(f"\nAfter scheduler:\n{weights=}")
```

Cost functions. In this section we will quickly look at cost functions that can be used when creating the neural network. Every cost function takes the target vector as its parameter, and returns a function valued only at X such that it may easily be differentiated.

```
def CostOLS(target):
    """
    Return OLS function valued only at X, so
    that it may be easily differentiated
    """

    def func(X):
        return (1.0 / target.shape[0]) * np.sum((target - X) ** 2)

    return func


def CostLogReg(target):
    """
    Return Logistic Regression cost function
    valued only at X, so that it may be easily differentiated
    """

    def func(X):
        return -(1.0 / target.shape[0]) * np.sum(
            (target * np.log(X + 10e-10)) + ((1 - target) * np.log(1 - X + 10e-10))
        )

    return func


def CostCrossEntropy(target):
    """
    Return cross entropy cost function valued only at X, so
    that it may be easily differentiated
    """

    def func(X):
        return -(1.0 / target.size) * np.sum(target * np.log(X + 10e-10))

    return func
```

Usage of cost functions. Below we will provide a short example of how these cost function may be used to obtain results if you wish to test them out on your own using AutoGrad's automatic differentiation.

```python
from autograd import grad

target = np.array([[1, 2, 3]]).T
a = np.array([[4, 5, 6]]).T

cost_func = CostCrossEntropy
cost_func_derivative = grad(cost_func(target))

valued_at_a = cost_func_derivative(a)
print(f"Derivative of cost function {cost_func.__name__} valued at a:\n{valued_at_a}")
```

Activation functions. Finally, before we look at the layers that make up the neural network, we will look at the activation functions which can be specified between the hidden layers and as the output function. Each function can be valued for any given vector or matrix X, and can be differentiated via derivate().

```python
import autograd.numpy as np
from autograd import elementwise_grad

def identity(X):
    return X


def sigmoid(X):
    try:
        return 1.0 / (1 + np.exp(-X))
    except FloatingPointError:
        return np.where(X > np.zeros(X.shape), np.ones(X.shape), np.zeros(X.shape))


def softmax(X):
    X = X - np.max(X, axis=-1, keepdims=True)
    delta = 10e-10
    return np.exp(X) / (np.sum(np.exp(X), axis=-1, keepdims=True) + delta)


def RELU(X):
    return np.where(X > np.zeros(X.shape), X, np.zeros(X.shape))


def LRELU(X):
    delta = 10e-4
    return np.where(X > np.zeros(X.shape), X, delta * X)


def derivate(func):
    if func.__name__ == "RELU":

        def func(X):
            return np.where(X > 0, 1, 0)

        return func
    elif func.__name__ == "LRELU":

        def func(X):
            delta = 10e-4
            return np.where(X > 0, 1, delta)

        return func

    else:
        return elementwise_grad(func)
```

Usage of activation functions. Below we present a short demonstration of how to use an activation function. The derivative of the activation function will be important when calculating the output delta term during backpropagation. Note that derivate() can also be used for cost functions for a more generalized approach.

```
z = np.array([[4, 5, 6]]).T
print(f"Input to activation function:\n{z}")

act_func = sigmoid
a = act_func(z)
print(f"\nOutput from {act_func.__name__} activation function:\n{a}")

act_func_derivative = derivate(act_func)
valued_at_z = act_func_derivative(a)
print(f"\nDerivative of {act_func.__name__} activation function valued at z:\n{valued_at_z}")
```

Convolution. In order to construct a convolutional neural network (CNN), it is crucial to comprehend the fundamental principles of convolution and how it aids in extracting information from images. Convolution, at its core, is merely a mathematical operation between two functions that yields another function. It is represented by an integral between two functions, which is typically expressed as:

$$(f * g)(t) := \int_{-\infty}^{\infty} f(\tau)g(t-\tau)d\tau.$$

Here, f and g are the two functions on which we want to perform an operation. The outcome of the convolution operation is represented by $(f * g)$, and it is derived by sliding the function g over f and computing the integral of their product at each position. If both functions are continuous, convolution takes the form shown above. However, if we discretize both f and g, the convolution operation will take the form of a sum between the elements of f and g:

$$(f * g)[n] = \sum_{m=0}^{n-1} f(m)g(n-m).$$

The key idea we utilize to extract the information contained in an image is to slide an $m \times n$ matrix g over an $m \times n$ matrix f. In our case, f represents the image, while g represents the kernel, oftentimes called a filter. However, since our convolution will be a two-dimensional variant, we need to extend our mathematical formula with an additional summation:

$$(f * g)(i,j) \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} f(m,n)g(i-m, j-n).$$

It is imperative to note that the size of the kernel g is significantly smaller than the size of the input image f, thereby reducing the amount of computation necessary for feature extraction. Furthermore, the kernel is usually a trainable parameter in a convolutional neural network, allowing the network to learn appropriate kernels for specific tasks.

To give you an example of how 2D convolution works in practice, suppose we have an image f of dimension 6×6

$$f = \begin{bmatrix} 4 & 1 & 2 & 9 & 8 & 6 \\ 9 & 5 & 9 & 5 & 8 & 5 \\ 1 & 5 & 9 & 7 & 6 & 4 \\ 2 & 9 & 8 & 3 & 7 & 1 \\ 8 & 1 & 6 & 4 & 2 & 2 \\ 1 & 0 & 5 & 7 & 8 & 2 \end{bmatrix}$$

and a 3×3 kernel g called a low-pass filter. Note that the kernel is usually rotated by 180 degrees during convolution, however this has no effect on this kernel.

$$g = \frac{1}{9} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$$

In order to filter the image, we have to extract a 3×3 element from the upper left corner of f, and perform element-wise multiplication of the extracted image pixels with the elements of the kernel g:

$$\begin{bmatrix} 4 & 1 & 2 \\ 9 & 5 & 9 \\ 1 & 5 & 9 \end{bmatrix} \cdot \begin{bmatrix} \frac{1}{9} & \frac{1}{9} & \frac{1}{9} \\ \frac{1}{9} & \frac{1}{9} & \frac{1}{9} \\ \frac{1}{9} & \frac{1}{9} & \frac{1}{9} \end{bmatrix} = \begin{bmatrix} \frac{4}{9} & \frac{1}{9} & \frac{2}{9} \\ \frac{9}{9} & \frac{5}{9} & \frac{9}{9} \\ \frac{1}{9} & \frac{5}{9} & \frac{9}{9} \end{bmatrix} = \boldsymbol{A}$$

Then, following the multiplication, we summarize all the elements of the resulting matrix $\boldsymbol{A}$:

$$(f * g)(0,0) = \sum_{i=0}^{2} \sum_{j=0}^{2} a_{i,j} = 5,$$

which corresponds to the first element of the filtered image $(f * g)$.

Here we use a stride of $S = 1$, a parameter denoted S which describes how many indexes we move the kernel g to the right before repeating the calculations above for the next 3×3 element of the image f. It is usually presumed that

$S = 1$, however, larger values for S can be used to reduce the dimentionality of the filtered image such that the convolution operation is more computationally efficient. In the context of a convolutional neural network, this will become very useful.

The full result of the convolution is:

$$(f * g) = \begin{bmatrix} 5 & 5.78 & 7 & 6.44 \\ 6.33 & 6.67 & 6.89 & 5.11 \\ 5.44 & 5.78 & 5.78 & 4 \\ 4.44 & 4.78 & 5.56 & 4 \end{bmatrix}$$

The result is markedly smaller in shape than the original image. This occurs when using convolution without first padding the image with additional columns and rows, allowing us to keep the original image shape after sliding the kernel over the image. How many rows and columns we wish to pad the image with depends strictly on the shape of the kernel, as we wish to pad the image with r additional rows and c additional columns.

$$r = \lfloor \frac{\text{kernelheight}}{2} \rfloor \cdot 2c = \lfloor \frac{\text{kernelwidth}}{2} \rfloor \cdot 2$$

Note the notation $\lfloor \frac{\text{kernelwidth}}{2} \rfloor$ means that we floor the result of the division, meaning we round down to a whole number in case $\frac{\text{kernelwidth}}{2}$ results in a floating point number.

Using those simple equations, we find out by how much we have to extend the dimensions of the original image. Before proceeding, however, we might ask what we shall fill the additional rows and columns with? One of the most common approaches to padding is zero-padding, which as the name suggest, involves filling the rows and columns with zeros. This is the approach that we will be using for this demonstration. If we apply this padding to out original 6×6 image, the result will be an 8×8 image as the kernel has a width and height of 3. Note that the original image is encapsuled by the zero-padded rows and columns:

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 1 & 2 & 9 & 8 & 6 & 0 \\ 0 & 9 & 5 & 9 & 5 & 8 & 5 & 0 \\ 0 & 1 & 5 & 9 & 7 & 6 & 4 & 0 \\ 0 & 2 & 9 & 8 & 3 & 7 & 1 & 0 \\ 0 & 8 & 1 & 6 & 4 & 2 & 2 & 0 \\ 0 & 1 & 0 & 5 & 7 & 8 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Below we have provided code that demonstrates padding and convolution. As you will see when we run the code, the size of the image will remain unchanged when using padding.

```
import numpy as np
```

```
def padding(image, kernel):
    # calculate r and c
    r = (kernel.shape[0] // 2) * 2
    c = (kernel.shape[1] // 2) * 2

    # padded image dimensions
    padded_height = image.shape[0] + r
    padded_width = image.shape[1] + c

    # for more readable code
    k_half_height = kernel.shape[0] // 2
    k_half_width = kernel.shape[1] // 2

    # zero matrix with padded dimensions
    padded_img = np.zeros((padded_height, padded_width))

    # place image into zero matrix
    padded_img[k_half_height : padded_height - k_half_height,
               k_half_width : padded_width - k_half_width] = image[:, :]

    return padded_img

def convolve(original_image, padded_image, kernel, stride=1):
    # rotate kernel by 180 degrees
    kernel = np.rot90(np.rot90(kernel))

    # note that kernel height // 2 is written as 'm'
    # and kernel width // 2 as 'n' in the mathematical notation
    m = kernel.shape[0] // 2
    n = kernel.shape[1] // 2

    r = (kernel.shape[0] // 2) * 2
    c = (kernel.shape[1] // 2) * 2

    # initialize output array
    convolved_image = np.zeros(original_image.shape)
    image_height = original_image.shape[0]
    image_width = original_image.shape[1]

    # the convolution
    for i in range(m, image_height + m, stride):
        for j in range(n, image_width + n, stride):
            convolved_image[i-m, j-n] = np.sum(
                padded_image[i : i + m, j : j + n]
                * kernel
            )

    return convolved_image

def convolve(image, kernel, stride=1):
    for i in range(2):
        kernel = np.rot90(kernel)

    k_half_height = kernel.shape[0] // 2
    k_half_width = kernel.shape[0] // 2

    conv_image = np.zeros(image.shape)
    pad_image = padding(image, kernel)

    for i in range(k_half_height, conv_image.shape[0] + k_half_height, stride):
        for j in range(k_half_width, conv_image.shape[1] + k_half_width, stride):
            conv_image[i - k_half_height, j - k_half_width] = np.sum(
                pad_image[
                    i - k_half_height : i + k_half_height + 1, j - k_half_width : j + k_half_width
                ]
                * kernel
            )

    return conv_image
```

Fun fact: When filtering images, you will see that convolution involves rotating the kernel by 180 degrees. However, this is not the case when applying convolution in a CNN, where the same operation that is not rotated by 180 degrees is called cross-correlation, which is normally implemented in most libraries.

```
original_image = np.array([[4, 1, 2, 9, 8, 6],
                 [9, 5, 9, 5, 8, 5],
                 [1, 5, 9, 7, 6, 4],
                 [2, 9, 8, 3, 7, 1],
                 [8, 1, 6, 4, 2, 2],
                 [1, 0, 5, 7, 8, 2]])

kernel = (1/9)*np.ones((3,3))

print(f"{original_image.shape=}")

# note that convolve() performs padding
convolved_image = convolve(original_image, kernel, stride=1)

print(f"{convolved_image.shape=}")
```

As you can see, the resulting image is of the same size as the original image. To round of our demonstration of convolution, we will present the results of convolution using commonly used kernels. In a CNN, the values of the kernels are randomly initialized, and then learned during training. These kernels will extract information regarding the picture, such as for example the edge detection filter demonstrated below extracts the edges present in the picture. Of course, there is no guarantee that the CNN will learn an edge detection filter, but this should provide some intuiton as to how the CNN is able to use kernels to make better predictions than a regular feed forward neural network.

```
# Now an example using a real image and first a gaussian low-pass filter and then a Sobel filter
import numpy as np
import imageio.v3 as imageio
import matplotlib.pyplot as plt
import time

def generate_gauss_mask(sigma, K=1):
    side = np.ceil(1 + 8 * sigma)
    y, x = np.mgrid[-side // 2 + 1 : (side // 2) + 1, -side // 2 + 1 : (side // 2) + 1]
    ker_coef = K / (2 * np.pi * sigma**2)
    g = np.exp(-((x**2 + y**2) / (2.0 * sigma**2)))

    return g, ker_coef
```

```
img_path = "data/IMG-2167.JPG"
image_of_cute_dog = imageio.imread(img_path, mode='L')

plt.imshow(image_of_cute_dog, cmap="gray", vmin=0, vmax=255, aspect="auto")
plt.title("Original image")
plt.show()

gauss, kernel = generate_gauss_mask(sigma=6)
gauss_kernel = gauss*kernel

filtered_image = convolve(image_of_cute_dog, gauss_kernel)
plt.imshow(filtered_image, cmap="gray", vmin=0, vmax=255, aspect="auto")
plt.title("Result of convolution with gauss kernel (blurring filter)")
plt.show()

sobel_kernel = np.array([[1, 2, 1],
                    [0, 0, 0],
                    [-1, -2, -1]])

filtered_image = convolve(image_of_cute_dog, sobel_kernel)

plt.imshow(filtered_image, cmap="gray", vmin=0, vmax=255, aspect="auto")
plt.title("Result of convolution with sobel kernel (edge detection filter)")
plt.show()
```

Layers. The code below initialises global variables for readability and describes the abstract class Layers. This is not important in order to understand the CNN, but is benefitial for organizing the code neatly.

