Lab 0: Preparation

NOTE: This is a lab project accompanying the following book [MLF] and it should be used together with the book.

[MLF] *H. Jiang*, "[Machine Learning Fundamentals: A Concise Introduction (http://wiki.eecs.yorku.ca/user/hj/research:mlfbook)](http://wiki.eecs.yorku.ca/user/hj/research:mlfbook)", Cambridge University Press, 2021. ([bibtex (http://www.cse.yorku.ca/~hj/mlf-jiang.bib)](http://www.cse.yorku.ca/~hj/mlf-jiang.bib))

The purpose of this lab is to introduce *vectorization*-based programming style, which is essential for implementing machine learning algorithms using some high-level programming languages (such as Python, Matlab), and then give some recipes on how to load data sets that will be used in all projects in the book [MLF].

Prerequisites: basic understanding on Python, Numpy and JAX.

I. Programming via Vectorization

Vectorization is a special programing style for numerical computation, in which we packs all arguments into vectors/matrices and casts all numerical operations as matrix operations. By doing so, we try to get rid of loops and array indexing so as to deliver clean and effecient programs even when they are written in high-level programming languages, such as Python, Matlab.

Vectorization: programming using vectors, matrices, and even tensors without explicitly looping, indexing, conditioning over vector/matrix/tensor elements.

Advantages:

1. vectorized codes are more concise and easier to read.
2. vectorized codes run much faster in high-level languages, such as Python/Numpy, Matlab and so on.
3. vectorized codes can easily utilize parallel units in powerful computing hardwares (such as multi-core CPUs or GPUs) to yield further speed-up.

The key idea in vectorization-based programming is to use linear algebra techniques to pack the data into vectors / matrices /tensors. In the following, let us use two simple examples to explain how to write efficient vectorization-based codes, and further show how much faster these vectorized codes can run compared with the regular programming style (in either CPUs or GPUs).

Example 0.1

clipping all elements in a vector/matrix to [0,1].

1.1 POOR programming style using loops, indexing and conditioning

```
In [ ]: def clip_loops(A):
          for i in range(A.shape[0]):
            for j in range(A.shape[1]):
              if (A[i,j] > 1):
                A[i,j] = 1
              elif (A[i,j] < 0):
                A[i,j] = 0

          return A
```

1.2 use a *numpy* function *clip( )* to do it efficiently

```
In [ ]: import numpy as np

        A = np.clip(A,0,1)
```

1.3 Running on a random matrix to compare their results and run-in speed.

```
In [ ]: import numpy as np

        X = np.random.normal(size=(5000,784))*1.5

        X1 = clip_loops(X)
        X2 = np.clip(X,0,1)

        print(np.sum((X1-X2)*(X1-X2)))

        %timeit clip_loops(X)
        %timeit np.clip(X,0,1)
```

```
0.0
1 loop, best of 5: 3.61 s per loop
100 loops, best of 5: 11.5 ms per loop
```

1.4 Summary:

1. Vectorized code is much more concise and easier to read.
2. Vectorization code is much faster than loops (about 300-400 times faster, 3.61 s vs 11.5 ms)

Example 0.2

Write a function to compute the sample covariance matrix from a set of data samples:
$$\mathcal{D} = \left\{ \mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N \right\}$$
as

$$\mathbf{S} = \frac{1}{N} \sum_{i=1}^{N} (\mathbf{x}_i - \bar{\mathbf{x}}) (\mathbf{x}_i - \bar{\mathbf{x}})^\mathsf{T}$$

(NOTE: the sample covariance matrix is discussed in *Section 4.2 Linear Dimension Reduction*, which is the main backbone in some popular machine learning methods such as PCA and LDA.)

2.1 regular (but poor) programing using loops

```
In [ ]:  import numpy as np

         ## input: matrix X as N by d, each row is a feature vector of d dimens
         ions
         def cov_loops(X):
           N = X.shape[0]
           d = X.shape[1]

           # compute the mean
           mean = np.zeros((d))
           for i in range(N):
             for j in range(d):
               mean[j] += X[i,j]
           for j in range(d):
             mean[j] /= N

           # compute the sample covariance matrix
           S = np.zeros((d,d))
           z = np.zeros((d))
           for i in range(N):
             for j in range(d):
               z[j] = X[i,j] - mean[j]
             for m in range(d):
               for n in range(d):
                 S[m,n] += z[m] * z[n]
           for m in range(d):
             for n in range(d):
               S[m,n] /=  N

           return S
```

