Assignment9_Solutions

June 30, 2021

```
In [94]: import pandas as pd
         import numpy as np
         from numpy.random import seed
         import matplotlib.pyplot as plt
         import skimage.measure
         import tensorflow as tf
         import torchvision.transforms as transforms
         import torchvision.datasets as datasets
         from tensorflow import keras
         from tensorflow.keras import layers
         from sklearn.preprocessing import StandardScaler
         from sklearn.ensemble import RandomForestClassifier, GradientBoostingClassifier
         from sklearn.linear_model import LogisticRegression
         from sklearn.model_selection import GridSearchCV, KFold, cross_val_predict, train_tes
         from sklearn.calibration import calibration_curve
         from keras.applications.vgg16 import VGG16
         from keras.utils.vis_utils import plot_model
         from keras.preprocessing.image import load_img
         from keras.preprocessing.image import img_to_array
         from keras.applications.vgg16 import preprocess_input
         from keras.applications.vgg16 import decode_predictions
         from keras.wrappers.scikit_learn import KerasClassifier
In [44]: # !pip install -q -U keras-tuner
In [45]: import kerastuner as kt
         from kerastuner import HyperModel
```

0.1 Biomedical Data Science & AI

0.2 Assignment 9

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0.2.1 Exercise 1 - Basics of NN

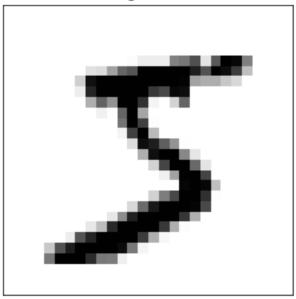
From the MNIST database load the handwritten digits dataset.

1.1. Normalize your dataset before training your model.

```
In [47]: # For normalization we scale the images to contain values in [0, 1]
    x_train = x_train.astype("float32") / 255
    x_test = x_test.astype("float32") / 255
    # Alternative approach:
    # x_train = tf.keras.utils.normalize(x_train, axis=1)

# Print the first image to get an idea of the data
    index = 0
    _classification = y_train[0]
    plt.imshow(x_train[0], cmap=plt.cm.binary); plt.title(f"Image of a {_classification}", plt.xticks([]); plt.yticks([]); plt.show()
```





```
In [48]: # Check, that all images have shape (28, 28, 1)
    x_train = np.expand_dims(x_train, -1)
    x_test = np.expand_dims(x_test, -1)
    input_shape = x_train[0].shape
```

```
print(x_train.shape[0], "train samples")
    print(x_test.shape[0], "test samples")

x_train shape: (60000, 28, 28, 1)
60000 train samples
10000 test samples

In [49]: # Check, if the number of classes is ten (since there are ten digits 0,...,9)
    num_classes = 10

    if num_classes == len(set(y_train)) == len(set(y_test)): print(f"There are {num_classes})
There are 10 classes.
```

1.2. Train a neural network once using Adam and once using AdaGrad optimizer. *Hint*: Set epochs to 20, neurons of hidden layer to 100 and use the ReLU as activation function.

print("x_train shape:", x_train.shape)

```
In [50]: num_epochs = 20
        num_hidden_neurons = 100
         activation_fct = "relu"
         # Alternative:
         \# \ activation\_fct = tf.nn.relu
         loss = "sparse_categorical_crossentropy"
In [51]: model = keras.Sequential(
                 # Input layer (size 28x28 -> 784)
                 keras.Input(shape=input_shape),
                 layers.Flatten(),
                 # One hidden layer (size 'num_hidden_neurons'=100)
                 layers.Dense(num_hidden_neurons, activation=activation_fct),
                 # Output layer (size 10)
                 # Use 'softmax' to get a probability for the digits 0,...,9 as classification
                 layers.Dense(num_classes, activation="softmax")
             ]
         )
         model.summary()
```

WARNING:tensorflow:Please add `keras.layers.InputLayer` instead of `keras.Input` to Sequential

3

Model: "sequential_120"