```
import math
import autograd.numpy as np
from copy import deepcopy, copy
from autograd import grad
from typing import Callable

# global variables for index readability
input_index = 0
node_index = 1
bias_index = 1
input_channel_index = 1
feature_maps_index = 1
height_index = 2
width_index = 3
kernel_feature_maps_index = 1
kernel_input_channels_index = 0


class Layer:
    def __init__(self, seed):
        self.seed = seed

    def _feedforward(self):
        raise NotImplementedError

    def _backpropagate(self):
        raise NotImplementedError
    def _reset_weights(self, previous_nodes):
        raise NotImplementedError
```

Convolution2DLayer: convolution in a hidden layer. After establishing the foundational understanding of applying convolution to spatial data, let us delve into the intricate workings of a convolutional layer in a Convolutional Neural Network (CNN). The primary function of convolution, as previously discussed, is to extract pertinent information from images while simultaneously decreasing the scale of our data. To initiate the image processing, we shall begin by partitioning the images into color channels (unless the image is grayscale), comprising three primary colors: red, green, and blue. We will subsequently utilize trainable kernels to construct a higher-dimensional encoding of each channel called feature maps. Successive layers will receive these feature maps as inputs, generating further encodings, albeit with reduced dimensions. The term trainable kernels denotes the initialization of pre-defined kernel-shaped weights, which we will then train via backpropagation, similar to how weights are trained in a Feedforward Neural Network.

To ensure seamless integration between our implementation of the convolutional layer and popular machine learning frameworks like Tensorflow (Keras) and PyTorch, we have adopted a design pattern that mirrors the construction of models using these APIs. This involves implementing our convolutional layer as a Python class or object, which allows for a more modular and flexible approach to building neural networks. By structuring our code in this way, users can easily incorporate our implementation into their existing machine learning pipelines without having to make significant changes to their codebase. Additionally, this design pattern promotes code reusability and makes it easier to maintain and update our convolutional layer implementation over time.

Note that the Convolution2DLayer takes in an activation function as a parameter, as it also performs non-linearity.

```
class Convolution2DLayer(Layer):
    def __init__(
        self,
        input_channels,
        feature_maps,
        kernel_height,
        kernel_width,
        v_stride,
        h_stride,
        pad,
        act_func: Callable,
        seed=None,
        reset_weights_independently=True,
    ):
        super().__init__(seed)
        self.input_channels = input_channels
        self.feature_maps = feature_maps
        self.kernel_height = kernel_height
        self.kernel_width = kernel_width
        self.v_stride = v_stride
        self.h_stride = h_stride
        self.pad = pad
        self.act_func = act_func

        # such that the layer can be used on its own
        # outside of the CNN module
        if reset_weights_independently == True:
            self._reset_weights_independently()

    def _feedforward(self, X_batch):
        # note that the shape of X_batch = [inputs, input_maps, img_height, img_width]

        # pad the input batch
        X_batch_padded = self._padding(X_batch)

        # calculate height_index and width_index after stride
        strided_height = int(np.ceil(X_batch.shape[height_index] / self.v_stride))
        strided_width = int(np.ceil(X_batch.shape[width_index] / self.h_stride))

        # create output array
        output = np.ndarray(
            (
                X_batch.shape[input_index],
                self.feature_maps,
                strided_height,
                strided_width,
            )
        )

        # save input and output for backpropagation
        self.X_batch_feedforward = X_batch
        self.output_shape = output.shape

        # checking for errors, no need to look here :)
        self._check_for_errors()

        # convolve input with kernel
        for img in range(X_batch.shape[input_index]):
            for chin in range(self.input_channels):
                for fmap in range(self.feature_maps):
                    out_h = 0
                    for h in range(0, X_batch.shape[height_index], self.v_stride):
                        out_w = 0
                        for w in range(0, X_batch.shape[width_index], self.h_stride):
                            output[img, fmap, out_h, out_w] = np.sum(
                                X_batch_padded[
                                    img,
                                    chin,
                                    h : h + self.kernel_height,
                                    w : w + self.kernel_width,
                                ]
                                * self.kernel[chin, fmap, :, :]
                            )
                            out_w += 1
                        out_h += 1

        # Pay attention to the fact that we're not rotating the kernel by 180 degrees when filter
        # the convolutional layer, as convolution in terms of Machine Learning is a procedure know
        # in image processing and signal processing

        # return a
        return self.act_func(output / (self.kernel_height))

    def _backpropagate(self, delta_term_next):
        # intiate matrices
        delta_term = np.zeros((self.X_batch_feedforward.shape))
        gradient_kernel = np.zeros((self.kernel.shape))

        # pad input for convolution
        X_batch_padded = self._padding(self.X_batch_feedforward)

        # Since an activation function is used at the output of the convolution layer, its deriva
        # has to be accounted for in the backpropagation -> as if ReLU was a layer on its own.
        act_derivative = derivate(self.act_func)
        delta_term_next = act_derivative(delta_term_next)

        # fill in 0's for values removed by vertical stride in feedforward
        if self.v_stride > 1:
            v_ind = 1
            for i in range(delta_term_next.shape[height_index]):
                for j in range(self.v_stride - 1):
                    delta_term_next = np.insert(
                        delta_term_next, v_ind, 0, axis=height_index
                    )
                v_ind += self.v_stride

        # fill in 0's for values removed by horizontal stride in feedforward
        if self.h_stride > 1:
            h_ind = 1
            for i in range(delta_term_next.shape[width_index]):
                for k in range(self.h_stride - 1):
                    delta_term_next = np.insert(
                        delta_term_next, h_ind, 0, axis=width_index
                    )
                h_ind += self.h_stride

        # crops out 0-rows and 0-columns
        delta_term_next = delta_term_next[
            :,
            :,
            : self.X_batch_feedforward.shape[height_index],
            : self.X_batch_feedforward.shape[width_index],
        ]

        # the gradient received from the next layer also needs to be padded
        delta_term_next = self._padding(delta_term_next)

        # calculate delta term by convolving next delta term with kernel
        for img in range(self.X_batch_feedforward.shape[input_index]):
            for chin in range(self.input_channels):
                for fmap in range(self.feature_maps):
                    for h in range(self.X_batch_feedforward.shape[height_index]):
                        for w in range(self.X_batch_feedforward.shape[width_index]):
                            delta_term[img, chin, h, w] = np.sum(
                                delta_term_next[
                                    img,
                                    fmap,
                                    h : h + self.kernel_height,
                                    w : w + self.kernel_width,
                                ]
                                * np.rot90(np.rot90(self.kernel[chin, fmap, :, :]))
                            )
        # calculate gradient for kernel for weight update
        # also via convolution
        for chin in range(self.input_channels):
            for fmap in range(self.feature_maps):
                for k_x in range(self.kernel_height):
                    for k_y in range(self.kernel_width):
                        gradient_kernel[chin, fmap, k_x, k_y] = np.sum(
                            X_batch_padded[
                                img,
                                chin,
                                h : h + self.kernel_height,
                                w : w + self.kernel_width,
                            ]
                            * delta_term_next[
                                img,
                                fmap,
                                h : h + self.kernel_height,
                                w : w + self.kernel_width,
                            ]
                        )
        # all kernels are updated with weight gradient of kernel
        self.kernel -= gradient_kernel

        # return delta term
        return delta_term

    def _padding(self, X_batch, batch_type="image"):

        # same padding for images
        if self.pad == "same" and batch_type == "image":
            padded_height = X_batch.shape[height_index] + (self.kernel_height // 2) * 2
            padded_width = X_batch.shape[width_index] + (self.kernel_width // 2) * 2
            half_kernel_height = self.kernel_height // 2
            half_kernel_width = self.kernel_width // 2

            # initialize padded array
            X_batch_padded = np.ndarray(
                (
                    X_batch.shape[input_index],
                    X_batch.shape[feature_maps_index],
                    padded_height,
                    padded_width,
                )
            )

            # zero pad all images in X_batch
            for img in range(X_batch.shape[input_index]):
                padded_img = np.zeros(
                    (X_batch.shape[feature_maps_index], padded_height, padded_width)
                )
                padded_img[
                    :,
                    half_kernel_height : padded_height - half_kernel_height,
                    half_kernel_width : padded_width - half_kernel_width,
                ] = X_batch[img, :, :, :]
                X_batch_padded[img, :, :, :] = padded_img[:, :, :]

            return X_batch_padded

        # same padding for gradients
        elif self.pad == "same" and batch_type == "grad":
            padded_height = X_batch.shape[height_index] + (self.kernel_height // 2) * 2
            padded_width = X_batch.shape[width_index] + (self.kernel_width // 2) * 2
            half_kernel_height = self.kernel_height // 2
            half_kernel_width = self.kernel_width // 2

            # initialize padded array
            delta_term_padded = np.zeros(
                (
                    X_batch.shape[input_index],
                    X_batch.shape[feature_maps_index],
                    padded_height,
                    padded_width,
                )
            )

            # zero pad delta term
            delta_term_padded[
                :, :, : X_batch.shape[height_index], : X_batch.shape[width_index]
            ] = X_batch[:, :, :, :]

            return delta_term_padded

        else:
            return X_batch

    def _reset_weights_independently(self):
        # sets seed to remove randomness inbetween runs
        if self.seed is not None:
            np.random.seed(self.seed)

        # initializes kernel matrix
        self.kernel = np.ndarray(
            (
                self.input_channels,
                self.feature_maps,
                self.kernel_height,
                self.kernel_width,
            )
        )

        # randomly initializes weights
        for chin in range(self.kernel.shape[kernel_input_channels_index]):
            for fmap in range(self.kernel.shape[kernel_feature_maps_index]):
                self.kernel[chin, fmap, :, :] = np.random.rand(
                    self.kernel_height, self.kernel_width
                )

    def _reset_weights(self, previous_nodes):
        # sets weights
        self._reset_weights_independently()

        # returns shape of output used for subsequent layer's weight initiation
        strided_height = int(
            np.ceil(previous_nodes.shape[height_index] / self.v_stride)
        )
        strided_width = int(np.ceil(previous_nodes.shape[width_index] / self.h_stride))
        next_nodes = np.ones(
            (
                previous_nodes.shape[input_index],
                self.feature_maps,
                strided_height,
                strided_width,
            )
        )
        return next_nodes / self.kernel_height

    def _check_for_errors(self):
        if self.X_batch_feedforward.shape[input_channel_index] != self.input_channels:
            raise AssertionError(
                f"ERROR: Number of input channels in data ({self.X_batch_feedforward.shape[input_
            )
```

Backpropagation in the convolutional layer. As you may have noticed, we have not yet explained how the backpropagation algorithm works in a convolutional layer. However, having covered all other major details about convolutional layers, we are now prepared to do so. It should come as no surprise that the calculation of delta terms at each convolutional layer takes the form of convolution. After the gradient has been propagated backwards through the flattening layer, where it was reshaped into an appropriate form, calculating the update value for the kernel is simply a matter of convolving the output gradient with the input of the layer for which we are updating the weights. For more detail, this article serves as an excellent resource, see https://pavisj.medium.com/convolutions-and-backpropagations-46026a8f5d2c

Demonstration. We can use the convolutional layer above to perform a simple convolution on an image of the now familiar cute dog.

```
import numpy as np
import imageio.v3 as imageio
import matplotlib.pyplot as plt

def plot_convolution_result(X, layer):
    plt.imshow(X[0, 0, :, :], vmin=0, vmax=255, cmap="gray")
    plt.title("Original image")
    plt.colorbar()
    plt.show()
    conv_result = layer._feedforward(X)
    plt.title("Result of convolutional layer")
    plt.imshow(conv_result[0, 0, :, :], vmin=0, vmax=255, cmap="gray")
    plt.colorbar()
    plt.show()

# create layer
layer = Convolution2DLayer(
    input_channels=3,
    feature_maps=1,
    kernel_height=4,
    kernel_width=4,
    v_stride=2,
    h_stride=2,
    pad="same",
    act_func=identity,
    seed=2023,
    )
```

```
# read in image path, make data correct format
img_path = img_path = "data/IMG-2167.JPG"
image_of_cute_dog = imageio.imread(img_path)
image_shape = image_of_cute_dog.shape
image_of_cute_dog = image_of_cute_dog.reshape(1, image_shape[0], image_shape[1], image_shape[2])
image_of_cute_dog = image_of_cute_dog.transpose(0, 3, 1, 2)

# plot the result of the convolution
plot_convolution_result(image_of_cute_dog, layer)
```

We cobserve that the result has half the pixels on each axis due to the fact that we've used a horizontal and vertical stride of 2. The result of this convolution is not very insightfull, as the kernel has completely random values for the first feedforward pass. However, as we perform multiple forward and backward passes, the results of the convolution should provide identifying features of the image it uses for classification.

Note that image data usually comes in many different shapes and sizes, but for our CNN we require the input data be formatted as

$$Numberofinputs, inputchannels, inputheight, inputwidth$$

. Occasionally, the data you come accross use will be formatted like this, but on many occasions reshaping and transposing the dimensions is sadly necessary.

Pooling Layer. The pooling layer is another widely used type of layer in convolutional neural networks that enables data downsampling to a more manageable size. Despite recent technological advancements that allow for convolution without excessive size reduction of the data, the pooling layer still remains a fundamental component of convolutional neural networks. It can be used before, after, or in between convolutional layers, although finding the optimal placement of layers and network depth requires experimentation to achieve the best performance for a given problem. The code we provide allows you to perform two types of pooling known as max pooling and average pooling.

```
class Pooling2DLayer(Layer):
    def __init__(
        self,
        kernel_height,
        kernel_width,
        v_stride,
        h_stride,
        pooling="max",
        seed=None,
    ):
        super().__init__(seed)
        self.kernel_height = kernel_height
        self.kernel_width = kernel_width
        self.v_stride = v_stride
        self.h_stride = h_stride
        self.pooling = pooling
```

```
def _feedforward(self, X_batch):
    # Saving the input for use in the backwardpass
    self.X_batch_feedforward = X_batch

    # check if user is silly
    self._check_for_errors()

    # Computing the size of the feature maps based on kernel size and the stride parameter
    strided_height = (
        X_batch.shape[height_index] - self.kernel_height
    ) // self.v_stride + 1
    if X_batch.shape[height_index] == X_batch.shape[width_index]:
        strided_width = strided_height
    else:
        strided_width = (
            X_batch.shape[width_index] - self.kernel_width
        ) // self.h_stride + 1

    # initialize output array
    output = np.ndarray(
        (
            X_batch.shape[input_index],
            X_batch.shape[feature_maps_index],
            strided_height,
            strided_width,
        )
    )

    # select pooling action, either max or average pooling
    if self.pooling == "max":
        self.pooling_action = np.max
    elif self.pooling == "average":
        self.pooling_action = np.mean

    # pool based on kernel size and stride
    for img in range(output.shape[input_index]):
        for fmap in range(output.shape[feature_maps_index]):
            for h in range(strided_height):
                for w in range(strided_width):
                    output[img, fmap, h, w] = self.pooling_action(
                        X_batch[
                            img,
                            fmap,
                            (h * self.v_stride) : (h * self.v_stride)
                            + self.kernel_height,
                            (w * self.h_stride) : (w * self.h_stride)
                            + self.kernel_width,
                        ]
                    )

    # output for feedforward in next layer
    return output

def _backpropagate(self, delta_term_next):
    # initiate delta term array
    delta_term = np.zeros((self.X_batch_feedforward.shape))

    for img in range(delta_term_next.shape[input_index]):
        for fmap in range(delta_term_next.shape[feature_maps_index]):
            for h in range(0, delta_term_next.shape[height_index], self.v_stride):
                for w in range(
                    0, delta_term_next.shape[width_index], self.h_stride
                ):
                    # max pooling
                    if self.pooling == "max":
                        # get window
                        window = self.X_batch_feedforward[
                            img,
                            fmap,
                            h : h + self.kernel_height,
                            w : w + self.kernel_width,
                        ]

