

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 programming 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: $\mathcal{D} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N\}$ as $\mathbf{S} = \frac{1}{N} \sum_{i=1}^N (\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})^T$ (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) programming using loops

In []:

```
import numpy as np

## input: matrix X as N by d, each row is a feature vector of d dimensions
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 Vectorized codes using *numpy* for CPUs

For the above sample covariance example, we use the following identity (refer to Q2.3 on page 64):
$$\sum_{i=1}^m \mathbf{x}_i \mathbf{x}_i^T = \mathbf{X} \mathbf{X}^T$$

In []:

```
import numpy as np

## input: matrix X as N by d, each row is a feature vector of d dimensions
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 dimensions
@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 could mean that an intermediate result is being cached.

3 loops, best of 3: 613 μ s 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 Un
corr. ECC |
| Fan  Temp   Perf   Pwr:Usage/Cap|      Memory-Usage | GPU-Util  C
ompute 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                        G
PU Memory |
|       ID    ID                                   |
sage      |
|=====+=====+=====
=====|
| 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) (<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 []:

```
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/dist-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/Colab Noteboo
ks/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 Notebooks/d
atasets/MNIST/t10k-images-idx3-ubyte')
test_data = np.reshape(test_data,(10000,28*28))
test_label = idx2numpy.convert_from_file('/content/drive/My Drive/Colab Noteboo
ks/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 []:

```
# install python_mnist

!pip install python_mnist
```

Requirement already satisfied: python_mnist in /usr/local/lib/python
3.7/dist-packages (0.7)

In []:

```
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 []:

```
# use a matplotlib function to display some MNIST images

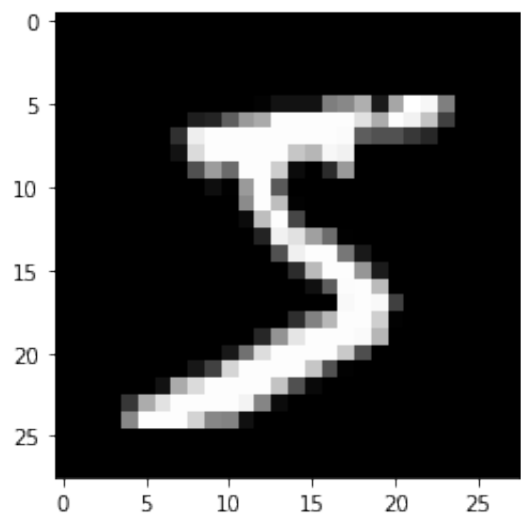
import matplotlib.pyplot as plt
import numpy as np

# functions to show an image

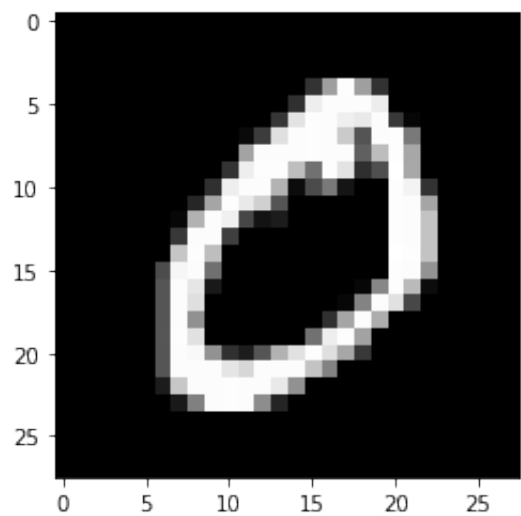
def show_img(num):
    img = train_data[num,:]
    img = img.reshape(28,-1)
    print(str(img.shape) + ' No.' + str(num) + ' label:' + str(train_label[num]))
    plt.imshow(img, cmap='gray')
    plt.show()

for i in range(10):
    show_img(i)
```

