report

September 29, 2020

1 Machine Learning Homework 01 – Report

1.1 1. – Solution

There were two problems to solve (problem 1 and problem 2). The first problem required implementing two functions to compute the pairwise distance matrix Z of a random $N \times D$ matrix X:

1. A function using a two-level nested loop, iterating through all pairs (i, j) and computing the corresponding entry $Z_{i,j}$
2. A function using numpy matrix operations (vectorization)

And the second problem required implementing two functions to compute the correlation matrix R of a random $N \times D$ matrix X:

1. A function using a two-level nested loop
2. A function using vectorization

For each of these problems, we were asked to profile the performance of the functions on random matrices of row-size N by plotting the running time as a function of N. Finally, the third problem required evaluating the running times of each function on three datasets in the `sklearn.datasets` library.

Since this report is written in a Jupyter Notebook, for simplicity's sake I will import libraries necessary for easily showing plots and other results in the notebook:

[1]:
```
import math
from timeit import timeit
from typing import Tuple

import numpy as np
from numpy.random import rand
from matplotlib import pyplot as plt
from sklearn.datasets import load_iris, load_breast_cancer, load_digits
from tqdm import tqdm
```

1.1.1 1.1. – Problem 1

1.1.1. – Pairwise Distance Matrix Using Loops The pairwise Euclidean distance betweeen vectors `v1` and `v2` can be computed using the following function:

[2]:
```python
def pairwise_distance_loop(v1, v2):
    diff = v1 - v2
    payload = 0
    for d in diff:
        payload += d**2
    return math.sqrt(payload)
```

This sums the squares of the element-wise difference between the input vectors and takes the square root of the result – the definition of pairwise Euclidean distance.

Then, using this helper function, we can solve the first subproblem by initializing an empty $N \times N$ matrix `z` and simply looping over each row of the matrix `x` and, for each row, looping over all other rows (including the same row) and updating the corresponding entry of `z`:

[3]:
```python
def compute_pairwise_distance_loop(x):
    """

    :param x: 2d numpy array of dimension num_vectors x feature_dim
    :return: num_vectors x num_vectors 2d numpy array in which each
             (i, j)-entry is the pairwise euclidean distance between
             rows indexed as `i` and `j`.

    """
    num_vectors = x.shape[0]      # number of vectors in dataset
    z = np.zeros((num_vectors, num_vectors))
    for i in range(num_vectors):
        for j in range(num_vectors):
            # Note: pairwise_distance(x[i, :], x[j, :]) will give either
            # a small, nonzero float or NaN when taking pairwise_distance on
            # i = j, so best to just impute it to zero manually.
            z[i][j] = 0.0 if i == j else pairwise_distance_loop(x[i], x[j])
    return z
```

The updating of `z[i][j]` is conditional upon whether the indices are the same – if they are, we are taking the pairwise distance between a row and itself. This should amount to zero, but Python's handling of this results in either a very small floating point number, or a value of `NaN`, so for simplicity it is just imputed to zero automatically upon witnessing `i == j` evaluate to `True`.

1.1.2. – Pairwise Distance Matrix Using Vectorization For the vectorization portion of the problem, we need to find a sequence of matrix operations to compute the pairwise distance matrix. That is, we need to find a way to represent a mapping from X to a matrix in which each (i, j) entry is $||\vec{x_i} - \vec{x_j}||$. It's known that

$$||\vec{x_i} - \vec{x_j}|| = \sqrt{||\vec{x_i}||^2 - 2\vec{x_i}^T\vec{x_j} + ||\vec{x_j}||^2}$$

so the problem is reduced to finding a matrix representation of each function on the corresponding vectors in the square root, which amounts to finding a matrix consisting of all entries with $||\vec{x_i}||^2$, a matrix consisting of all entries with $||\vec{x_i}||^2$, and a matrix consisting of all entries with $2\vec{x_i}^T\vec{x_j}$;

from there, we can just add/subtract the matrices and take the square root. We will take this case-by-case; the solution to this is as follows:

1. (all entries $= 2\vec{x_i}^T\vec{x_j}$) When one multiplies an $N \times D$ matrix by its transpose, the result is an $N \times N$ matrix with entries equal to the dot product of row vectors in X at row indices i and j for row i in X and column j in X^T. This is exactly the representation for $\vec{x_i}^T\vec{x_j}$, so we can just add the matrix to itself to get the representation for $= 2\vec{x_i}^T\vec{x_j}$. In Python (using numpy), this computation is represented as