                        # find max values indices in window
                        max_h, max_w = np.unravel_index(
                            window.argmax(), window.shape
                        )

                        # set values in new, upsampled delta term
                        delta_term[
                            img,
                            fmap,
                            (h + max_h),
                            (w + max_w),
                        ] += delta_term_next[img, fmap, h, w]

                    # average pooling
                    if self.pooling == "average":
                        delta_term[
                            img,
                            fmap,
                            h : h + self.kernel_height,
                            w : w + self.kernel_width,
                        ] = (
                            delta_term_next[img, fmap, h, w]
                            / self.kernel_height
                            / self.kernel_width
                        )
    # returns input to backpropagation in previous layer
    return delta_term

def _reset_weights(self, previous_nodes):
    # calculate strided height, strided width
    strided_height = (
        previous_nodes.shape[height_index] - self.kernel_height
    ) // self.v_stride + 1
    if previous_nodes.shape[height_index] == previous_nodes.shape[width_index]:
        strided_width = strided_height
    else:
        strided_width = (
            previous_nodes.shape[width_index] - self.kernel_width
        ) // self.h_stride + 1

    # initiate output array
    output = np.ones(
        (
            previous_nodes.shape[input_index],
            previous_nodes.shape[feature_maps_index],
            strided_height,
            strided_width,
        )
    )
    # returns output with shape used for reset weights in next layer
    return output

def _check_for_errors(self):
    # check if input is smaller than kernel size -> error
    assert (
        self.X_batch_feedforward.shape[width_index] >= self.kernel_width
    ), f"ERROR: Pooling kernel width_index ({self.kernel_width}) larger than data width_index
    assert (
        self.X_batch_feedforward.shape[height_index] >= self.kernel_height
    ), f"ERROR: Pooling kernel height_index ({self.kernel_height}) larger than data height_inc
```

Flattening Layer. Before we can begin building our first CNN model, we need to introduce the flattening layer. As its name suggests, the flattening layer transforms the data into a one-dimensional vector that can be fed into the feedforward layers of our network. This layer plays a crucial role in preparing the data for further processing in the network. Additionally, the flattening layer is responsible for reshaping the gradient to the proper shape during backpropagation. This ensures that the kernels are correctly updated, allowing for effective learning in the network.

```
class FlattenLayer(Layer):
    def __init__(self, act_func=LRELU, seed=None):
        super().__init__(seed)
        self.act_func = act_func

    def _feedforward(self, X_batch):
        # save input for backpropagation
        self.X_batch_feedforward_shape = X_batch.shape
        # Remember, the data has the following shape: (I, FM, H, W, ) in the convolutional layers
        # whilst the data has the shape (I, FM * H * W) in the fully connected layers
        # I = Inputs, FM = Feature Maps, H = Height and W = Width.
        X_batch = X_batch.reshape(
            X_batch.shape[input_index],
            X_batch.shape[feature_maps_index]
            * X_batch.shape[height_index]
            * X_batch.shape[width_index],
        )

        # add bias to a
        self.z_matrix = X_batch
        bias = np.ones((X_batch.shape[input_index], 1)) * 0.01
        self.a_matrix = np.hstack([bias, X_batch])

        # return a, the input to feedforward in next layer
        return self.a_matrix

    def _backpropagate(self, weights_next, delta_term_next):
        activation_derivative = derivate(self.act_func)

        # calculate delta term
        delta_term = (
            weights_next[bias_index:, :] @ delta_term_next.T
        ).T * activation_derivative(self.z_matrix)

        # FlattenLayer does not update weights
        # reshapes delta layer to convolutional layer data format [Input, Feature_Maps, Height, W
        return delta_term.reshape(self.X_batch_feedforward_shape)

    def _reset_weights(self, previous_nodes):
        # note that the previous nodes to the FlattenLayer are from the convolutional layers
        previous_nodes = previous_nodes.reshape(
            previous_nodes.shape[input_index],
            previous_nodes.shape[feature_maps_index]
            * previous_nodes.shape[height_index]
            * previous_nodes.shape[width_index],
        )

        # return shape used in reset_weights in next layer
        return previous_nodes.shape[node_index]

    def get_prev_a(self):
        return self.a_matrix
```

Fully Connected Layers. Finally, the result from the flatten layer will pass to a series of fully connected layers, which function as a normal feed forward neural network. The fully connected layers are split into two classes; FullyConnectedLayer which acts as a hidden layer, and OutputLayer, which acts as the single output layer at the end of the CNN. If one wishes to use this codebase to construct a normal feed forward neural network, it must start with a FlattenLayer due to techincal details regarding weight intitialization. However many FullyConnectedLayers can be added to the CNN, and in each layer the amount of nodes, which activation function and scheduler to use can be specified. In practice, the scheduler will be specified in the CNN object initialization, and inherited if no other scheduler is specified.

```
class FullyConnectedLayer(Layer):
    # FullyConnectedLayer per default uses LRELU and Adam scheduler
    # with an eta of 0.0001, rho of 0.9 and rho2 of 0.999
    def __init__(
        self,
        nodes: int,
        act_func: Callable = LRELU,
        scheduler: Scheduler = Adam(eta=1e-4, rho=0.9, rho2=0.999),
        seed: int = None,
    ):
        super().__init__(seed)
        self.nodes = nodes
        self.act_func = act_func
        self.scheduler_weight = copy(scheduler)
        self.scheduler_bias = copy(scheduler)

        # initiate matrices for later
        self.weights = None
        self.a_matrix = None
        self.z_matrix = None

    def _feedforward(self, X_batch):
        # calculate z
        self.z_matrix = X_batch @ self.weights

        # calculate a, add bias
        bias = np.ones((X_batch.shape[input_index], 1)) * 0.01
        self.a_matrix = self.act_func(self.z_matrix)
        self.a_matrix = np.hstack([bias, self.a_matrix])

        # return a, the input for feedforward in next layer
        return self.a_matrix

    def _backpropagate(self, weights_next, delta_term_next, a_previous, lam):
        # take the derivative of the activation function
        activation_derivative = derivate(self.act_func)

        # calculate the delta term
        delta_term = (
            weights_next[bias_index:, :] @ delta_term_next.T
        ).T * activation_derivative(self.z_matrix)

        # intitiate matrix to store gradient
        # note that we exclude the bias term, which we will calculate later
        gradient_weights = np.zeros(
            (
                a_previous.shape[input_index],
                a_previous.shape[node_index] - bias_index,
                delta_term.shape[node_index],
            )
        )

        # calculate gradient = delta term * previous a
        for i in range(len(delta_term)):
            gradient_weights[i, :, :] = np.outer(
                a_previous[i, bias_index:], delta_term[i, :]
            )

        # sum the gradient, divide by input_index
        gradient_weights = np.mean(gradient_weights, axis=input_index)
        # for the bias gradient we do not multiply by previous a
        gradient_bias = np.mean(delta_term, axis=input_index).reshape(
            1, delta_term.shape[node_index]
        )

        # regularization term
        gradient_weights += self.weights[bias_index:, :] * lam

        # send gradients into scheduler
        # returns update matrix which will be used to update the weights and bias
        update_matrix = np.vstack(
            [
                self.scheduler_bias.update_change(gradient_bias),
                self.scheduler_weight.update_change(gradient_weights),
            ]
        )

        # update weights
        self.weights -= update_matrix

        # return weights and delta term, input for backpropagation in previous layer
        return self.weights, delta_term

    def _reset_weights(self, previous_nodes):
        # sets seed to remove randomness inbetween runs
        if self.seed is not None:
            np.random.seed(self.seed)
        # add bias, initiate random weights
        bias = 1
        self.weights = np.random.randn(previous_nodes + bias, self.nodes)

        # returns number of nodes, used for reset_weights in next layer
        return self.nodes

    def _reset_scheduler(self):
        # resets scheduler per epoch
        self.scheduler_weight.reset()
        self.scheduler_bias.reset()

    def get_prev_a(self):
        # returns a matrix, used in backpropagation
        return self.a_matrix


class OutputLayer(FullyConnectedLayer):
    def __init__(
        self,
        nodes: int,
        output_func: Callable = LRELU,
        cost_func: Callable = CostCrossEntropy,
        scheduler: Scheduler = Adam(eta=1e-4, rho=0.9, rho2=0.999),
        seed: int = None,
    ):
        super().__init__(nodes, output_func, copy(scheduler), seed)
        self.cost_func = cost_func

        # initiate matrices for later
        self.weights = None
        self.a_matrix = None
        self.z_matrix = None

        # decides if the output layer performs binary or multi-class classification
        self._set_pred_format()

    def _feedforward(self, X_batch: np.ndarray):
        # calculate a, z
        # note that bias is not added as this would create an extra output class
        self.z_matrix = X_batch @ self.weights
        self.a_matrix = self.act_func(self.z_matrix)

        # returns prediction
        return self.a_matrix

    def _backpropagate(self, target, a_previous, lam):
        # note that in the OutputLayer the activation function is the output function
        activation_derivative = derivate(self.act_func)

        # calculate output delta terms
        # for multi-class or binary classification
        if self.pred_format == "Multi-class":
            delta_term = self.a_matrix - target
        else:
            cost_func_derivative = grad(self.cost_func(target))
            delta_term = activation_derivative(self.z_matrix) * cost_func_derivative(
                self.a_matrix
            )
        # intiate matrix that stores gradient
        gradient_weights = np.zeros(
            (
                a_previous.shape[input_index],
                a_previous.shape[node_index] - bias_index,
                delta_term.shape[node_index],
            )
        )

        # calculate gradient = delta term * previous a
        for i in range(len(delta_term)):
            gradient_weights[i, :, :] = np.outer(
                a_previous[i, bias_index:], delta_term[i, :]
            )

        # sum the gradient, divide by input_index
        gradient_weights = np.mean(gradient_weights, axis=input_index)
        # for the bias gradient we do not multiply by previous a
        gradient_bias = np.mean(delta_term, axis=input_index).reshape(
            1, delta_term.shape[node_index]
        )

        # regularization term
        gradient_weights += self.weights[bias_index:, :] * lam

        # send gradients into scheduler
        # returns update matrix which will be used to update the weights and bias
        update_matrix = np.vstack(
            [
                self.scheduler_bias.update_change(gradient_bias),
                self.scheduler_weight.update_change(gradient_weights),
            ]
        )

        # update weights
        self.weights -= update_matrix

        # return weights and delta term, input for backpropagation in previous layer
        return self.weights, delta_term

    def _reset_weights(self, previous_nodes):
        # sets seed to remove randomness inbetween runs
        if self.seed is not None:
            np.random.seed(self.seed)

        # add bias, initiate random weights
        bias = 1
        self.weights = np.random.rand(previous_nodes + bias, self.nodes)

        # returns number of nodes, used for reset_weights in next layer
        return self.nodes

    def _reset_scheduler(self):
        # resets scheduler per epoch
        self.scheduler_weight.reset()
        self.scheduler_bias.reset()

    def _set_pred_format(self):
        # sets prediction format to either regression, binary or multi-class classification
        if self.act_func.__name__ is None or self.act_func.__name__ == "identity":
            self.pred_format = "Regression"
        elif self.act_func.__name__ == "sigmoid" or self.act_func.__name__ == "tanh":
            self.pred_format = "Binary"
        else:
            self.pred_format = "Multi-class"

    def get_pred_format(self):
        # returns format of prediction
        return self.pred_format
```

Optimized Convolution2DLayer. For our CNN, we have also implemented an optimized version of the Convolution2DLayer, Convolution2DLayerOPT, which runs much faster. See VII. Remarks for discussion. This layer will per default be used by the CNN due to its computational advantages, but is much less readable. We've documented it such that specially interested students can understand the principles behind it, but it is not recommended to read. In short, we reshape and transpose parts of the image such that the convolutional operation can be swapped out for a simple matrix multiplication.

```
class Convolution2DLayerOPT(Convolution2DLayer):
    """
    Am optimized version of the convolution layer above which
    utilizes an approach of extracting windows of size equivalent
    in size to the filter. The convoution is then performed on those
    windows instead of a full feature map.
    """

    def __init__(
        self,
        input_channels,
        feature_maps,
        kernel_height,
        kernel_width,
        v_stride,
        h_stride,
        pad,
        act_func: Callable,
        seed=None,
        reset_weights_independently=True,
    ):
        super().__init__(
            input_channels,
            feature_maps,
            kernel_height,
            kernel_width,
            v_stride,
            h_stride,
            pad,
            act_func,
            seed,
        )
        # true if layer is used outside of CNN
        if reset_weights_independently == True:
            self._reset_weights_independently()

    def _feedforward(self, X_batch):
        # The optimized _feedforward method is difficult to understand but computationally more e
        # for a more "by the book" approach, please look at the _feedforward method of Convolutio
        # save the input for backpropagation
        self.X_batch_feedforward = X_batch

        # check that there are the correct amount of input channels
        self._check_for_errors()

        # calculate new shape after stride
        strided_height = int(np.ceil(X_batch.shape[height_index] / self.v_stride))
        strided_width = int(np.ceil(X_batch.shape[width_index] / self.h_stride))

        # get windows of the image for more computationally efficient convolution
        # the idea is that we want to align the dimensions that we wish to matrix
        # multiply, then use a simple matrix multiplication instead of convolution.
        # then, we reshape the size back to its intended shape
        windows = self._extract_windows(X_batch)
        windows = windows.transpose(1, 0, 2, 3, 4).reshape(
            X_batch.shape[input_index],
            strided_height * strided_width,
            -1,
        )

        # reshape the kernel for more computationally efficient convolution
        kernel = self.kernel
        kernel = kernel.transpose(0, 2, 3, 1).reshape(
            kernel.shape[kernel_input_channels_index]
            * kernel.shape[height_index]
            * kernel.shape[width_index],
            -1,
        )

        # use simple matrix calculation to obtain output
        output = (
            (windows @ kernel)
            .reshape(
                X_batch.shape[input_index],
                strided_height,
                strided_width,
                -1,
            )
            .transpose(0, 3, 1, 2)
        )

        # The output is reshaped and rearranged to appropriate shape
        return self.act_func(
            output / (self.kernel_height * X_batch.shape[feature_maps_index])
        )

    def _backpropagate(self, delta_term_next):
        # The optimized _backpropagate method is difficult to understand but computationally more
        # for a more "by the book" approach, please look at the _backpropagate method of Convolut
        act_derivative = derivate(self.act_func)
        delta_term_next = act_derivative(delta_term_next)

        # calculate strided dimensions
        strided_height = int(
            np.ceil(self.X_batch_feedforward.shape[height_index] / self.v_stride)
        )
        strided_width = int(
            np.ceil(self.X_batch_feedforward.shape[width_index] / self.h_stride)
        )
```

```
# copy kernel
kernel = self.kernel

# get windows, reshape for matrix multiplication
windows = self._extract_windows(self.X_batch_feedforward, "image").reshape(
    self.X_batch_feedforward.shape[input_index]
    * strided_height
    * strided_width,
    -1,
)