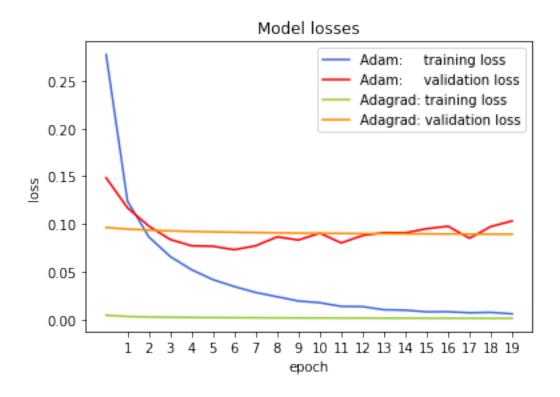
```
Layer (type)
           Output Shape
                     Param #
______
flatten_120 (Flatten)
           (None, 784)
_____
dense 298 (Dense)
           (None, 100)
                     78500
-----
dense 299 (Dense)
          (None, 10)
                     1010
______
Total params: 79,510
Trainable params: 79,510
Non-trainable params: 0
In [52]: # Compile the model with 'adam'
   model.compile(loss=loss, optimizer="adam", metrics=["accuracy"])
   # Train the model
   # Also pass the validation data, because this way the history will contain
   # the loss and accuracy w.r.t. to the validation data too (for later use)
   %time history_adam = model.fit(x_train, y_train, epochs=num_epochs, validation_data=(
   # Save the score (validation loss and validation accuracy) for later use
   score_adam = model.evaluate(x_test, y_test, verbose=0)
Epoch 1/20
Epoch 2/20
Epoch 3/20
Epoch 4/20
Epoch 5/20
Epoch 6/20
Epoch 7/20
Epoch 8/20
Epoch 9/20
Epoch 10/20
Epoch 11/20
Epoch 12/20
```

```
Epoch 13/20
Epoch 14/20
Epoch 15/20
Epoch 16/20
Epoch 17/20
Epoch 18/20
Epoch 19/20
Epoch 20/20
CPU times: user 1min 45s, sys: 8.15 s, total: 1min 53s
Wall time: 1min 25s
In [53]: # Now do the same using AdaGrad. First compile the model
  model.compile(loss=loss, optimizer="adagrad", metrics=["accuracy"])
  # Train the model
  %time history_adagrad = model.fit(x_train, y_train, epochs=num_epochs, validation_date
  # Save the score (validation loss and validation accuracy) for later use
  score_adagrad = model.evaluate(x_test, y_test, verbose=0)
Epoch 1/20
Epoch 2/20
Epoch 3/20
Epoch 4/20
Epoch 5/20
Epoch 6/20
Epoch 7/20
Epoch 8/20
Epoch 9/20
```

```
Epoch 10/20
Epoch 11/20
Epoch 12/20
Epoch 13/20
Epoch 14/20
Epoch 15/20
Epoch 16/20
Epoch 17/20
Epoch 18/20
Epoch 19/20
Epoch 20/20
CPU times: user 1min 36s, sys: 6.44 s, total: 1min 42s
Wall time: 1min 20s
In [54]: # Compare the scores of the two models
                                       Validation loss: {score_adam[0]:.2f},\tValidation accuracy: {score_a
              print(f'ADAM:
              print(f'ADAGRAD: Validation loss: {score_adagrad[0]:.2f},\tValidation accuracy: {score_
              Validation loss: 0.10,
                                                             Validation accuracy: 97.74 %
ADAM:
                                                             Validation accuracy: 98.07 %
ADAGRAD: Validation loss: 0.09,
```