   ```
   d1 = np.matmul(x, np.transpose(x))
   ```

2. (all entries $= ||\vec{x_i}||^2$) When one multiplies an $N \times D$ matrix by its transpose, the result is an $N \times N$ matrix with entries equal to the dot product of row vectors in X at row indices i and j for row i in X and column j in X^T. The diagonal of this matrix is exactly the (column) vector consisting of entries $\vec{x_i} \cdot \vec{x_i}$, and since $||\vec{x}|| = \sqrt{\Sigma x^2}$ for $x \in \ \vec{x_i}$, and $\Sigma x^2 = \vec{x_i} \cdot \vec{x_i}$, we conclude that $\vec{x_i} \cdot \vec{x_i} = ||\vec{x_i}^2||$. To get a matrix in which each entry is $||\vec{x_i}^2||$, therefore, take the diagonal of the product of X with its transpose, and multiply it (as a column vector) with a row vector of all ones. In Python (numpy) this is:

   ```
   d2 = np.matmul(np.diag(d1).reshape(-1, 1), np.ones(num_vectors).reshape(1, -1))
   ```

3. (all entries $= ||\vec{x_j}||^2$) Since we want to add $\vec{x_j}$ at the j column in Z, we can obtain this by taking the transpose of the matrix representing all entries $= ||\vec{x_i}||^2$. In numpy this is:

   ```
   d3 = np.transpose(d2)
   ```

And now we add `d2` and `d3`, subtract twice `d1`, and take the square root of the result. This gets us the correct matrix representation. The whole function looks like this:

[4]:
```
def compute_pairwise_distance_ops(x):
    num_vectors = x.shape[0]  # number of vectors in dataset
    d1 = np.matmul(x, np.transpose(x))
    d2 = np.matmul(np.diag(d1).reshape(-1, 1), np.ones(num_vectors).reshape(1,␣
 ↪-1))
    d3 = np.transpose(d2)

    return np.sqrt(np.subtract(np.add(d2, d3), np.add(d1, d1)))
```

For sanity check, let's see if we get the same answer using both functions on the same random matrix:

[5]:
```
r = rand(10, 8)
m = compute_pairwise_distance_loop(r)
n = compute_pairwise_distance_ops(r)
sanity = np.round_(m-n)
print(sanity)
```

```
[[ 0. -0.  0.  0. -0.  0. -0. -0. -0. -0.]
 [-0.  0.  0.  0.  0.  0. -0.  0.  0.  0.]
 [ 0.  0.  0.  0.  0. -0. -0. -0. -0. -0.]
 [ 0.  0.  0.  0.  0.  0.  0.  0.  0.  0.]
 [-0.  0.  0.  0.  0. -0. -0.  0. -0. -0.]
```

```
[ 0.   0. -0.  0. -0.  0.  0.  0.  0.  0.]
[-0. -0. -0.  0. -0.  0.  0.  0.  0.  0.]
[-0.  0. -0.  0.  0.  0.  0.  0.  0.  0.]
[-0.  0. -0.  0. -0.  0.  0.  0.  0.  0.]
[-0.  0. -0.  0. -0.  0.  0.  0.  0.  0.]]
```

Which checks out.

1.1.2 1.2. – Problem 2

1.2.1. – Correlation Matrix Using Loops Given a random $N \times D$ matrix X, at each (i, j) entry of the $D \times D$ correlation matrix R, $R_{i,j}$ is computed as the quotient of the sample variance of the column vectors at indices i and j ($s_{0,0}$) and the product of standard deviations of column vectors of X at i and j (σ_i, σ_j). I implemented helper functions `covar` and `sd` to make the primary function more compact. The sample variance is computed as the sum of products between differences of column vectors at i and j, each subtracted by the sample mean at that dimension, and then divided by the total number of row vectors (observations) in X. This is implemented in the following way:

[6]:
```python
def variance_(x, position: Tuple[int, int]):
    num_vectors = x.shape[0]
    # feature_dim = x.shape[1]
    """sample_mean = np.zeros(num_vectors)
    for i in range(num_vectors):
        sample_mean += x[:, i]
    sample_mean /= num_vectors"""
    sample_mean = 0
    for i in range(num_vectors):
        sample_mean += x[i][position[1]]
    sample_mean /= num_vectors
    s = 0
    for i in range(num_vectors):
        s += (x[i][position[0]] - sample_mean) * (x[i][position[1]] -␣
↪sample_mean)
    payload = s/num_vectors
    return payload
```

While the standard deviation at an index i is just the square root of the sample variance between X's column vector at i and itself. It is implemented using the `covar` helper function in the following way:

[7]:
```python
def sd(x, idx):
    return math.sqrt(variance_(x, (idx, idx)))
```