# initialize output gradient, reshape and transpose into correct shape
# for matrix multiplication
output_grad_tr = delta_term_next.transpose(0, 2, 3, 1).reshape(
    self.X_batch_feedforward.shape[input_index]
    * strided_height
    * strided_width,
    -1,
)

# calculate gradient kernel via simple matrix multiplication and reshaping
gradient_kernel = (
    (windows.T @ output_grad_tr)
    .reshape(
        kernel.shape[kernel_input_channels_index],
        kernel.shape[height_index],
        kernel.shape[width_index],
        kernel.shape[kernel_feature_maps_index],
    )
    .transpose(0, 3, 1, 2)
)

# for computing the input gradient
windows_out, upsampled_height, upsampled_width = self._extract_windows(
    delta_term_next, "grad"
)

# calculate new window dimensions
new_windows_first_dim = (
    self.X_batch_feedforward.shape[input_index]
    * upsampled_height
    * upsampled_width
)
# ceil allows for various asymmetric kernels
new_windows_sec_dim = int(np.ceil(windows_out.size / new_windows_first_dim))

# reshape for matrix multiplication
windows_out = windows_out.transpose(1, 0, 2, 3, 4).reshape(
    new_windows_first_dim, new_windows_sec_dim
)

# reshape for matrix multiplication
kernel_reshaped = kernel.reshape(self.input_channels, -1)

# calculating input gradient for next convolutional layer
input_grad = (windows_out @ kernel_reshaped.T).reshape(
    self.X_batch_feedforward.shape[input_index],
    upsampled_height,
    upsampled_width,
    kernel.shape[kernel_input_channels_index],
        )
        input_grad = input_grad.transpose(0, 3, 1, 2)

        # Update the weights in the kernel
        self.kernel -= gradient_kernel

        # Output the gradient to propagate backwards
        return input_grad

    def _extract_windows(self, X_batch, batch_type="image"):
        """
        Receives as input the X_batch with shape (inputs, feature_maps, image_height, image_width,
        and extract windows of size kernel_height * kernel_width for every image and every featur
        It then returns an np.ndarray of shape (image_height * image_width, inputs, feature_maps,
        which will be used either to filter the images in feedforward or to calculate the gradien
        """

        # initialize list of windows
        windows = []

        if batch_type == "image":
            # pad the images
            X_batch_padded = self._padding(X_batch, batch_type="image")
            img_height, img_width = X_batch_padded.shape[2:]
            # For each location in the image...
            for h in range(
                0,
                X_batch.shape[height_index],
                self.v_stride,
            ):
                for w in range(
                    0,
                    X_batch.shape[width_index],
                    self.h_stride,
                ):
                    # ...obtain an image patch of the original size (strided)

                    # get window
                    window = X_batch_padded[
                        :,
                        :,
                        h : h + self.kernel_height,
                        w : w + self.kernel_width,
                    ]

                    # append to list of windows
                    windows.append(window)

            # return numpy array instead of list
            return np.stack(windows)

        # In order to be able to perform backprogagation by the method of window extraction,
        # here is a modified approach to extracting the windows which allow for the necessary
        # upsampling of the gradient in case the on of the stride parameters is larger than one.

        if batch_type == "grad":

            # In the case of one of the stride parameters being odd, we have to take some
            # extra care in calculating the upsampled size of X_batch. We solve this
            # by simply flooring the result of dividing stride by 2.
            if self.v_stride < 2 or self.v_stride % 2 == 0:
```

```
    v_stride = 0
else:
    v_stride = int(np.floor(self.v_stride / 2))

if self.h_stride < 2 or self.h_stride % 2 == 0:
    h_stride = 0
else:
    h_stride = int(np.floor(self.h_stride / 2))

upsampled_height = (X_batch.shape[height_index] * self.v_stride) - v_stride
upsampled_width = (X_batch.shape[width_index] * self.h_stride) - h_stride

# When upsampling, we need to insert rows and columns filled with zeros
# into each feature map. How many of those we have to insert is purely
# dependant on the value of stride parameter in the vertical and horizontal
# direction.
if self.v_stride > 1:
    v_ind = 1
    for i in range(X_batch.shape[height_index]):
        for j in range(self.v_stride - 1):
            X_batch = np.insert(X_batch, v_ind, 0, axis=height_index)
        v_ind += self.v_stride

if self.h_stride > 1:
    h_ind = 1
    for i in range(X_batch.shape[width_index]):
        for k in range(self.h_stride - 1):
            X_batch = np.insert(X_batch, h_ind, 0, axis=width_index)
        h_ind += self.h_stride

# Since the insertion of zero-filled rows and columns isn't perfect, we have
# to assure that the resulting feature maps will have the expected upsampled height
# and width by cutting them og at desired dimensions.

X_batch = X_batch[:, :, :upsampled_height, :upsampled_width]

X_batch_padded = self._padding(X_batch, batch_type="grad")

# initialize list of windows
windows = []

# For each location in the image...
for h in range(
    0,
    X_batch.shape[height_index],
    self.v_stride,
):
    for w in range(
        0,
        X_batch.shape[width_index],
        self.h_stride,
    ):
        # ...obtain an image patch of the original size (strided)

        # get window
        window = X_batch_padded[
            :, :, h : h + self.kernel_height, w : w + self.kernel_width
        ]

        # append window to list
        windows.append(window)
```

```
            # return numpy array, unsampled dimensions
            return np.stack(windows), upsampled_height, upsampled_width

    def _check_for_errors(self):
        # compares input channels of data to input channels of Convolution2DLayer
        if self.X_batch_feedforward.shape[input_channel_index] != self.input_channels:
            raise AssertionError(
                f"ERROR: Number of input channels in data ({self.X_batch_feedforward.shape[input_c
            )
```

The Convolutional Neural Network (CNN). Finally, we present the code for the CNN. The CNN class organizes all the layers, and allows for training on image data.

```
import math
import autograd.numpy as np
import sys
import warnings
from autograd import grad, elementwise_grad
from random import random, seed
from copy import deepcopy
from typing import Tuple, Callable
from sklearn.utils import resample

warnings.simplefilter("error")


class CNN:
    def __init__(
        self,
        cost_func: Callable = CostCrossEntropy,
        scheduler: Scheduler = Adam(eta=1e-4, rho=0.9, rho2=0.999),
        seed: int = None,
    ):
        """
        Description:
        ------------
            Instantiates CNN object

        Parameters:
        ------------
            I   output_func (costFunctions) cost function for feed forward neural network part of
                such as "CostLogReg", "CostOLS" or "CostCrossEntropy"

            II  scheduler (Scheduler) optional parameter, default set to Adam. Can also be set to
                schedulers such as AdaGrad, Momentum, RMS_prop and Constant. Note that schedulers
                to be instantiated first with proper parameters (for example eta, rho and rho2 fo

            III seed (int) used for seeding all random operations
        """
        self.layers = list()
        self.cost_func = cost_func
        self.scheduler = scheduler
        self.schedulers_weight = list()
        self.schedulers_bias = list()
        self.seed = seed
        self.pred_format = None
```

```python
def add_FullyConnectedLayer(
    self, nodes: int, act_func=LRELU, scheduler=None
) -> None:
    """
    Description:
    ------------
        Add a FullyConnectedLayer to the CNN, i.e. a hidden layer in the feed forward neural
        network part of the CNN. Often called a Dense layer in literature

    Parameters:
    ------------
        I   nodes (int) number of nodes in FullyConnectedLayer
        II  act_func (activationFunctions) activation function of FullyConnectedLayer,
            such as "sigmoid", "RELU", "LRELU", "softmax" or "identity"
        III scheduler (Scheduler) optional parameter, default set to Adam. Can also be set to
            schedulers such as AdaGrad, Momentum, RMS_prop and Constant
    """
    assert self.layers, "FullyConnectedLayer should follow FlattenLayer in CNN"

    if scheduler is None:
        scheduler = self.scheduler

    layer = FullyConnectedLayer(nodes, act_func, scheduler, self.seed)
    self.layers.append(layer)

def add_OutputLayer(self, nodes: int, output_func=sigmoid, scheduler=None) -> None:
    """
    Description:
    ------------
        Add an OutputLayer to the CNN, i.e. a the final layer in the feed forward neural
        network part of the CNN

    Parameters:
    ------------
        I   nodes (int) number of nodes in OutputLayer. Set nodes=1 for binary classification
            nodes = number of classes for multi-class classification
        II  output_func (activationFunctions) activation function for the output layer, such
            "identity" for regression, "sigmoid" for binary classification and "softmax" for
            classification
        III scheduler (Scheduler) optional parameter, default set to Adam. Can also be set to
            schedulers such as AdaGrad, Momentum, RMS_prop and Constant
    """
    assert self.layers, "OutputLayer should follow FullyConnectedLayer in CNN"

    if scheduler is None:
        scheduler = self.scheduler

    output_layer = OutputLayer(
        nodes, output_func, self.cost_func, scheduler, self.seed
    )
    self.layers.append(output_layer)
    self.pred_format = output_layer.get_pred_format()

def add_FlattenLayer(self, act_func=LRELU) -> None:
    """
    Description:
    ------------
        Add a FlattenLayer to the CNN, which flattens the image data such that it is formatte
        be used in the feed forward neural network part of the CNN
    """
```

```
        self.layers.append(FlattenLayer(act_func=act_func, seed=self.seed))

    def add_Convolution2DLayer(
        self,
        input_channels=1,
        feature_maps=1,
        kernel_height=3,
        kernel_width=3,
        v_stride=1,
        h_stride=1,
        pad="same",
        act_func=LRELU,
        optimized=True,
    ) -> None:
        """
        Description:
        ------------
            Add a Convolution2DLayer to the CNN, i.e. a convolutional layer with a 2 dimensional k
            the first layer added to the CNN

        Parameters:
        ------------
            I   input_channels (int) specifies amount of input channels. For monochrome images, us
                = 1, and input_channels = 3 for colored images, where each channel represents one
            II  feature_maps (int) amount of feature maps in CNN
            III kernel_height (int) height of the kernel, also called 'convolutional filter' in li
            IV  kernel_width (int) width of the kernel, also called 'convolutional filter' in lite
            V   v_stride (int) value of vertical stride for dimentionality reduction
            VI  h_stride (int) value of horizontal stride for dimentionality reduction
            VII pad (str) default = "same" ensures output size is the same as input size (given s
           VIII act_func (activationFunctions) default = "LRELU", nonlinear activation function
             IX optimized (bool) default = True, uses Convolution2DLayerOPT if True which is much
                compared to Convolution2DLayer, which is a more straightforward, understandable in
        """
        if optimized:
            conv_layer = Convolution2DLayerOPT(
                input_channels,
                feature_maps,
                kernel_height,
                kernel_width,
                v_stride,
                h_stride,
                pad,
                act_func,
                self.seed,
                reset_weights_independently=False,
            )
        else:
            conv_layer = Convolution2DLayer(
                input_channels,
                feature_maps,
                kernel_height,
                kernel_width,
                v_stride,
                h_stride,
                pad,
                act_func,
                self.seed,
                reset_weights_independently=False,
            )
        self.layers.append(conv_layer)
```

```
def add_PoolingLayer(
    self, kernel_height=2, kernel_width=2, v_stride=1, h_stride=1, pooling="max"
) -> None:
    """
    Description:
    ------------
        Add a Pooling2DLayer to the CNN, i.e. a pooling layer that reduces the dimentionality
        the image data. It is not necessary to use a Pooling2DLayer when creating a CNN, but
        can be used to speed up the training

    Parameters:
    ------------
        I   kernel_height (int) height of the kernel used for pooling
        II  kernel_width (int) width of the kernel used for pooling
        III v_stride (int) value of vertical stride for dimentionality reduction
        IV  h_stride (int) value of horizontal stride for dimentionality reduction
        V   pooling (str) either "max" or "average", describes type of pooling performed
    """
    pooling_layer = Pooling2DLayer(
        kernel_height, kernel_width, v_stride, h_stride, pooling, self.seed
    )
    self.layers.append(pooling_layer)

def fit(
    self,
    X: np.ndarray,
    t: np.ndarray,
    epochs: int = 100,
    lam: float = 0,
    batches: int = 1,
    X_val: np.ndarray = None,
    t_val: np.ndarray = None,
) -> dict:
    """
    Description:
    ------------
        Fits the CNN to input X for a given amount of epochs. Performs feedforward and backpro
        can utilize batches, regulariziation and validation if desired.

    Parameters:
    ------------
        X (numpy array) with input data in format [images, input channels,
        image height, image_width]
        t (numpy array) target labels for input data
        epochs (int) amount of epochs
        lam (float) regulariziation term lambda
        batches (int) amount of batches input data splits into
        X_val (numpy array) validation data
        t_val (numpy array) target labels for validation data

    Returns:
    ------------
        scores (dict) a dictionary with "train_error", "train_acc", "val_error", val_acc" keys
        that contain numpy arrays with float values of all accuracies/errors over all epochs.
        Can be used to create plots. Also used to update the progress bar during training
    """

    # setup
    if self.seed is not None:
        np.random.seed(self.seed)
    # initialize weights
    self._initialize_weights(X)

    # create arrays for score metrics
    scores = self._initialize_scores(epochs)

    assert batches <= t.shape[0]
    batch_size = X.shape[0] // batches

    try:
        for epoch in range(epochs):
            for batch in range(batches):
                # minibatch gradient descent
                # If the for loop has reached the last batch, take all thats left
                if batch == batches - 1:
                    X_batch = X[batch * batch_size :, :, :, :]
                    t_batch = t[batch * batch_size :, :]
                else:
                    X_batch = X[
                        batch * batch_size : (batch + 1) * batch_size, :, :, :
                    ]
                    t_batch = t[batch * batch_size : (batch + 1) * batch_size, :]

                self._feedforward(X_batch)
                self._backpropagate(t_batch, lam)

            # reset schedulers for each epoch (some schedulers pass in this call)
            for layer in self.layers:
                if isinstance(layer, FullyConnectedLayer):
                    layer._reset_scheduler()

            # computing performance metrics
            scores = self._compute_scores(scores, epoch, X, t, X_val, t_val)

            # printing progress bar
            print_length = self._progress_bar(
                epoch,
                epochs,
                scores,
            )
    # allows for stopping training at any point and seeing the result
    except KeyboardInterrupt:
        pass

    # visualization of training progression (similiar to tensorflow progression bar)
    sys.stdout.write("\r" + " " * print_length)
    sys.stdout.flush()
    self._progress_bar(
        epochs,
        epochs,
        scores,
    )
    sys.stdout.write("")

    return scores

def _feedforward(self, X_batch) -> np.ndarray:
    """
    Description:
    ------------
```

```
            Performs the feedforward pass for all layers in the CNN. Called from fit()
        """
        a = X_batch
        for layer in self.layers:
            a = layer._feedforward(a)

        return a

    def _backpropagate(self, t_batch, lam) -> None:
        """
        Description:
        ------------
            Performs backpropagation for all layers in the CNN. Called from fit()
        """
        assert len(self.layers) >= 2
        reversed_layers = self.layers[::-1]