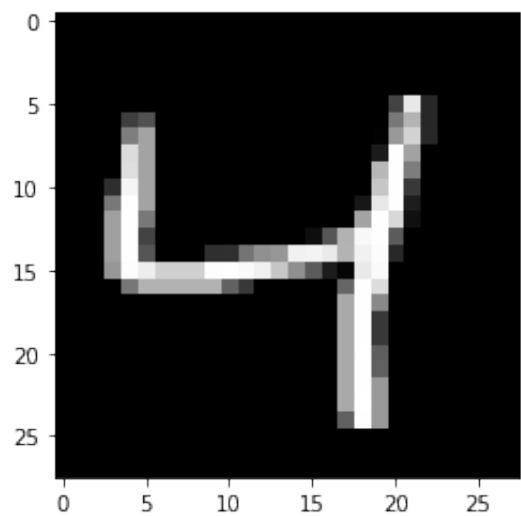
```
(28, 28) No.0 label:5
```



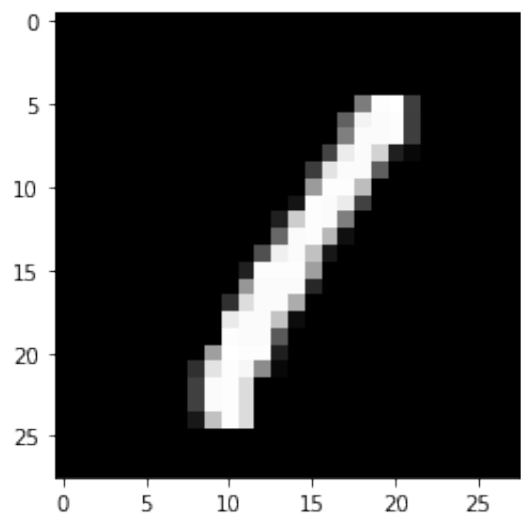
(28, 28) No.1 label:0



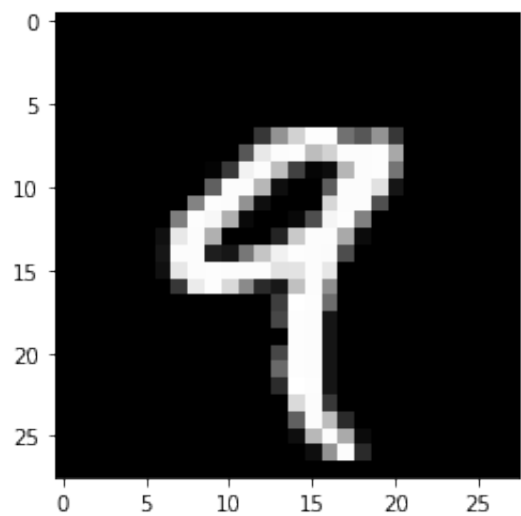
(28, 28) No.2 label:4



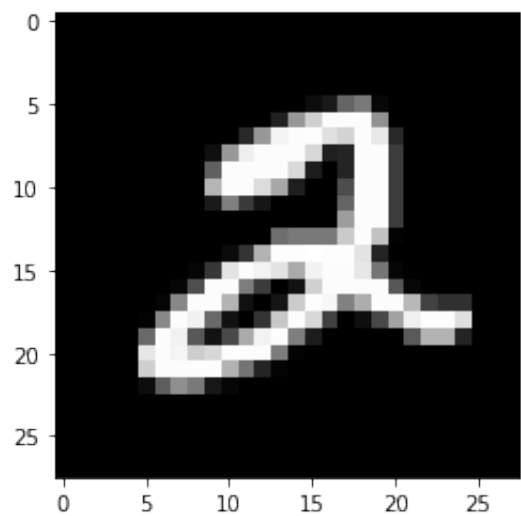
(28, 28) No.3 label:1



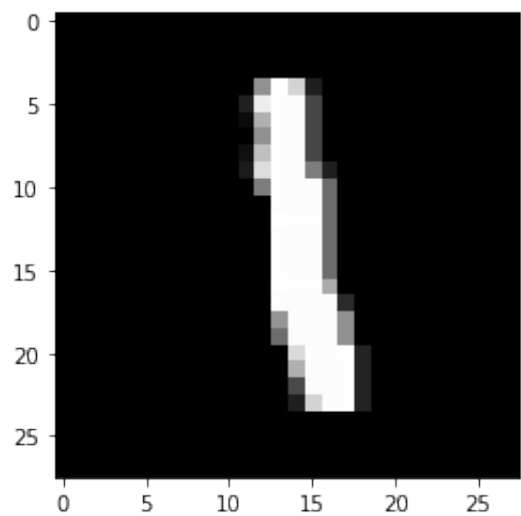
(28, 28) No.4 label:9



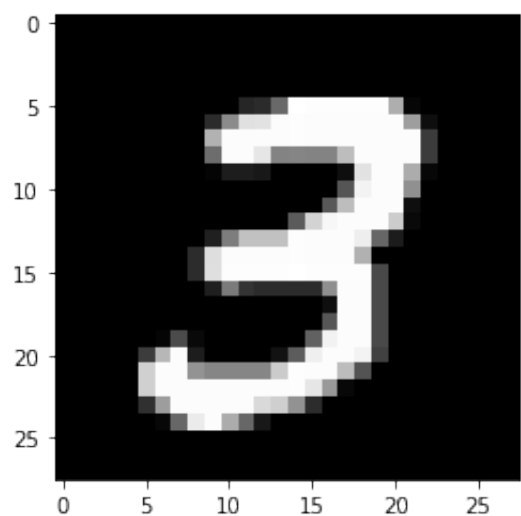
(28, 28) No.5 label:2



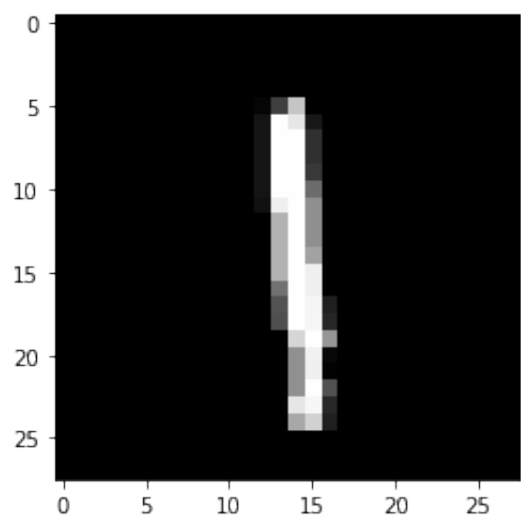
(28, 28) No.6 label:1



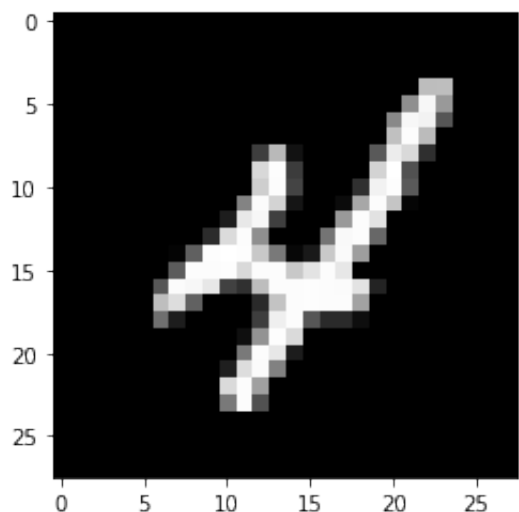
(28, 28) No.7 label:3



(28, 28) No.8 label:1



(28, 28) No.9 label:4



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-WW0Kydm81eytMHNbdIHr5o/view?usp=sharing) (<https://drive.google.com/file/d/1UOJmn44xf-WW0Kydm81eytMHNbdIHr5o/view?usp=sharing>), and upload it into your Google drive, then link your Google drive to your Colab session as described previously.

Refer to [here](https://www.cs.toronto.edu/~delve/data/boston/bostonDetail.html) (<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/datasets/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 \(https://www.kaggle.com/c/house-prices-advanced-regression-techniques\)](https://www.kaggle.com/c/house-prices-advanced-regression-techniques) or [here \(https://drive.google.com/drive/folders/1w2hM-TIzvFFYHp_5JCVEGTA3DWNNskx9?usp=sharing\)](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 described previously. The data description is [here \(https://drive.google.com/file/d/1sSEHUamh5JJGxMvk17GkrgHBpzUf7Q-n/view?usp=sharing\)](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 features (refer to the data description)
#           they need be pre-processed to numbers prior to model training 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 \(https://drive.google.com/drive/folders/1agkY7npAHZav-e1yYIVBJNgfux5AsmIX?usp=sharing\)](https://drive.google.com/drive/folders/1agkY7npAHZav-e1yYIVBJNgfux5AsmIX?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 Euclidean distances (i.e., L_2 norm) between all vectors in a set of data samples: $\mathcal{D} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N\}$ where each $\mathbf{x}_i \in \mathbb{R}^d$. Store all these pair-wise distances in a symmetric matrix $\mathbf{E} \in \mathbb{R}^{N \times N}$, where each element e_{ij} indicates the distance between \mathbf{x}_i and \mathbf{x}_j .

1. Implement it using regular loop-based programming style.
2. Implement it using 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 \mathbf{Q} for three different kernel types: linear, polynomial and RBF functions.

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