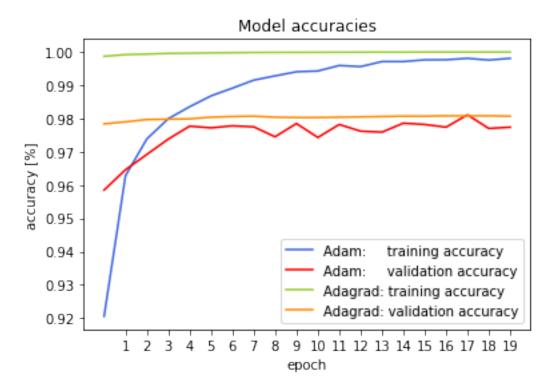
1.3. Plot the *SparseCategoricalCrossentropy* loss for both models. Plot the computed accuracy for both models. Which model performed better while training?

```
plt.ylabel('loss')
plt.xlabel('epoch')
plt.xticks(range(1, num_epochs))
plt.legend(['Adam: training loss', 'Adam: validation loss', 'Adagrad: training plt.show()
```



1.4. Compute the model accuracy on the test set for both optimizers. Which model performed better?

```
plt.title('Model accuracies')
plt.ylabel('accuracy [%]')
plt.xlabel('epoch')
plt.xticks(range(1, num_epochs))
plt.legend(['Adam: training accuracy', 'Adam: validation accuracy', 'Adagrad:
plt.show()
```



1.5. Familiarize yourself with Layer Normalization and explain how it works. Layer normalization is the process of normalizing the activations of layers *for each given example* in a batch *independently.*

Thus it is similar to batch normalization, but does not have the same limitations. Limitations of batch normalization that layer normalization does not have are: - normalization accross a batch and thus dependent of the other examples in the batch - no obvious application to *recurrent NN* (*RNN*): The summed inputs often vary with the length of the sequence! - no application to online learning algorithms

Furthermore, unlike batch normalization, layer normalization performs exactly the same computation at training and *validation*.

Important **benefits** of batch normalization are also given by layer normalization: - stabilizes the hidden state dynamics in recurrent networks - can substantially reduce the training time

Mathematical description of layer normalization:

Let - a^l be the vector representation of the summed inputs to the neurons in layer l, - W^l be the weights between layer l - 1 and l, - x^l the inputs for layer l, - b^l the bias of layer l and - f activation function.

It is

$$a_i^l = w_i^{l \mathsf{T}} x^l, \qquad \qquad x_i^{l+1} = f(a_i^l + b_i^l)$$

For layer normalization, adjust the mean and variance of every layer to be the mean and variance over *all hidden units in the same layer*. Let *l* be a layer with *H* neurons. Define

$$\mu^l := rac{1}{H} \sum_{i=1}^{H} a_i^l, \qquad \qquad \sigma^l := \sqrt{rac{1}{H} \sum_{i=1}^{H} (a_i^l - \mu^l)^2}$$

Source:

• "Layer Normalization" by Jimmy Lei Ba, Jamie Ryan Kiros and Geoffrey E. Hinton (2016)

1.6. Use the same dataset to train a neural network with Layer Normalization.

```
In [59]: model = keras.Sequential(
                 # Input layer (size 28x28 -> 784)
                keras.Input(shape=input_shape),
                layers.Flatten(),
                 # TODO: since the input was originally normalized, if this necessary here too
                 layers.LayerNormalization(axis=1),
                 # One hidden layer (size 'num_hidden_neurons'=100)
                 layers.Dense(num_hidden_neurons, activation=activation_fct),
                 layers.LayerNormalization(axis=1),
                 # Output layer (size 10)
                 # Use 'softmax' to get a probability for the digits 0,...,9 as classification
                 layers.Dense(num_classes, activation="softmax")
             ]
         )
        model.summary()
WARNING:tensorflow:Please add `keras.layers.InputLayer` instead of `keras.Input` to Sequential
Model: "sequential_121"
Layer (type)
                           Output Shape
                                                     Param #
                         (None, 784)
flatten_121 (Flatten)
layer_normalization (LayerNo (None, 784)
                                                       1568
                            (None, 100)
dense_300 (Dense)
                                                       78500
layer_normalization_1 (Layer (None, 100)
                                                       200
```

```
dense_301 (Dense)
        (None, 10)
                1010
______
Total params: 81,278
Trainable params: 81,278
Non-trainable params: 0
In [60]: # Lets use AdaGrad, since it performed better. First compile the model
  model.compile(loss=loss, optimizer="adagrad", metrics=["accuracy"])
  # Train the model
  %time history = model.fit(x_train, y_train, epochs=num_epochs, validation_data=(x_tes
  # Save the score (validation loss and validation accuracy) for later use
  score = model.evaluate(x_test, y_test, verbose=0)
Epoch 1/20
Epoch 2/20
Epoch 3/20
Epoch 4/20
Epoch 5/20
Epoch 6/20
Epoch 7/20
Epoch 8/20
Epoch 9/20
Epoch 10/20
Epoch 11/20
Epoch 12/20
Epoch 13/20
Epoch 14/20
Epoch 15/20
```