        # for every layer, backwards
        for i in range(len(reversed_layers) - 1):
            layer = reversed_layers[i]
            prev_layer = reversed_layers[i + 1]

            # OutputLayer
            if isinstance(layer, OutputLayer):
                prev_a = prev_layer.get_prev_a()
                weights_next, delta_next = layer._backpropagate(t_batch, prev_a, lam)

            # FullyConnectedLayer
            elif isinstance(layer, FullyConnectedLayer):
                assert (
                    delta_next is not None
                ), "No OutputLayer to follow FullyConnectedLayer"
                assert (
                    weights_next is not None
                ), "No OutputLayer to follow FullyConnectedLayer"
                prev_a = prev_layer.get_prev_a()
                weights_next, delta_next = layer._backpropagate(
                    weights_next, delta_next, prev_a, lam
                )

            # FlattenLayer
            elif isinstance(layer, FlattenLayer):
                assert (
                    delta_next is not None
                ), "No FullyConnectedLayer to follow FlattenLayer"
                assert (
                    weights_next is not None
                ), "No FullyConnectedLayer to follow FlattenLayer"
                delta_next = layer._backpropagate(weights_next, delta_next)

            # Convolution2DLayer and Convolution2DLayerOPT
            elif isinstance(layer, Convolution2DLayer):
                assert (
                    delta_next is not None
                ), "No FlattenLayer to follow Convolution2DLayer"
                delta_next = layer._backpropagate(delta_next)

            # Pooling2DLayer
            elif isinstance(layer, Pooling2DLayer):
                assert delta_next is not None, "No Layer to follow Pooling2DLayer"
                delta_next = layer._backpropagate(delta_next)
            # Catch error
            else:
                raise NotImplementedError

    def _compute_scores(
        self,
        scores: dict,
        epoch: int,
        X: np.ndarray,
        t: np.ndarray,
        X_val: np.ndarray,
        t_val: np.ndarray,
    ) -> dict:
        """
        Description:
        ------------
            Computes scores such as training error, training accuracy, validation error
            and validation accuracy for the CNN depending on if a validation set is used
            and if the CNN performs classification or regression

        Returns:
        ------------
            scores (dict) a dictionary with "train_error", "train_acc", "val_error", val_acc" key
            that contain numpy arrays with float values of all accuracies/errors over all epochs.
            Can be used to create plots. Also used to update the progress bar during training
        """

        pred_train = self.predict(X)
        cost_function_train = self.cost_func(t)
        train_error = cost_function_train(pred_train)
        scores["train_error"][epoch] = train_error

        if X_val is not None and t_val is not None:
            cost_function_val = self.cost_func(t_val)
            pred_val = self.predict(X_val)
            val_error = cost_function_val(pred_val)
            scores["val_error"][epoch] = val_error

        if self.pred_format != "Regression":
            train_acc = self._accuracy(pred_train, t)
            scores["train_acc"][epoch] = train_acc
            if X_val is not None and t_val is not None:
                val_acc = self._accuracy(pred_val, t_val)
                scores["val_acc"][epoch] = val_acc

        return scores

    def _initialize_scores(self, epochs) -> dict:
        """
        Description:
        ------------
            Initializes scores such as training error, training accuracy, validation error
            and validation accuracy for the CNN

        Returns:
        ------------
            A dictionary with "train_error", "train_acc", "val_error", val_acc" keys that
            will contain numpy arrays with float values of all accuracies/errors over all epochs
            when passed through the _compute_scores() function during fit()
        """
        scores = dict()

        train_errors = np.empty(epochs)
        train_errors.fill(np.nan)
        val_errors = np.empty(epochs)
        val_errors.fill(np.nan)

        train_accs = np.empty(epochs)
        train_accs.fill(np.nan)
        val_accs = np.empty(epochs)
        val_accs.fill(np.nan)

        scores["train_error"] = train_errors
        scores["val_error"] = val_errors
        scores["train_acc"] = train_accs
        scores["val_acc"] = val_accs

        return scores

    def _initialize_weights(self, X: np.ndarray) -> None:
        """
        Description:
        ------------
            Initializes weights for all layers in CNN

        Parameters:
        ------------
            I   X (np.ndarray) input of format [img, feature_maps, height, width]
        """
        prev_nodes = X
        for layer in self.layers:
            prev_nodes = layer._reset_weights(prev_nodes)

    def predict(self, X: np.ndarray, *, threshold=0.5) -> np.ndarray:
        """
        Description:
        ------------
            Predicts output of input X

        Parameters:
        ------------
            I   X (np.ndarray) input [img, feature_maps, height, width]
        """

        prediction = self._feedforward(X)

        if self.pred_format == "Binary":
            return np.where(prediction > threshold, 1, 0)
        elif self.pred_format == "Multi-class":
            class_prediction = np.zeros(prediction.shape)
            for i in range(prediction.shape[0]):
                class_prediction[i, np.argmax(prediction[i, :])] = 1
            return class_prediction
        else:
            return prediction

    def _accuracy(self, prediction: np.ndarray, target: np.ndarray) -> float:
        """
        Description:
        ------------
            Calculates accuracy of given prediction to target
        Parameters:
        ------------
            I   prediction (np.ndarray): output of predict() fuction
            (1s and 0s in case of classification, and real numbers in case of regression)
            II  target (np.ndarray): vector of true values (What the network should predict)

        Returns:
        ------------
            A floating point number representing the percentage of correctly classified instances
        """
        assert prediction.size == target.size
        return np.average((target == prediction))

    def _progress_bar(self, epoch: int, epochs: int, scores: dict) -> int:
        """
        Description:
        ------------
            Displays progress of training
        """
        progression = epoch / epochs
        epoch -= 1
        print_length = 40
        num_equals = int(progression * print_length)
        num_not = print_length - num_equals
        arrow = ">" if num_equals > 0 else ""
        bar = "[" + "=" * (num_equals - 1) + arrow + "-" * num_not + "]"
        perc_print = self._fmt(progression * 100, N=5)
        line = f"  {bar} {perc_print}% "

        for key, score in scores.items():
            if np.isnan(score[epoch]) == False:
                value = self._fmt(score[epoch], N=4)
                line += f"| {key}: {value} "
        print(line, end="\r")
        return len(line)

    def _fmt(self, value: int, N=4) -> str:
        """
        Description:
        ------------
            Formats decimal numbers for progress bar
        """
        if value > 0:
            v = value
        elif value < 0:
            v = -10 * value
        else:
            v = 1
        n = 1 + math.floor(math.log10(v))
        if n >= N - 1:
            return str(round(value))
            # or overflow
        return f"{value:.{N-n-1}f}"
```

Usage of CNN code. Using the CNN codebase is very simple. We begin by initiating a CNN object, which takes a cost function, a scheduler and a seed as its arguments. If a scheduler is not provided, it will per default initiate an

Adam scheduler with eta=1e-4, and if a seed is not provided, the CNN will not be seeded, meaning it will run with a different random seed every run. Below we demonstrate an initiation of our CNN.

```
adam_scheduler = Adam(eta=1e-3, rho=0.9, rho2=0.999)
cnn = CNN(cost_func=CostCrossEntropy, scheduler=adam_scheduler, seed=2023)
```

Now that we have our CNN object, we can begin to add layers to it! Many of the add_layer functions have default values, for example add_Convolution2DLayer() has a default v_stride and h_stride of 1. However, these can of course be set to any value you please. Note that the input channels of a subsequent convolutional layer must equal the previous convolutional layer's feature maps.

```
cnn.add_Convolution2DLayer(
    input_channels=1,
    feature_maps=1,
    kernel_height=3,
    kernel_width=3,
    act_func=LRELU,
)

cnn.add_FlattenLayer()

cnn.add_FullyConnectedLayer(30, LRELU)

cnn.add_FullyConnectedLayer(20, LRELU)

cnn.add_OutputLayer(10, softmax)
```

Here we have created a CNN with the following architecture:

1. A convolutional layer with 1 input channel, with a kernel height of 2 and a width of 2, which uses LRELU as its non-linearity function. This layer outputs 1 feature map, which feed into the subsequent layer.

2. A flatten layer

3. A hidden layer with 30 nodes, with LRELU as its activation function

4. Another hidden layer but with 20 nodes

5. The output layer, with softmax as its activation function and 10 nodes. We use 10 nodes because we will be using a dataset with 10 classes.

Now, before we can train the model, we need to load in our data. We will use the MNIST dataset and use 10000 28 × 28 images.

```
from sklearn.datasets import fetch_openml
from sklearn.model_selection import train_test_split

def onehot(target: np.ndarray):
    onehot = np.zeros((target.size, target.max() + 1))
    onehot[np.arange(target.size), target] = 1
    return onehot

# get dataset
dataset = fetch_openml("mnist_784", parser="auto")
mnist = dataset.data.to_numpy(dtype="float")[:10000, :]

# scale data
for i in range(mnist.shape[1]):
    mnist[:, i] /= 255

# reshape to add single input channel to data shape [inputs, input_channels, height, width]
mnist = mnist.reshape(mnist.shape[0], 1, 28, 28)

# one hot encode target as we are doing multi-class classification
target = onehot(np.array([int(i) for i in dataset.target.to_numpy()[:10000]]))

# split into training and validation data
x_train, x_val, y_train, y_val = train_test_split(mnist, target)
```

Now we may train our model. Note that we can utilize regularization in the CNN by using the lam (lambda) parameter in fit(), and utilize different types of gradient descent by specifying the amount of batches via the batches parameter as shown below.

The functionfit() returns a score dictionary of the training error and accuracy (and validation error and accuracy if a validation set is provided) which can be used to plot the error and accuracy of the model over epochs.

```
scores = cnn.fit(
    x_train,
    y_train,
    lam=1e-5,
    batches=10,
    epochs=100,
    X_val=x_val,
    t_val=y_val,
)

plt.plot(scores["train_acc"], label="Training")
plt.plot(scores["val_acc"], label="Validation")
plt.ylim([0.8,1])
plt.xlabel("Epochs")
plt.ylabel("Accuracy")
plt.legend()
plt.show()
```

Considering we only trained the model for 100 epochs without any tuning of the hyperparameters, this result is pretty good.

The codebase allows for great flexibility in CNN architectures. Pooling layers can be added before, inbetween or after convolutional layers, but due to the great optimizations made within Convolution2DLayerOPT, we recommend using the v_stride and h_stride parameters in add_Convolution2DLayer() to reduce the dimentionality of the problem as the pooling layer is slow in comparison. To use the unoptimized version of Convolution2DLayer, simply pass optimized=False as an argument in add_Convolution2DLayer().

If one wishes to perform binary classification using the CNN, simply use the cost function 'CostLogReg' when initializing the CNN and use 1 node at the OutputLayer.

Below we have created another, more untraditional architecture using our code to demonstrate its flexibility and different attributes such as asymmetric stride that might become useful when constructing your own CNN.

```
adam_scheduler = Adam(eta=1e-3, rho=0.9, rho2=0.999)
cnn = CNN(cost_func=CostCrossEntropy, scheduler=adam_scheduler, seed=2023)

cnn.add_Convolution2DLayer(
    input_channels=1,
    feature_maps=7,
    kernel_height=7,
    kernel_width=1,
    act_func=LRELU,
)

cnn.add_PoolingLayer(
    kernel_height=2,
    kernel_width=2,
    pooling="average",
)

cnn.add_PoolingLayer(
    kernel_height=2,
    kernel_width=2,
    pooling="max",
)

cnn.add_Convolution2DLayer(
    input_channels=7,
    feature_maps=1,
    kernel_height=4,
    kernel_width=4,
    v_stride=2,
    h_stride=3,
    act_func=LRELU,
    optimized=False,
)

cnn.add_Convolution2DLayer(
    input_channels=1,
    feature_maps=1,
    kernel_height=2,
    kernel_width=2,
    act_func=sigmoid,
    optimized=True,
)

cnn.add_PoolingLayer(
    kernel_height=2,
    kernel_width=2,
    pooling="max"
)

cnn.add_FlattenLayer()

cnn.add_FullyConnectedLayer(100, LRELU)
cnn.add_FullyConnectedLayer(10, sigmoid)

cnn.add_FullyConnectedLayer(101, identity)

cnn.add_OutputLayer(10, softmax)
```

Here we see the use of asymmetrical 1D kernels such as the 7 × 1 kernel in the first convolutional layer, both max and average pooling, asymmetric stride in the unoptimized convolutional layer, more pooling, a flatten layer, a hidden layer with 100 nodes using LRELU, another hidden layer with 10 hidden nodes that uses the sigmoid activation function, and another hidden layer with 101 nodes which utilizes no activation function (identity). Finally, we arrive at the output layer with 10 nodes, which uses softmax as its activation function.

Additional Remarks. The stride parameter controls the distance between each convolution and the kernel/filter. If our image is padded, stride is the only parameter that determines the size of the output from a convolutional layer. However, if we decide not to perform any padding, the size of the output feature map depends on both the stride and kernel size. It is important to note that neither the stride nor the kernel has to be symmetrical. This means that we can use a rectangular filter if we choose, and the stride in the vertical direction (axis=0 in Python) does not need to be the same as the stride in the horizontal direction (axis=1 in Python). It may even be the case that asymmetric combinations of stride or kernel dimensions, or both, yield better results than symmetric values for these parameters.

```
def convolve(image, kernel, stride=1):
    for i in range(2):
        kernel = np.rot90(kernel)

    k_half_height = kernel.shape[0] // 2
    k_half_width = kernel.shape[0] // 2

    conv_image = np.zeros(image.shape)
    pad_image = padding(image, kernel)

    for i in range(k_half_height, conv_image.shape[0] + k_half_height, stride):
        for j in range(k_half_width, conv_image.shape[1] + k_half_width, stride):
            conv_image[i - k_half_height, j - k_half_width] = np.sum(
                pad_image[
                    i - k_half_height : i + k_half_height + 1, j - k_half_width : j + k_half_width
                ]
                * kernel
            )

    return conv_image
```

Remarks on the speed. Despite the naive convolution algorithm shown above working finely, it is extremely slow, requiring approximately 20-30 seconds to process a single image. The time complexity of 2D convolution, which is

O(NMnm), rapidly becomes a constraint and may, at worst, make computations infeasible. Consequently, optimizing the naive 2D convolution algorithm is a necessity, as the execution time of the algorithm significantly increases as the input data size expands. This can pose a bottleneck in applications that necessitate real-time processing of large data volumes, such as image and video processing, deep learning, and scientific simulations.

To address this issue, we shall present two widely used optimization techniques: the separable kernel approach and Fast Fourier Transform (FFT). Both of these methods can drastically reduce the computational complexity of convolution and enhance the overall efficiency of processing substantial data quantities. While we shall refrain from delving into the intricacies of these algorithms, we strongly encourage you to examine at least the application of FFT to optimize computations.

Convolution using separable kernels.