2.2 Vecctorized codes using *numpy* for CPUs

For the above sample convariance example, we use the following identity (refer to Q2.3 on page 64):

$$\sum_{i=1}^{m} \mathbf{x}_i \mathbf{x}_i^\mathsf{T} = \mathbf{X}\mathbf{X}^\mathsf{T}$$

```
In [ ]:  import numpy as np

         ## input: matrix X as N by d, each row is a feature vector of d dimens
         ions
         def cov_vec(X):
           mean = np.mean(X, axis=0)

           return (X-mean) @ (X-mean).T / X.shape[0]
```

2.3 Vectorized codes using JAX for GPUs

Vectorized codes can be further accelerated in GPUs using some python library such as JAX.

```
In [ ]:  import jax.numpy as jnp
         from jax import jit

         ## input: matrix X as N by d, each row is a feature vector of d dimens
         ions
         @jit
         def cov_jax(X):
           X = jnp.array(X)
           mean = jnp.mean(X, axis=0)

           return (X-mean) @ (X-mean).T / X.shape[0]
```

2.4 Running on some random samples, and compare the results and running speed of the above three implementations.

```
In [ ]:  import numpy as np

         # N=300 samples, whose dimensions are d=784
         X = np.random.normal(size=(300,784))

         %timeit -n1 -r1  cov_loops(X)
         %timeit -n3 -r3  cov_vec(X)
         %timeit -n3 -r3  cov_jax(X)

         S1 = cov_loops(X)
         S2 = cov_vec(X)
         S3 = cov_jax(X)

         print(np.trace(S1), np.trace(S2), np.trace(S3))
```

```
1 loop, best of 1: 2min 23s per loop
3 loops, best of 3: 6.63 ms per loop
The slowest run took 1337.56 times longer than the fastest. This cou
ld mean that an intermediate result is being cached.
3 loops, best of 3: 613 µs per loop
779.8513112292864 779.8513112292862 779.8513
```

Compare CPU vs. GPU implementations on a larger sample set:

```
In [ ]:  import numpy as np

         # N=5000 samples, whose dimensions are d=784
         X = np.random.normal(size=(5000,784))

         %timeit cov_vec(X)
         %timeit cov_jax(X)

         S2 = cov_vec(X)
         S3 = cov_jax(X)

         print( np.trace(S2), np.trace(S3))
```

```
1 loop, best of 5: 1.18 s per loop
The slowest run took 31.36 times longer than the fastest. This could
mean that an intermediate result is being cached.
1 loop, best of 5: 7.92 ms per loop
783.0682494218952 783.06824
```

2.5 Summary:

1. Vectorization is about 20000+ times faster than loops (143s vs. 6.63ms)
2. GPUs can further speed it up about 10 times (6.63ms vs 0.613ms)
3. GPUs can accelerate more for larger matrices, about 150+ times faster at above (1.18s vs 7.92ms)

```
In [ ]:  # show the GPU type used in the above computation

         !nvidia-smi
```

```
Tue Jan 11 20:29:15 2022
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 495.46       Driver Version: 460.32.03    CUDA Version: 11.2      |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|                               |                      |               MIG M. |
|===============================+======================+======================|
|   0  Tesla K80           Off  | 00000000:00:04.0 Off |                    0 |
| N/A   58C    P8    30W / 149W |      0MiB / 11441MiB |      0%      Default |
|                               |                      |                  N/A |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                                  |
|  GPU   GI   CI        PID   Type   Process name                  GPU Memory |
|        ID   ID                                                   Usage      |
|=============================================================================|
|  No running processes found                                                 |
+-----------------------------------------------------------------------------+
```

II. Loading Data Sets

1. loading the MNIST data set

The MNIST data set is used in Lab Project I (page 92), Lab Project II (page 129) and Lab Project IV (page 200).