Epoch 16/20

1.6.a. Compute the SparseCategoricalCrossentropy loss and model accuracy.

```
In [61]: print(f'ADAGRAD with layer normlization:\nValidation loss: {score[0]:.2f},\tValidation addressed with layer normlization:

Validation loss: 0.17, Validation accuracy: 95.22 %
```

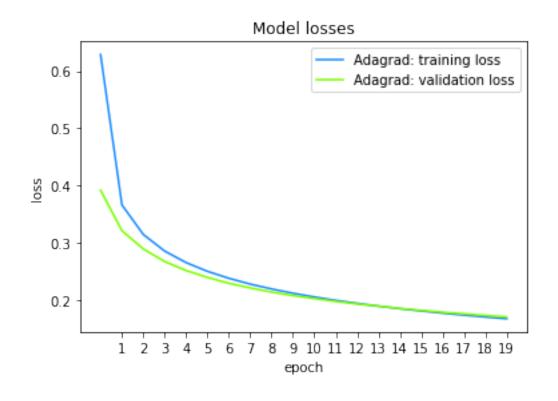
1.6.b. Evaluate the model performance using the test dataset.

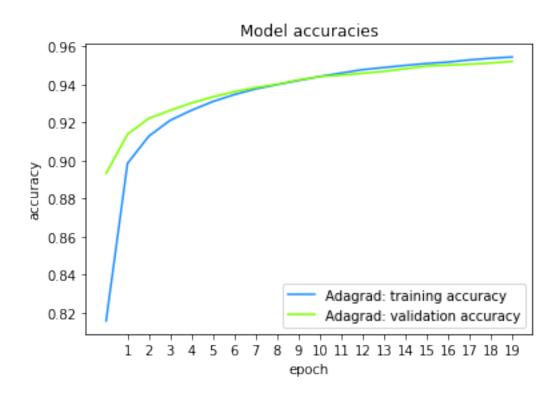
```
In [62]: singular = ['loss', 'accuracy']
    plural = ['losses', 'accuracies']

for i in range(len(singular)):
    mode = singular[i]

    plt.plot(history.history[mode], c="dodgerblue")
    plt.plot(history.history[f"val_{mode}"], c="chartreuse")

    plt.title(f"Model {plural[i]}")
    plt.ylabel(mode)
    plt.xlabel('epoch')
    plt.xticks(range(1, num_epochs))
    plt.legend([f"Adagrad: training {mode}", f"Adagrad: validation {mode}"])
    plt.show()
```





Just from looking at the plots we can see that the training went as desired: The loss steadily decreased while the accuracy increased.

Interestingly, the to be expected relation that the loss on the validation set is higher and the accuracy lower than on the training set is only the case after already 5 and 10 epochs.

We can see that around epoch 10, the loss on the training data gets lower, than on the validation loss. But the loss on the validation data still decreases, thus one can continue the training.