```
def conv2DSep(image, kernel, coef, stride=1, pad="zero"):
    for i in range(2):
        kernel = np.rot90(kernel)

    # The kernel is quadratic, thus we only need one of its dimensions
    half_dim = kernel.shape[0] // 2

    ker1 = np.array(kernel[0, :])
    ker2 = np.array(kernel[:, 0])

    if pad == "zero":
        conv_image = np.zeros(image.shape)
        pad_image = padding(image, kernel)
    else:
        conv_image = np.zeros(
            (image.shape[0] - kernel.shape[0], image.shape[1] - kernel.shape[1])
        )
        pad_image = image[:, :]

    for i in range(half_dim, conv_image.shape[0] + half_dim, stride):
        for j in range(half_dim, conv_image.shape[1] + half_dim, stride):
            conv_image[i - half_dim, j - half_dim] = (
                pad_image[
                    i - half_dim : i + half_dim + 1, j - half_dim : j + half_dim + 1
                ]
                @ ker1
                @ ker2.T
                * coef
            )

    return conv_image

img_path = img_path = "data/IMG-2167.JPG"
image_of_cute_dog = imageio.imread(img_path, mode="L")
start_time = time.time()
filtered_image = conv2DSep(image_of_cute_dog, kernel=sobel_kernel, coef=1)
print(f'Time taken for convolution with seperated kernel on 128x128 image {time.time() - start_ti
plt.imshow(filtered_image, cmap="gray", vmin=0, vmax=255, aspect="auto")
plt.show()
```

By taking advantage of the capabilities of separable kernels, we can effectively cut the computational expense of filtering an image in half. Yet, if we seek even more rapid processing, we can turn to the Fast Fourier Transform (FFT) algorithm provided by the numpy library. By utilizing FFT to transform the input image and filter into the frequency domain, we can perform convolution in this domain. This approach significantly reduces the number of operations needed and results in a marked speedup relative to other convolution techniques. In addition, it is worth noting that the FFT is widely regarded as one of the most critical algorithms developed to date, with applications ranging from digital signal processing to scientific computing.

Convolution in the Fourier domain.

```
start_time = time.time()
img_fft = np.fft.fft2(image_of_cute_dog)
kernel_fft = np.fft.fft2(sobel_kernel, s=image_of_cute_dog.shape)

conv_image = img_fft * kernel_fft

filtered_image = np.fft.ifft2(conv_image)
print(f'Time take for convolution in the fourier domain: {time.time() - start_time}')
plt.imshow(filtered_image.real, cmap="gray", vmin=0, vmax=255, aspect="auto")
plt.show()
```

It is evident that executing convolution in the Fourier domain yields the quickest computation time. Nonetheless, one should exercise caution, particularly when dealing with images of relatively small dimensions, as one of the other methods may prove to be more expeditious than FFT-enhanced convolution. The overhead involved in transferring both the image and filter into the Fourier domain, followed by their subsequent transformation back into the spatial domain, results in a minor inconvenience. Therefore, it is imperative to remain cognizant of this fact when utilizing FFT as the primary optimization technique.

From NNs and CNNs to recurrent neural networks (RNNs)

There are limitation of NNs, one of which being that FFNNs are not designed to handle sequential data (data for which the order matters) effectively because they lack the capabilities of storing information about previous inputs; each input is being treated indepen- dently. This is a limitation when dealing with sequential data where past information can be vital to correctly process current and future inputs.

Feedback connections

In contrast to NNs, recurrent networks introduce feedback connections, meaning the information is allowed to be carried to subsequent nodes across different time steps. These cyclic or feedback connections have the objective of providing the network with some kind of memory, making RNNs particularly suited for time-series data, natural language processing, speech recognition, and several other problems for which the order of the data is crucial. The RNN architectures vary greatly in how they manage information flow and memory in the network.

Vanishing gradients

Different architectures often aim at improving some sub-optimal characteristics of the network. The simplest form of recurrent network, commonly called simple or vanilla RNN, for example, is known to suffer from the problem of vanishing gradients. This problem arises due to the nature of backpropagation in time. Gradients of the cost/loss function may get exponentially small (or large) if there are many layers in the network, which is the case of RNN when the sequence gets long.

Recurrent neural networks (RNNs): Overarching view

Till now our focus has been, including convolutional neural networks as well, on feedforward neural networks. The output or the activations flow only in one direction, from the input layer to the output layer.

A recurrent neural network (RNN) looks very much like a feedforward neural network, except that it also has connections pointing backward.

RNNs are used to analyze time series data such as stock prices, and tell you when to buy or sell. In autonomous driving systems, they can anticipate car trajectories and help avoid accidents. More generally, they can work on sequences of arbitrary lengths, rather than on fixed-sized inputs like all the nets we have discussed so far. For example, they can take sentences, documents, or audio samples as input, making them extremely useful for natural language processing systems such as automatic translation and speech-to-text.

Sequential data only?

An important issue is that in many deep learning methods we assume that the input and output data can be treated as independent and identically distributed, normally abbreviated to **iid**. This means that the data we use can be seen as mutually independent.

This is however not the case for most data sets used in RNNs since we are dealing with sequences of data with strong inter-dependencies. This applies in particular to time series, which are sequential by contruction.

Differential equations

As an example, the solutions of ordinary differential equations can be represented as a time series, similarly, how stock prices evolve as function of time is another example of a typical time series, or voice records and many other examples.

Not all sequential data may however have a time stamp, texts being a typical example thereof, or DNA sequences.

The main focus here is on data that can be structured either as time series or as ordered series of data. We will not focus on for example natural language processing or similar data sets.

A simple regression example using TensorFlow with Keras

```
# Start importing packages
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import tensorflow as tf
from tensorflow.keras import datasets, layers, models
from tensorflow.keras.layers import Input
from tensorflow.keras.models import Model, Sequential
from tensorflow.keras.layers import Dense, SimpleRNN, LSTM, GRU
from tensorflow.keras import optimizers
from tensorflow.keras import regularizers
from tensorflow.keras.utils import to_categorical

# convert into dataset matrix
def convertToMatrix(data, step):
 X, Y =[], []
 for i in range(len(data)-step):
  d=i+step
  X.append(data[i:d,])
  Y.append(data[d,])
 return np.array(X), np.array(Y)

step = 4
N = 1000
Tp = 800

t=np.arange(0,N)
x=np.sin(0.02*t)+2*np.random.rand(N)
df = pd.DataFrame(x)
df.head()
# Setting up training data
values=df.values
train,test = values[0:Tp,:], values[Tp:N,:]
# add step elements into train and test
test = np.append(test,np.repeat(test[-1,],step))
train = np.append(train,np.repeat(train[-1,],step))
trainX,trainY =convertToMatrix(train,step)
testX,testY =convertToMatrix(test,step)
trainX = np.reshape(trainX, (trainX.shape[0], 1, trainX.shape[1]))
testX = np.reshape(testX, (testX.shape[0], 1, testX.shape[1]))
# Defining the model with a simple RNN
model = Sequential()
model.add(SimpleRNN(units=32, input_shape=(1,step), activation="relu"))
model.add(Dense(8, activation="relu"))
model.add(Dense(1))
model.compile(loss='mean_squared_error', optimizer='rmsprop')
model.summary()
# Training
model.fit(trainX,trainY, epochs=100, batch_size=16, verbose=2)
trainPredict = model.predict(trainX)
testPredict= model.predict(testX)
predicted=np.concatenate((trainPredict,testPredict),axis=0)
trainScore = model.evaluate(trainX, trainY, verbose=0)
```

```
print(trainScore)
plt.plot(df)
plt.plot(predicted)
plt.show()
```

Corresponding example using PyTorch

The structure of the code here is as follows

1. Generate a sine function and splits it into training and validation sets
2. Create a custom data set for sequence generation
3. Define an RNN model with one RNN layer and a final plain linear layer
4. Train the model using the mean-squared error as cost function and the Adam optimizer
5. Generate predictions using recursive forecasting
6. Plot the results and training/validation loss curves

The model takes sequences of 20 previous values to predict the next value of the sine function. The recursive prediction uses the model's own predictions to generate future values, showing how well it maintains the sine wave pattern over time.

The final plots show the the predicted values vs. the actual sine wave for the validation period and the training and validation cost function curves to monitor for overfitting.

```
import torch
import torch.nn as nn
import numpy as np
import matplotlib.pyplot as plt

# Generate synthetic sine wave data
t = torch.linspace(0, 4*np.pi, 1000)
data = torch.sin(t)

# Split data into training and validation
train_data = data[:800]
val_data = data[800:]

# Hyperparameters
seq_len = 20
batch_size = 32
hidden_size = 64
num_epochs = 100
learning_rate = 0.001

# Create dataset and dataloaders
class SineDataset(torch.utils.data.Dataset):
   def __init__(self, data, seq_len):
       self.data = data
       self.seq_len = seq_len
```

```
    def __len__(self):
        return len(self.data) - self.seq_len

    def __getitem__(self, idx):
        x = self.data[idx:idx+self.seq_len]
        y = self.data[idx+self.seq_len]
        return x.unsqueeze(-1), y  # Add feature dimension

train_dataset = SineDataset(train_data, seq_len)
val_dataset = SineDataset(val_data, seq_len)

train_loader = torch.utils.data.DataLoader(train_dataset, batch_size=batch_size, shuffle=True)
val_loader = torch.utils.data.DataLoader(val_dataset, batch_size=batch_size, shuffle=False)

# Define RNN model
class RNNModel(nn.Module):
    def __init__(self, input_size, hidden_size, output_size):
        super(RNNModel, self).__init__()
        self.rnn = nn.RNN(input_size, hidden_size, batch_first=True)
        self.fc = nn.Linear(hidden_size, output_size)

    def forward(self, x):
        out, _ = self.rnn(x)  # out: (batch_size, seq_len, hidden_size)
        out = out[:, -1, :]   # Take last time step output
        out = self.fc(out)
        return out

model = RNNModel(input_size=1, hidden_size=hidden_size, output_size=1)
criterion = nn.MSELoss()
optimizer = torch.optim.Adam(model.parameters(), lr=learning_rate)

# Training loop
train_losses = []
val_losses = []

for epoch in range(num_epochs):
    model.train()
    epoch_train_loss = 0
    for x_batch, y_batch in train_loader:
        optimizer.zero_grad()
        y_pred = model(x_batch)
        loss = criterion(y_pred, y_batch.unsqueeze(-1))
        loss.backward()
        optimizer.step()
        epoch_train_loss += loss.item()

    # Validation
    model.eval()
    epoch_val_loss = 0
    with torch.no_grad():
        for x_val, y_val in val_loader:
            y_pred_val = model(x_val)
            val_loss = criterion(y_pred_val, y_val.unsqueeze(-1))
            epoch_val_loss += val_loss.item()

    # Calculate average losses
    train_loss = epoch_train_loss / len(train_loader)
    val_loss = epoch_val_loss / len(val_loader)
    train_losses.append(train_loss)
    val_losses.append(val_loss)
    print(f'Epoch {epoch+1}/{num_epochs}, Train Loss: {train_loss:.4f}, Val Loss: {val_loss:.4f}')

# Generate predictions
model.eval()
initial_sequence = train_data[-seq_len:].reshape(1, seq_len, 1)
predictions = []
current_sequence = initial_sequence.clone()

with torch.no_grad():
    for _ in range(len(val_data)):
        pred = model(current_sequence)
        predictions.append(pred.item())
        # Update sequence by removing first element and adding new prediction
        current_sequence = torch.cat([current_sequence[:, 1:, :], pred.unsqueeze(1)], dim=1)

# Plot results
plt.figure(figsize=(12, 6))
plt.plot(t[800:].numpy(), val_data.numpy(), label='True values')
plt.plot(t[800:].numpy(), predictions, label='Predictions')
plt.title('Sine Wave Prediction')
plt.xlabel('Time')
plt.ylabel('Value')
plt.legend()
plt.show()