1. download the original MNIST data from **http://yann.lecun.com/exdb/mnist/ (http://yann.lecun.com/exdb/mnist/)** (OR here (https://drive.google.com/drive/folders/1r20aRjc2iu9O3kN3Xj9jNYY2uMgcERY1?usp=sharing))
2. rename the downloaded file as: *train-images-idx3-ubyte*, *train-labels-idx1-ubyte*, *t10k-images-idx3-ubyte*, and *t10k-labels-idx1-ubyte*.
3. upload these files into your Google drive (in order to use Google Colab)
4. link your Google drive to the Colab session by doing:

```
In [2]:  from google.colab import drive
         drive.mount('/content/drive')

         Mounted at /content/drive
```

1. i) use idx2numpy to convert idx to numpy arrays

```
In [ ]:  # install idx2numpy

         !pip install idx2numpy

         Requirement already satisfied: idx2numpy in /usr/local/lib/python3.7
         /dist-packages (1.2.3)
         Requirement already satisfied: numpy in /usr/local/lib/python3.7/dis
         t-packages (from idx2numpy) (1.19.5)
         Requirement already satisfied: six in /usr/local/lib/python3.7/dist-
         packages (from idx2numpy) (1.15.0)
```

```
In [ ]:  import idx2numpy
         import numpy as np

         # load training images and labels
         train_data=idx2numpy.convert_from_file('/content/drive/My Drive/Colab
         Notebooks/datasets/MNIST/train-images-idx3-ubyte')
         train_data = np.reshape(train_data,(60000,28*28))
         train_label = idx2numpy.convert_from_file('/content/drive/My Drive/Col
         ab Notebooks/datasets/MNIST/train-labels-idx1-ubyte')
         print(train_data.shape)
         print(train_label.shape)

         # load testing images and labels
         test_data=idx2numpy.convert_from_file('/content/drive/My Drive/Colab N
         otebooks/datasets/MNIST/t10k-images-idx3-ubyte')
         test_data = np.reshape(test_data,(10000,28*28))
         test_label = idx2numpy.convert_from_file('/content/drive/My Drive/Cola
         b Notebooks/datasets/MNIST/t10k-labels-idx1-ubyte')
         print(test_data.shape)
         print(test_label.shape)
```

```
(60000, 784)
(60000,)
(10000, 784)
(10000,)
```

1. ii) OR use python-mnist to load into numpy

```
In [3]:  # install python_mnist

         !pip install python_mnist
```

```
Collecting python_mnist
  Downloading python_mnist-0.7-py2.py3-none-any.whl (9.6 kB)
Installing collected packages: python-mnist
Successfully installed python-mnist-0.7
```

```
In [4]:  from mnist import MNIST
         import numpy as np
         mnist_loader = MNIST('/content/drive/My Drive/Colab Notebooks/datasets
         /MNIST')
         train_data, train_label = mnist_loader.load_training()
         test_data, test_label = mnist_loader.load_testing()
         train_data = np.array(train_data)
         train_label = np.array(train_label)
         test_data = np.array(test_data)
         test_label = np.array(test_label)

         print(train_data.shape)
         print(train_label.shape)
         print(test_data.shape)
         print(test_label.shape)
```

```
(60000, 784)
(60000,)
(10000, 784)
(10000,)
```

In [17]:
```python
# use a matplotlib function to display some MNIST images

import matplotlib.pyplot as plt
import numpy as np

# functions to show an image

def show_img(num):
  img = train_data[num,:]
  img = img.reshape(28,-1)
  print(str(img.shape) + '  No.' +  str(num) + '  label:' + str(train_
label[num]))
  plt.imshow(img, cmap='gray')
  plt.show()

fig = plt.figure()

for i in range(9):
  img = train_data[i,:]
  img = img.reshape(28,-1)
  ax = fig.add_subplot(3,3,i+1)
  ax.title.set_text(str(train_label[i]))
  plt.imshow(img, cmap='gray')

plt.show(block=True)
```
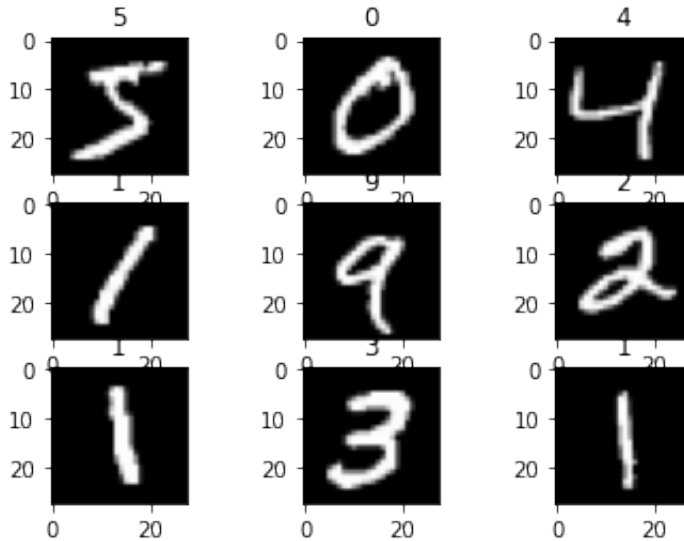
2. Loading the Boston House data set

The Boston House data set is used in Q7.7 on page 150.