0.2.2 Exercise 2 - Hyper Parameter Optimization

2.1. What are the main challenges with hyper-parameter optimization for neural networks? Typical challenges with hyper-parameter optimization (HPO) for NN are: - hyper-parameters may be *continuous* or *discrete/categorical* (thus: use methods like grid search, random search,...) - different *sensitivity* of the model with respect to different parameters - large number of hyper-parameters - complex models - time-consuming model evaluations - the choice of hyper-parameters may influence the *duration of training* significantly - non-linear hyper-parameter interactions

Source:

- "On Hyperparameter Optimization of Machine Learning Algorithms: Theory and Practice" by Li Yang and Abdallah Shami (2010)
- **2.2.** Inform yourself about variants of Bayesian-HPO and explain them in detail. Bayesian optimization is a method to model the generalization performance of a learning algorithm as a sample from a Gaussian process (GP). That means to find the minimum of a function f(x) on some bounded set $X \subset \mathbb{R}^D$ by constructing a probabilisitic model for f(x) and exploit it to make the next evaluations of f in X.

Since the evaluations f(x) are expensive to perform (train and evaluate the learning algorithm on the new hyper-parameters x), it is justified, that more effort in the selection of the x is made.

DEFINITION: Gaussian process (GP)

A GP is a (prior) distribution on functions $f: X \to \mathbb{R}$ such that any finite set of N points $\{x_n \in X\}_{n=1}^N$ induces a multivariate Gaussian distribution on \mathbb{R}^N .

Now assume that f(x) is drawn from a GP piror and that the observations/data are of the form $\{x_n, y_n\}_{n=1}^N$ where $y_n \sim \mathcal{N}(f(x_n), \nu)$ where ν is the *variance of noise* in the data.

Sources:

- "A Tutorial on Bayesian Optimization of Expensive Cost Functions, with Application to Active User Modeling and Hierarchical Reinforcement Learning" by Eric Brochu, Vlad M. Cora and Nando de Freitas (2010)
- "Practical Bayesian Optimization of Machine Learning Algorithms" by Jasper Snoek, Hugo Larochelle and Ryan P. Adams (2021)
- "Hyperopt: A Python Library for Optimizing the Hyperparameters of Machine Learning Algorithms" by James Bergstra, Dan Yamins and David D. Cox (2013)
- 2.3. Using the same MNIST dataset, optimize the activation function for the output layer and the number of dropout units in the NN model using the following methods.

```
In [63]: ###### For preparation do the same as in exercise 1.1.: #####
         # Load the data:
         # Split between train and test sets w.r.t. data 'x' and class vectors 'y'
         (X_train, y_train), (X_test, y_test) = keras.datasets.mnist.load_data()
         # For normalization we scale the images to contain values in [0, 1]
         X_train = X_train.astype("float32") / 255
         X_test = X_test.astype("float32") / 255
         # Check, that all images have shape (28, 28, 1)
         X_train = np.expand_dims(X_train, -1)
         X_test = np.expand_dims(X_test, -1)
         input_shape = X_train[0].shape
In [64]: num classes = 10
  2.3.a. Grid search
In [65]: # Create a wrapper for the model (required by KerasClassifier)
         def build_model(activation = 'relu', rate = 0.2):
             model = keras.models.Sequential()
             model.add(keras.layers.Flatten())
             # Input layer
             model.add(keras.layers.Dense(128, activation = 'relu'))
             # Hidden layer
             model.add(keras.layers.Dense(100, activation = 'relu'))
             model.add(keras.layers.Dropout(rate = rate))
             # Output layer
             model.add(keras.layers.Dense(10, activation = activation))
             model.compile(loss ='sparse_categorical_crossentropy', optimizer = 'adam', metric
             return model
In [66]: # create nn model with Keras Classifier
         nn_model = KerasClassifier(build_fn = build_model, verbose = 0)
In [67]: # Define the grid search parameters
         param_grid = {
             'activation': ['relu', 'softmax', 'sigmoid'],
             'rate': [0.2, 0.4, 0.6, 0.8]
         }
         grid_search = GridSearchCV(
             estimator = nn_model,
             param_grid = param_grid,
         )
```

```
In [68]: # Apply the grid Search
         %time grid_search_result = grid_search.fit(X_train, y_train)
CPU times: user 5min 47s, sys: 22.8 s, total: 6min 10s
Wall time: 5min 38s
In [69]: # Grid Search Performance
         print(f"Best parameter settings are:\n{grid_search_result.best_params_}")
         print(f"\n\nWith an accuracy of {grid_search_result.best_score_*100:.2f} %.")
Best parameter settings are:
{'activation': 'sigmoid', 'rate': 0.2}
With an accuracy of 95.70 %.
  2.3.a. Random search
In [73]: class SequentialHyperModel(HyperModel):
             def __init__(self, input_shape, num_classes):
                 self.input_shape = input_shape
                 self.num_classes = num_classes
             def build(self, hp):
                 model = keras.models.Sequential()
                 model.add(keras.layers.Flatten())
                 # Input layer
                 model.add(keras.layers.Dense(self.input_shape, activation = 'relu'))
                 # Hidden layer
                 model.add(keras.layers.Dense(100, activation = 'relu'))
                 model.add(keras.layers.Dropout(rate = hp.Choice('rate', values = [0.2, 0.4, 0
                 # Output layer
                 model.add(keras.layers.Dense(self.num_classes, activation = hp.Choice('activa')
                 model.compile(loss = 'sparse_categorical_crossentropy', optimizer = 'adam', me
                 return model
In [74]: # Create a hypermodel instance
         hypermodel = SequentialHyperModel(input_shape = 128, num_classes = num_classes)
In [75]: # Create a Random Search hyperparameter tuner
         tuner = kt.RandomSearch(
             hypermodel = hypermodel,
             objective = 'accuracy',
```

```
max_trials = 10,
            directory = 'RSHO',
            project_name = 'Random Search'
        )
In [78]: # Execute the search by the tuner
        %time tuner.search(x = X_train, y = y_train, epochs = 10, verbose = 0)
INFO:tensorflow:Oracle triggered exit
CPU times: user 9min 23s, sys: 36.8 s, total: 9min 59s
Wall time: 6min 45s
In [79]: # Report the found parameters
        tuner_results = tuner.get_best_hyperparameters()[0]
        best_model = tuner.get_best_models(num_models = 1)[0]
        loss, accuracy = best_model.evaluate(X_test, y_test)
In [80]: print("Best params are:\nrate: {}, activation: {}".format(
            tuner_results.get('rate'),
            tuner_results.get('activation')
        ))
        print(f"\n\nWith an accuracy of {accuracy*100:.2f} % and a loss of {loss}.")
Best params are:
rate: 0.2, activation: softmax
With an accuracy of 97.51 % and a loss of 0.10285230726003647.
  2.3.a. Bayesian Hyper-parameter optimization
In [81]: # Create a Bayesian Optimization hyperparameter tuner
        tuner = kt.BayesianOptimization(
            hypermodel = hypermodel,
            objective = 'accuracy',
            max_trials = 10,
            directory = 'BHO',
            project_name = 'BayesianOptimisation'
        )
In [83]: # Execute the search by the tuner
        %time tuner.search(x = X_train, y = y_train, epochs = 10, verbose = 0)
```

0.2.3 Exercise 3 - Transfer Learning & CNNs

3.1. Load the VGG16 pre-trained model using Keras Applications API. Use the model to classify the dog images in canines.zip after pre-processing each image by doing the following: (See MachineLearningMastery for reference)

block1_pool (MaxPooling2D) (None, 112, 112, 64) 0

block2_conv1 (Conv2D) (None, 112, 112, 128) 73856

block2_conv2 (Conv2D) (None, 112, 112, 128) 147584

block2_pool (MaxPooling2D)	(None, 56, 56, 128)	0
block3_conv1 (Conv2D)	(None, 56, 56, 256)	295168
block3_conv2 (Conv2D)	(None, 56, 56, 256)	590080
block3_conv3 (Conv2D)	(None, 56, 56, 256)	590080
block3_pool (MaxPooling2D)	(None, 28, 28, 256)	0
block4_conv1 (Conv2D)	(None, 28, 28, 512)	1180160
block4_conv2 (Conv2D)	(None, 28, 28, 512)	2359808
block4_conv3 (Conv2D)	(None, 28, 28, 512)	2359808
block4_pool (MaxPooling2D)	(None, 14, 14, 512)	0
block5_conv1 (Conv2D)	(None, 14, 14, 512)	2359808
block5_conv2 (Conv2D)	(None, 14, 14, 512)	2359808
block5_conv3 (Conv2D)	(None, 14, 14, 512)	2359808
block5_pool (MaxPooling2D)	(None, 7, 7, 512)	0
flatten (Flatten)	(None, 25088)	0
fc1 (Dense)	(None, 4096)	102764544
fc2 (Dense)	(None, 4096)	16781312
predictions (Dense)	(None, 1000)	4097000
Total params: 138.357.544		