# Plot training and validation loss
plt.figure(figsize=(10, 5))
plt.plot(train_losses, label='Training Loss')
plt.plot(val_losses, label='Validation Loss')
plt.title('Training and Validation Loss')
plt.xlabel('Epoch')
plt.ylabel('Loss')
plt.legend()
plt.show()
```

RNNs

RNNs are very powerful, because they combine two properties:

1. Distributed hidden state that allows them to store a lot of information about the past efficiently.

2. Non-linear dynamics that allows them to update their hidden state in complicated ways.

With enough neurons and time, RNNs can compute anything that can be computed by your computer.

What kinds of behaviour can RNNs exhibit?

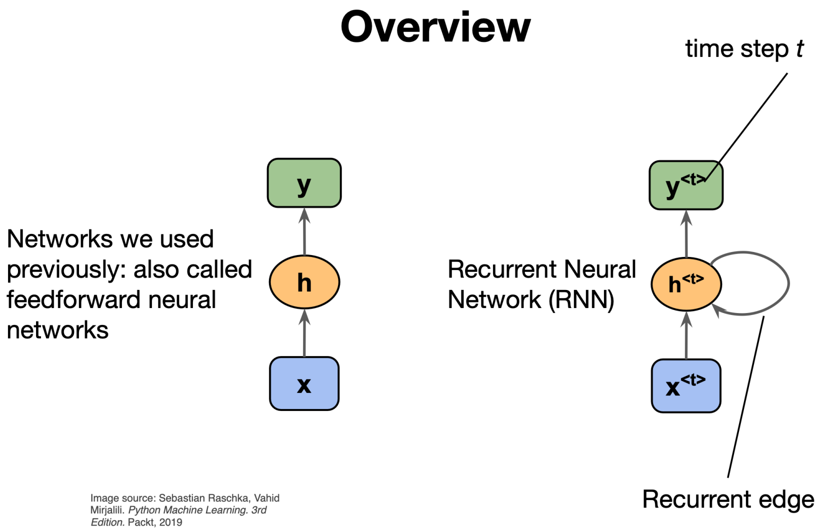
1. They can oscillate.

2. They can settle to point attractors.

3. They can behave chaotically.
4. RNNs could potentially learn to implement lots of small programs that each capture a nugget of knowledge and run in parallel, interacting to produce very complicated effects.

But the extensive computational needs of RNNs makes them very hard to train.

Basic layout, Figures from Sebastian Rashcka et al, Machine learning with Sickit-Learn and PyTorch



Overview

time step *t*
y
h
x
Networks we used previously: also called feedforward neural networks
Recurrent Neural Network (RNN)
$y^{<t>}$
$h^{<t>}$
$x^{<t>}$
Recurrent edge

Image source: Sebastian Raschka, Vahid Mirjalili. *Python Machine Learning. 3rd Edition.* Packt, 2019

Solving differential equations with RNNs

To gain some intuition on how we can use RNNs for time series, let us tailor the representation of the solution of a differential equation as a time series.

Consider the famous differential equation (Newton's equation of motion for damped harmonic oscillations, scaled in terms of dimensionless time)

$$\frac{d^2x}{dt^2} + \eta\frac{dx}{dt} + x(t) = F(t),$$

where η is a constant used in scaling time into a dimensionless variable and $F(t)$ is an external force acting on the system. The constant η is a so-called damping.

Two first-order differential equations

In solving the above second-order equation, it is common to rewrite it in terms of two coupled first-order equations with the velocity

$$v(t) = \frac{dx}{dt},$$

and the acceleration

$$\frac{dv}{dt} = F(t) - \eta v(t) - x(t).$$

With the initial conditions $v_0 = v(t_0)$ and $x_0 = x(t_0)$ defined, we can integrate these equations and find their respective solutions.

Velocity only

Let us focus on the velocity only. Discretizing and using the simplest possible approximation for the derivative, we have Euler's forward method for the updated velocity at a time step $i+1$ given by

$$v_{i+1} = v_i + \Delta t \frac{dv}{dt}_{|_{v=v_i}} = v_i + \Delta t \left(F_i - \eta v_i - x_i\right).$$

Defining a function

$$h_i(x_i, v_i, F_i) = v_i + \Delta t \left(F_i - \eta v_i - x_i\right),$$

we have

$$v_{i+1} = h_i(x_i, v_i, F_i).$$

Linking with RNNs

The equation

$$v_{i+1} = h_i(x_i, v_i, F_i).$$

can be used to train a feed-forward neural network with inputs v_i and outputs v_{i+1} at a time t_i. But we can think of this also as a recurrent neural network with inputs v_i, x_i and F_i at each time step t_i, and producing an output v_{i+1}.

Noting that

$$v_i = v_{i-1} + \Delta t \left(F_{i-1} - \eta v_{i-1} - x_{i-1}\right) = h_{i-1}.$$

we have

$$v_i = h_{i-1}(x_{i-1}, v_{i-1}, F_{i-1}),$$

and we can rewrite

$$v_{i+1} = h_i(x_i, h_{i-1}, F_i).$$

Minor rewrite

We can thus set up a recurring series which depends on the inputs x_i and F_i and the previous values h_{i-1}. We assume now that the inputs at each step (or time t_i) is given by x_i only and we denote the outputs for $\tilde{y}_i$ instead of v_{i_1}, we have then the compact equation for our outputs at each step t_i

$$y_i = h_i(x_i, h_{i-1}).$$

We can think of this as an element in a recurrent network where our network (our model) produces an output y_i which is then compared with a target value through a given cost/loss function that we optimize. The target values at a given step t_i could be the results of a measurement or simply the analytical results of a differential equation.

RNNs in more detail

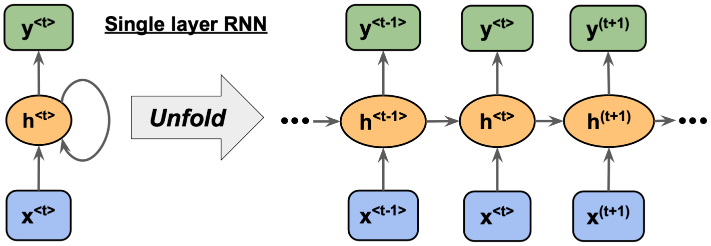
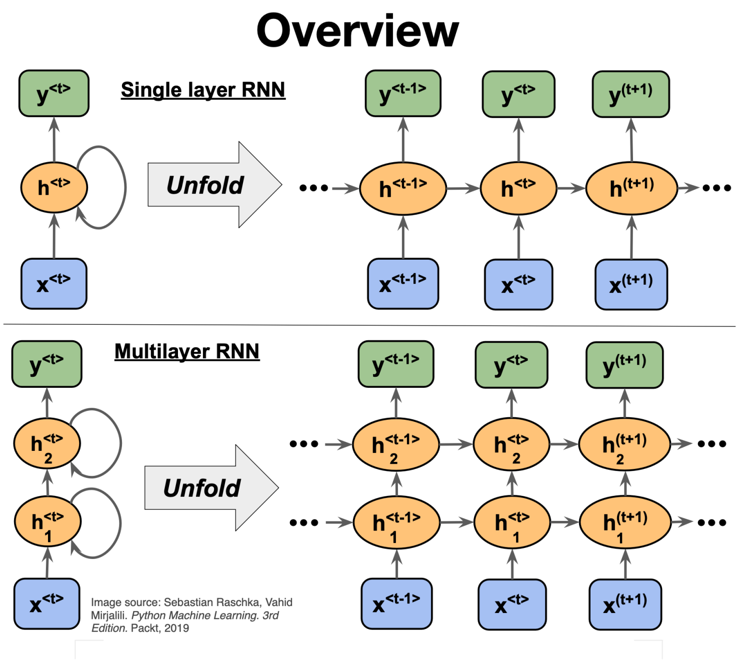


Image source: Sebastian Raschka, Vahid Mirjalili. *Python Machine Learning. 3rd Edition.* Packt, 2019

RNNs in more detail, part 2



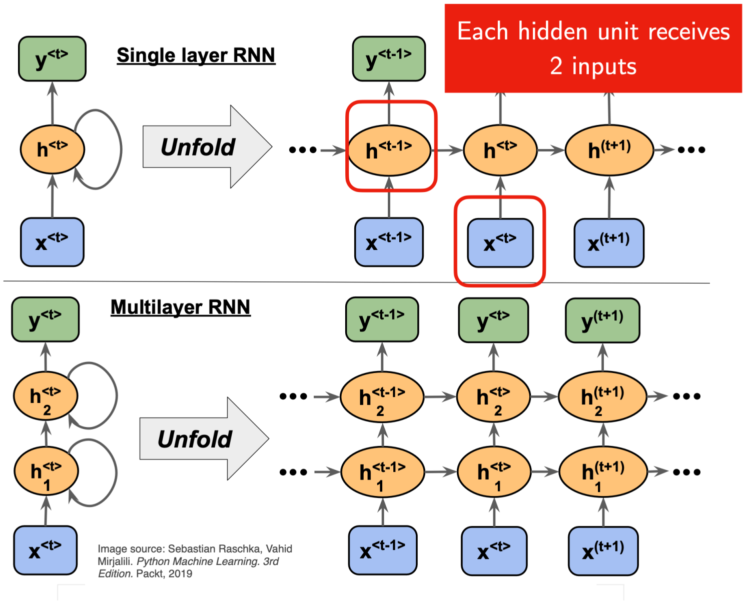
Overview

Single layer RNN

Multilayer RNN

Image source: Sebastian Raschka, Vahid Mirjalili. *Python Machine Learning. 3rd Edition.* Packt, 2019

RNNs in more detail, part 3



Each hidden unit receives 2 inputs

Image source: Sebastian Raschka, Vahid Mirjalili. *Python Machine Learning. 3rd Edition.* Packt, 2019

RNNs in more detail, part 4

Different Types of Sequence Modeling Tasks

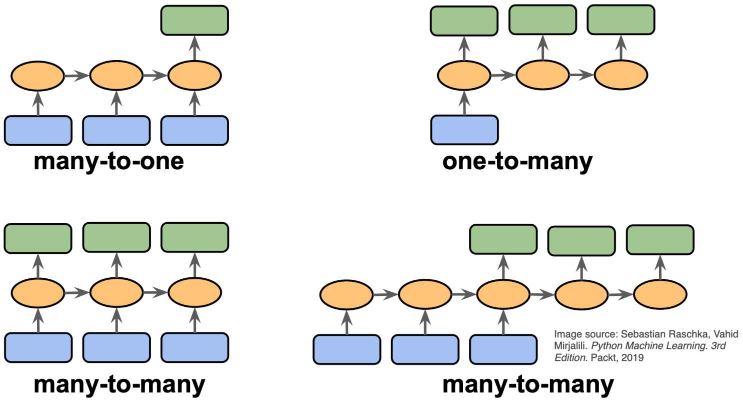
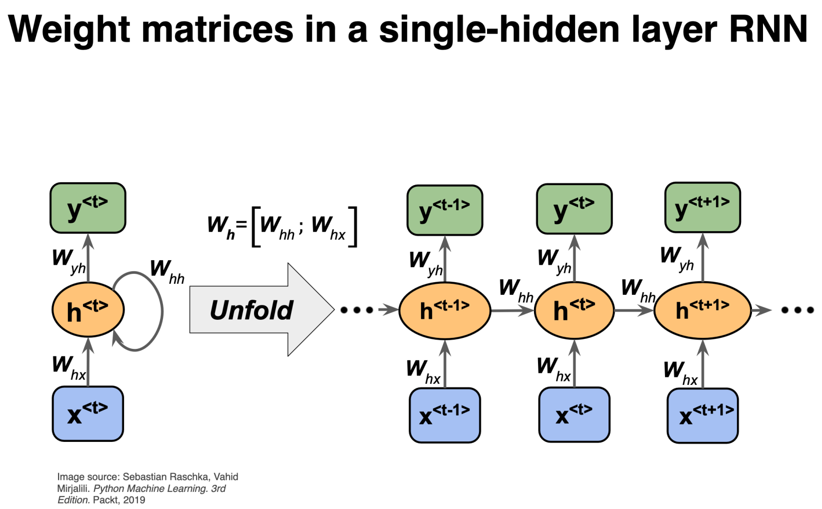


Image source: Sebastian Raschka, Vahid Mirjalili. *Python Machine Learning. 3rd Edition.* Packt, 2019

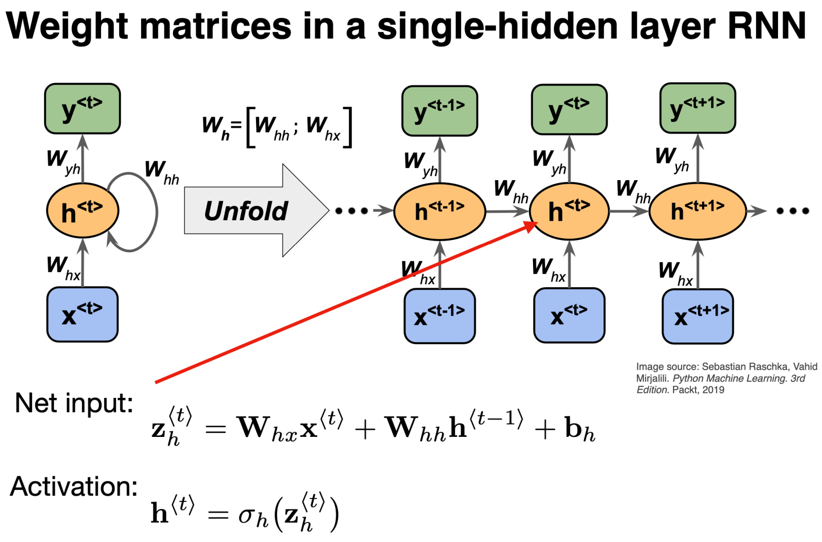
RNNs in more detail, part 5



Weight matrices in a single-hidden layer RNN

Image source: Sebastian Raschka, Vahid Mirjalili. *Python Machine Learning. 3rd Edition.* Packt, 2019

RNNs in more detail, part 6

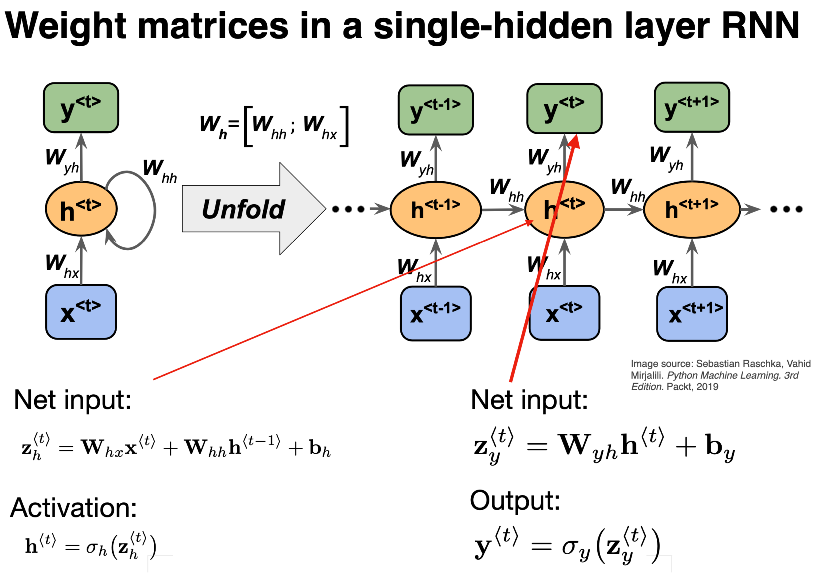


Weight matrices in a single-hidden layer RNN

Image source: Sebastian Raschka, Vahid Mirjalili. *Python Machine Learning. 3rd Edition.* Packt, 2019

Net input: $\mathbf{z}_h^{\langle t \rangle} = \mathbf{W}_{hx}\mathbf{x}^{\langle t \rangle} + \mathbf{W}_{hh}\mathbf{h}^{\langle t-1 \rangle} + \mathbf{b}_h$

Activation: $\mathbf{h}^{\langle t \rangle} = \sigma_h\big(\mathbf{z}_h^{\langle t \rangle}\big)$



Weight matrices in a single-hidden layer RNN

Image source: Sebastian Raschka, Vahid Mirjalili. *Python Machine Learning. 3rd Edition.* Packt, 2019

Net input:

$$\mathbf{z}_h^{\langle t \rangle} = \mathbf{W}_{hx}\mathbf{x}^{\langle t \rangle} + \mathbf{W}_{hh}\mathbf{h}^{\langle t-1 \rangle} + \mathbf{b}_h$$

Activation:

$$\mathbf{h}^{\langle t \rangle} = \sigma_h\big(\mathbf{z}_h^{\langle t \rangle}\big)$$

Net input:

$$\mathbf{z}_y^{\langle t \rangle} = \mathbf{W}_{yh}\mathbf{h}^{\langle t \rangle} + \mathbf{b}_y$$

Output:

$$\mathbf{y}^{\langle t \rangle} = \sigma_y\big(\mathbf{z}_y^{\langle t \rangle}\big)$$

Backpropagation through time

We can think of the recurrent net as a layered, feed-forward net with shared weights and then train the feed-forward net with weight constraints.

We can also think of this training algorithm in the time domain:

1. The forward pass builds up a stack of the activities of all the units at each time step.

2. The backward pass peels activities off the stack to compute the error derivatives at each time step.

3. After the backward pass we add together the derivatives at all the different times for each weight.

The backward pass is linear

1. There is a big difference between the forward and backward passes.

2. In the forward pass we use squashing functions (like the logistic) to prevent the activity vectors from exploding.

3. The backward pass, is completely linear. If you double the error derivatives at the final layer, all the error derivatives will double.

The forward pass determines the slope of the linear function used for backpropagating through each neuron

The problem of exploding or vanishing gradients

- What happens to the magnitude of the gradients as we backpropagate through many layers?
    1. If the weights are small, the gradients shrink exponentially.
    2. If the weights are big the gradients grow exponentially.

- Typical feed-forward neural nets can cope with these exponential effects because they only have a few hidden layers.