First download boston.csv (https://drive.google.com/file/d/1UOJmn44xf-WW0KydM81eytMHNbdlHr5o/view?usp=sharing), and upload it into your Google drive, then link your Google drive to your Colab session as decribed previously.

Refer to here (https://www.cs.toronto.edu/~delve/data/boston/bostonDetail.html) for the description of the data

```
In [ ]: import pandas as pd
        import numpy as np

        raw_data = pd.read_csv('/content/drive/My Drive/Colab Notebooks/datase
        ts/boston.csv', header=None)
        data_rows = np.reshape(raw_data.to_numpy(), (506,14))
        data = data_rows[:,:13]
        target = data_rows[:,13]

        print(data.shape)
        print(target.shape)

        (506, 13)
        (506,)
```

3. Loading the Ames Housing data set

The Ames Housing data set is used in Lab Project V (page 216).

First download the data set from Kaggle (https://www.kaggle.com/c/house-prices-advanced-regression-techniques) or here (https://drive.google.com/drive/folders/1w2hM-TIzvFFYHp_5JCVEGTA3DWNNskx9?usp=sharing), and upload it into your Google drive, then link your Google drive to your Colab session as decribed previously. The data description is here (https://drive.google.com/file/d/1sSEHUamh5JJGxMvk17GkrgHBpzUf7Q-n/view?usp=sharing).

```
In [ ]:  import pandas as pd

         train_dataframe = pd.read_csv("/content/drive/My Drive/Colab Notebooks
         /datasets/AmesHouse/train.csv")
         test_dataframe = pd.read_csv("/content/drive/My Drive/Colab Notebooks/
         datasets/AmesHouse/test.csv")

         print(train_dataframe.shape)
         print(test_dataframe.shape)

         # WARNING: both train_dataframe and test_dataframe contain symbolic fe
         atures (refer to the data description)
         #          they need be pre-processed to numbers prior to model traini
         ng and testing

         (1460, 81)
         (1459, 80)
```

4. Loading the MLF Gaussian data set

The MLF Gaussian data set is used in Lab Project VI (page 287).

First download the data set from here (https://drive.google.com/drive/folders/1agkY7npAHzav-e1yYlVBJNgfux5AsmlX?usp=sharing), and upload the file to your Google drive, and link your Google drive to the Colab session as above.

```
In [ ]:  import pandas as pd

         train_dataframe = pd.read_csv("/content/drive/My Drive/Colab Notebooks
         /datasets/MLF-Gauss/train-gaussian.csv")
         test_dataframe = pd.read_csv("/content/drive/My Drive/Colab Notebooks/
         datasets/MLF-Gauss/test-gaussian.csv")
         train_data = train_dataframe.to_numpy()
         test_data = test_dataframe.to_numpy()

         print(train_data.shape)
         print(test_data.shape)

         (1891, 4)
         (830, 4)
```

Exercises

Problem 0.1:

Write a program to compute pair-wise Euclean distances (i.e., L_2 norm) between all vectors in a set of data samples:

$$\mathcal{D} = \left\{ \mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N \right\}$$

where each $\mathbf{x}_i \in \mathbb{R}^d$. Store all these pair-wise distances in a symmetric marix $\mathbf{E} \in \mathbb{R}^{N \times N}$, where each element e_{ij} indicates the distance between $\mathbf{x}_i$ and $\mathbf{x}_j$.

1. Implement it using regular loop-based programing style.
2. Implement it use vectorization.
3. Generate some random samples, compare the above two implementations in terms of running speed.

Problem 0.2:

Refer to Q6.8 (page 130), write some programs to compute the SVM matrix Q for three different kernel types: linear, polynomial and RBF functions.

1. Implement it using regular loop-based programing style.
2. Use vectorization to re-write vectorized codes to compute the matrix Q for all three kernel types.
3. Generate some random samples, compare the above two implementations in terms of running speed.