Total params: 138,357,544
Trainable params: 138,357,544

Non-trainable params: 0

3.1.a. Load each image and set the size to 224 x 224 pixels.

3.1.b. Convert the image pixels to a numpy array and reshape it according to the model's input requirements.

3.1.c. Use the model to print out the predicted class and its probability for each image.

```
In [91]: image_target_size = (224, 224)
         for image_number in range(1,9):
           # Load an image from file
           image = load_img("dog"+str(image_number)+".jpg", target_size=image_target_size)
           # Convert the image pixels to a numpy array
           image = img_to_array(image)
           # Reshape the data for the model
           image = image.reshape((1, image.shape[0], image.shape[1], image.shape[2]))
           # Prepare the image for the VGG model
           image = preprocess_input(image)
           # Predict the probability across all output classes
           %time yhat = model.predict(image)
           # Convert the probabilities to class labels
           label = decode_predictions(yhat)
           # Retrieve the most likely result, e.g. highest probability
           label = label[0][0]
           # Print the classification
           print('Image Number %d:\t %s (%.2f\%)\n' % (image number, label[1], label[2]*100))
CPU times: user 1.08 s, sys: 701 ts, total: 1.08 s
Wall time: 613 ms
Image Number 1:
                        Doberman (93.43%)
CPU times: user 1.08 s, sys: 1.38 ms, total: 1.08 s
Wall time: 599 ms
                        Pembroke (74.57%)
Image Number 2:
CPU times: user 1.09 s, sys: 2.19 ms, total: 1.09 s
Wall time: 631 ms
Image Number 3:
                        golden_retriever (78.78%)
CPU times: user 1.07 s, sys: 6.86 ms, total: 1.08 s
Wall time: 600 ms
Image Number 4:
                        Border collie (70.29%)
CPU times: user 1.09 s, sys: 2.89 ms, total: 1.09 s
Wall time: 631 ms
Image Number 5:
                        Great_Dane (45.38%)
CPU times: user 1.08 s, sys: 5.51 ms, total: 1.08 s
```

```
Wall time: 619 ms
Image Number 6: Great_Dane (90.89%)

CPU times: user 1.08 s, sys: 4.67 ms, total: 1.08 s
Wall time: 597 ms
Image Number 7: Eskimo_dog (49.96%)

CPU times: user 1.07 s, sys: 6.74 ms, total: 1.08 s
Wall time: 611 ms
Image Number 8: Doberman (35.42%)
```

3.2. Downscale the given matrix by applying the following pooling operations: Note: It is not specified, what the pooling size should be. We will use 3×3 .





3.2.a. Average Pool

3.3. Load the CIFAR10 dataset using Keras datasets API and normalize the images' pixel values. Train a convolutional neural network to classify the dataset images with the following architecture:

3.3.a. Convolutional Base:

- 1. An input convolution layer with 32 filters and a kernel size of (3,3). Adjust your input shape to that of the CIFAR images' format
- 2. Two convolution layers, each with 64 filters and a kernel size of (3,3)
- 3. Two Max Pool layers, with a pool size of 2×2

3.3.b. Two dense layers, with 64 and 10 units respectively. Adjust the output of the convolutional base such that it satisfies the input requirements of the dense layers.

3.3.c. Use the following parameters to train the network:

- 1. Sparse categorical cross entropy as your loss function
- 2. Adam optimizer
- 3. 10 epochs
- 4. ReLU activation for your layers

Compile your model, then plot the accuracy across each epoch.