- In an RNN trained on long sequences (e.g. 100 time steps) the gradients can easily explode or vanish.
    1. We can avoid this by initializing the weights very carefully.

- Even with good initial weights, its very hard to detect that the current target output depends on an input from many time-steps ago.

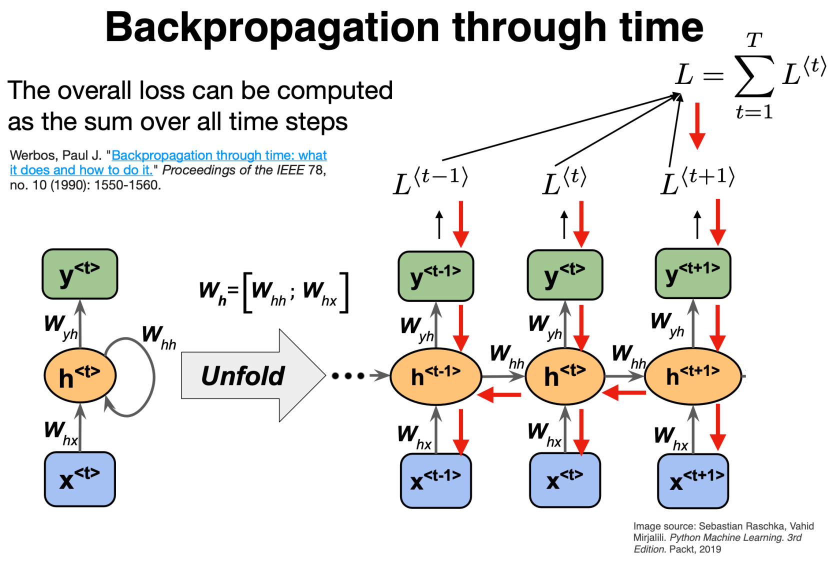
RNNs have difficulty dealing with long-range dependencies.

Mathematical setup

The expression for the simplest Recurrent network resembles that of a regular feed-forward neural network, but now with the concept of temporal dependencies

$$\begin{aligned}
\mathbf{a}^{(t)} &= U * \mathbf{x}^{(t)} + W * \mathbf{h}^{(t-1)} + \mathbf{b}, \\
\mathbf{h}^{(t)} &= \sigma_h(\mathbf{a}^{(t)}), \\
\mathbf{y}^{(t)} &= V * \mathbf{h}^{(t)} + \mathbf{c}, \\
\hat{\mathbf{y}}^{(t)} &= \sigma_y(\mathbf{y}^{(t)}).
\end{aligned}$$

Back propagation in time through figures, part 1



Backpropagation through time

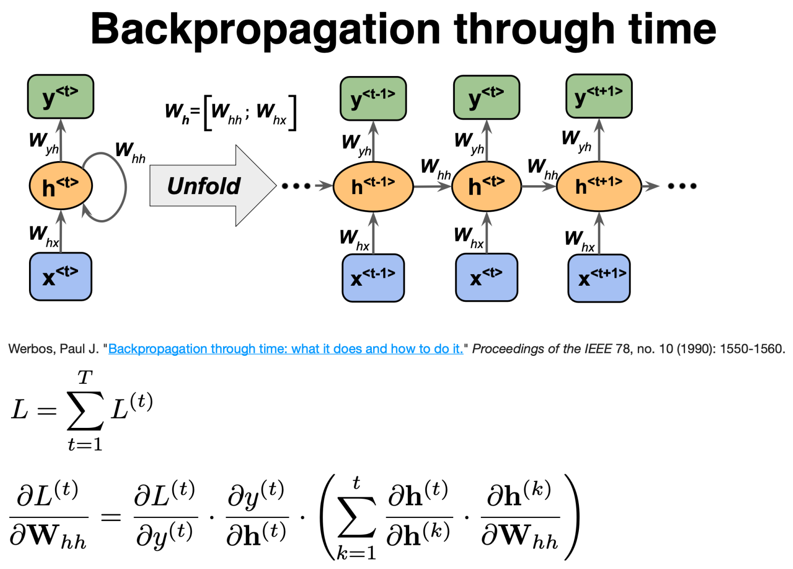
The overall loss can be computed as the sum over all time steps

Werbos, Paul J. "Backpropagation through time: what it does and how to do it." *Proceedings of the IEEE* 78, no. 10 (1990): 1550-1560.

$$L = \sum_{t=1}^{T} L^{\langle t \rangle}$$

Image source: Sebastian Raschka, Vahid Mirjalili. *Python Machine Learning. 3rd Edition.* Packt, 2019

Back propagation in time, part 2



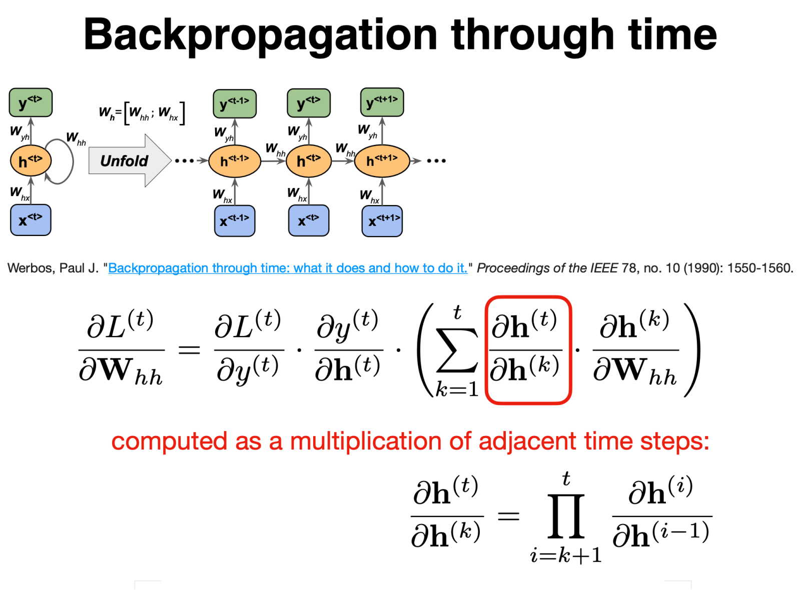
Backpropagation through time

Werbos, Paul J. "Backpropagation through time: what it does and how to do it." *Proceedings of the IEEE* 78, no. 10 (1990): 1550-1560.

$$L = \sum_{t=1}^{T} L^{(t)}$$

$$\frac{\partial L^{(t)}}{\partial \mathbf{W}_{hh}} = \frac{\partial L^{(t)}}{\partial y^{(t)}} \cdot \frac{\partial y^{(t)}}{\partial \mathbf{h}^{(t)}} \cdot \left(\sum_{k=1}^{t} \frac{\partial \mathbf{h}^{(t)}}{\partial \mathbf{h}^{(k)}} \cdot \frac{\partial \mathbf{h}^{(k)}}{\partial \mathbf{W}_{hh}} \right)$$

Back propagation in time, part 3



Backpropagation through time

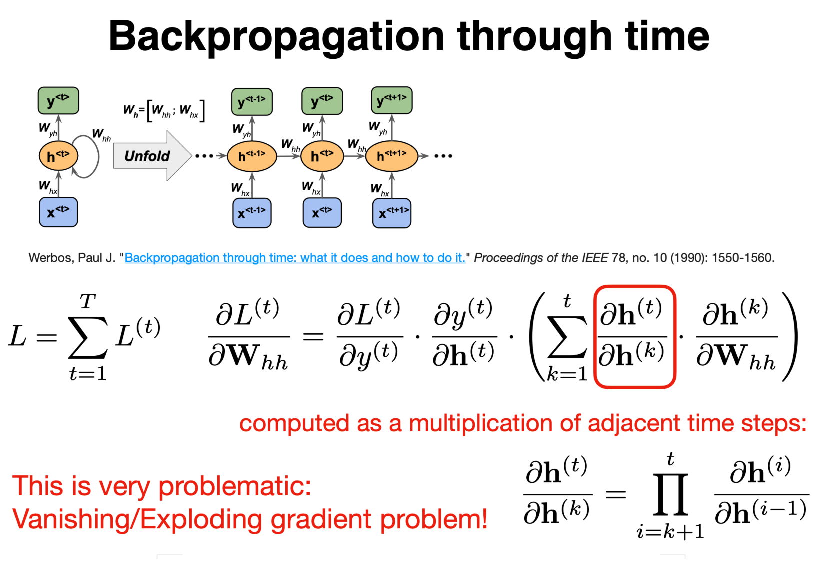
Werbos, Paul J. "Backpropagation through time: what it does and how to do it." *Proceedings of the IEEE* 78, no. 10 (1990): 1550-1560.

$$\frac{\partial L^{(t)}}{\partial \mathbf{W}_{hh}} = \frac{\partial L^{(t)}}{\partial y^{(t)}} \cdot \frac{\partial y^{(t)}}{\partial \mathbf{h}^{(t)}} \cdot \left(\sum_{k=1}^{t} \boxed{\frac{\partial \mathbf{h}^{(t)}}{\partial \mathbf{h}^{(k)}}} \cdot \frac{\partial \mathbf{h}^{(k)}}{\partial \mathbf{W}_{hh}} \right)$$

computed as a multiplication of adjacent time steps:

$$\frac{\partial \mathbf{h}^{(t)}}{\partial \mathbf{h}^{(k)}} = \prod_{i=k+1}^{t} \frac{\partial \mathbf{h}^{(i)}}{\partial \mathbf{h}^{(i-1)}}$$

Back propagation in time, part 4



Backpropagation through time

Werbos, Paul J. "Backpropagation through time: what it does and how to do it." *Proceedings of the IEEE* 78, no. 10 (1990): 1550-1560.

$$L = \sum_{t=1}^{T} L^{(t)} \qquad \frac{\partial L^{(t)}}{\partial \mathbf{W}_{hh}} = \frac{\partial L^{(t)}}{\partial y^{(t)}} \cdot \frac{\partial y^{(t)}}{\partial \mathbf{h}^{(t)}} \cdot \left(\sum_{k=1}^{t} \boxed{\frac{\partial \mathbf{h}^{(t)}}{\partial \mathbf{h}^{(k)}}} \cdot \frac{\partial \mathbf{h}^{(k)}}{\partial \mathbf{W}_{hh}} \right)$$

computed as a multiplication of adjacent time steps:

This is very problematic:
Vanishing/Exploding gradient problem!

$$\frac{\partial \mathbf{h}^{(t)}}{\partial \mathbf{h}^{(k)}} = \prod_{i=k+1}^{t} \frac{\partial \mathbf{h}^{(i)}}{\partial \mathbf{h}^{(i-1)}}$$

Back propagation in time in equations

To derive the expression of the gradients of $\mathcal{L}$ for the RNN, we need to start recursively from the nodes closer to the output layer in the temporal unrolling scheme - such as $\mathbf{y}$ and $\mathbf{h}$ at final time $t = \tau$,

$$
\begin{aligned}
(\nabla_{\mathbf{y}^{(t)}} \mathcal{L})_i &= \frac{\partial \mathcal{L}}{\partial L^{(t)}} \frac{\partial L^{(t)}}{\partial y_i^{(t)}}, \\
\nabla_{\mathbf{h}^{(\tau)}} \mathcal{L} &= \mathbf{V}^{\mathsf{T}} \nabla_{\mathbf{y}^{(\tau)}} \mathcal{L}.
\end{aligned}
$$

Chain rule again

For the following hidden nodes, we have to iterate through time, so by the chain rule,

$$
\nabla_{\mathbf{h}^{(t)}} \mathcal{L} = \left(\frac{\partial \mathbf{h}^{(t+1)}}{\partial \mathbf{h}^{(t)}} \right)^{\mathsf{T}} \nabla_{\mathbf{h}^{(t+1)}} \mathcal{L} + \left(\frac{\partial \mathbf{y}^{(t)}}{\partial \mathbf{h}^{(t)}} \right)^{\mathsf{T}} \nabla_{\mathbf{y}^{(t)}} \mathcal{L}.
$$

Gradients of loss functions

Similarly, the gradients of $\mathcal{L}$ with respect to the weights and biases follow,

$$
\begin{aligned}
\nabla_{\mathbf{c}} \mathcal{L} &= \sum_t \left(\frac{\partial \mathbf{y}^{(t)}}{\partial \mathbf{c}} \right)^{\mathsf{T}} \nabla_{\mathbf{y}^{(t)}} \mathcal{L} \\
\nabla_{\mathbf{b}} \mathcal{L} &= \sum_t \left(\frac{\partial \mathbf{h}^{(t)}}{\partial \mathbf{b}} \right)^{\mathsf{T}} \nabla_{\mathbf{h}^{(t)}} \mathcal{L} \\
\nabla_{\mathbf{V}} \mathcal{L} &= \sum_t \sum_i \left(\frac{\partial \mathcal{L}}{\partial y_i^{(t)}} \right) \nabla_{\mathbf{V}^{(t)}} y_i^{(t)} \\
\nabla_{\mathbf{W}} \mathcal{L} &= \sum_t \sum_i \left(\frac{\partial \mathcal{L}}{\partial h_i^{(t)}} \right) \nabla_{\mathbf{w}^{(t)}} h_i^{(t)} \\
\nabla_{\mathbf{U}} \mathcal{L} &= \sum_t \sum_i \left(\frac{\partial \mathcal{L}}{\partial h_i^{(t)}} \right) \nabla_{\mathbf{U}^{(t)}} h_i^{(t)}.
\end{aligned}
$$

Summary of RNNs

Recurrent neural networks (RNNs) have in general no probabilistic component in a model. With a given fixed input and target from data, the RNNs learn the intermediate association between various layers. The inputs, outputs, and internal representation (hidden states) are all real-valued vectors.

In a traditional NN, it is assumed that every input is independent of each other. But with sequential data, the input at a given stage t depends on the input from the previous stage $t-1$

Summary of a typical RNN

1. Weight matrices U, W and V that connect the input layer at a stage t with the hidden layer h_t, the previous hidden layer h_{t-1} with h_t and the hidden layer h_t connecting with the output layer at the same stage and producing an output $\tilde{y}_t$, respectively.

2. The output from the hidden layer h_t is oftem modulated by a $\tanh$ function $h_t = \sigma_h(x_t, h_{t-1}) = \tanh(Ux_t + Wh_{t-1} + b)$ with b a bias value

3. The output from the hidden layer produces $\tilde{y}_t = \sigma_y(Vh_t + c)$ where c is a new bias parameter.

4. The output from the training at a given stage is in turn compared with the observation y_t thorugh a chosen cost function.

The function g can any of the standard activation functions, that is a Sigmoid, a Softmax, a ReLU and other. The parameters are trained through the so-called back-propagation through time (BPTT) algorithm.

Four effective ways to learn an RNN and preparing for next week

1. Long Short Term Memory Make the RNN out of little modules that are designed to remember values for a long time.

2. Hessian Free Optimization: Deal with the vanishing gradients problem by using a fancy optimizer that can detect directions with a tiny gradient but even smaller curvature.

3. Echo State Networks: Initialize the input a hidden and hidden-hidden and output-hidden connections very carefully so that the hidden state has a huge reservoir of weakly coupled oscillators which can be selectively driven by the input.

   - ESNs only need to learn the hidden-output connections.

4. Good initialization with momentum Initialize like in Echo State Networks, but then learn all of the connections using momentum