Finally, the primary function to solve the problem is implemented by taking the quotient $\frac{s_{i,j}}{\sigma_i \sigma_j}$ while looping over indices of X:

[8]:
```python
def compute_correlation_matrix_loop(x):
    feature_dim = x.shape[1]
    z = np.zeros((feature_dim, feature_dim))
```

```
    for i in range(feature_dim):
        for j in range(feature_dim):
            if (sd_i := sd(x, i) != 0) and (sd_j := sd(x, j) != 0):
                z[i][j] = variance_(x, (i, j)) / (sd_i * sd_j)
            else:
                z[i][j] = 0
    return z
```

The reason for the conditional is that the standard deviation at one of the indices will be zero when the column is filled with zeros, and will yield a divide by zero error. To circumvent this, we will just catch these cases and impute to zero, rather than removing the columns from the dataset. This is relevant in the `digits` dataset from `scikit-learn`.

1.2.2. – Correlation Matrix Using Vectorization The problem of computing the correlation matrix in a vectorized way amounts to computing the variance-covariance matrix S and then computing the the correlation matrix from this. To compute the variance-covariance matrix S, each (i, j) entry in S must be equal to the sum of products between differences of column vectors at i and j in X, each subtracted by the sample mean at that dimension, and then divided by the total number of row vectors (observations) in X. This can be broken down into smaller components.

First, let's find a way to represent subtracting sample means of column vectors from those column vectors. The matrix of mean column vectors is obtained by multiplying an $N \times N$ matrix of all ones by X, and then dividing by the total number of vectors in X. To compute the entry-wise differencee between the mean column vector and the corresponding column vector in X, subtract the matrix of mean column vectors from X. This is implemented in Python as:

```
num_vectors = x.shape[0]
y = np.subtract(x, np.divide(np.matmul(np.ones((num_vectors, num_vectors)), x), num_vectors
```

And to obtain the variance-covariance matrix, multiply by the transpose of this matrix, and divide by the total number of vectors, completing the definition of variance for each entry in the new matrix S. In Python:

```
vcv = np.divide(np.matmul(np.transpose(y), y), num_vectors)
```

Now to get from the variance-covariance matrix to the correlation matrix, we need to find a way to represent the division of each entry in S by the standard deviations of the i and j columns. We know that $\sigma_i = \sqrt{s_{i,i}}$, so we can divide each entry by the square roots of the i-th and j-th elements of the diagonal of S – that is to say, multiply by the inverse of each of these elements. This can be done by multiplying this inverted square-root diagonal matrix by the variance-covariance matrix, and then multiplying again by the inverted square-root diagonal matrix. In all, the function looks like this:

[9]:
```
def compute_correlation_matrix_ops(x):
    num_vectors = x.shape[0]
    y = np.subtract(x, np.divide(np.matmul(np.ones((num_vectors, num_vectors)),
 ↪x), num_vectors))
    vcv = np.divide(np.matmul(np.transpose(y), y), num_vectors)
    try:
        d = np.linalg.inv(np.sqrt(np.diag(np.diag(vcv))))
```

```
    except:
        d = np.zeros(vcv.shape)
    corr_matrix = np.matmul(np.matmul(d, vcv), d)
    return corr_matrix
```

The `try/except` block is used for a similar reason as the conditional statement in the loop-based method – to handle matrices that contain columns of all zeros. In this case, the issue is that the matrix in question is non-invertible, thus using `np.linalg.inv()` raises an error on such matrices.

Again, let's do a sanity check to make sure the functions give the same output:

[10]:
```
r = rand(7, 12)
m = compute_pairwise_distance_loop(r)
n = compute_pairwise_distance_ops(r)
sanity = np.round_(m-n)
print(sanity)
```

```
[[ 0. -0. -0. -0. -0. -0. -0.]
 [-0.  0.  0. -0.  0. -0.  0.]
 [-0.  0.  0. -0. -0. -0.  0.]
 [-0. -0. -0.  0. -0. -0. -0.]
 [-0.  0. -0. -0.  0. -0.  0.]
 [-0. -0. -0. -0. -0.  0.  0.]
 [-0.  0.  0. -0.  0.  0.  0.]]
```

Great!

1.2 2. Experiments

1.2.1 2.1. Setting

The functions were evaluated based on their running times on random square matrices, as well as on datasets built into `scikit-learn` – the datasets `iris`, `breast_cancer`, and `digits`. I used `numpy` to generate the random matrices, `scikit-learn` to get the three datasets, the Python `timeit` library to get the running times, `matplotlib` for plotting comparisons of the running times, and `tqdm` for progress bars (to know how long the whole loop would take).

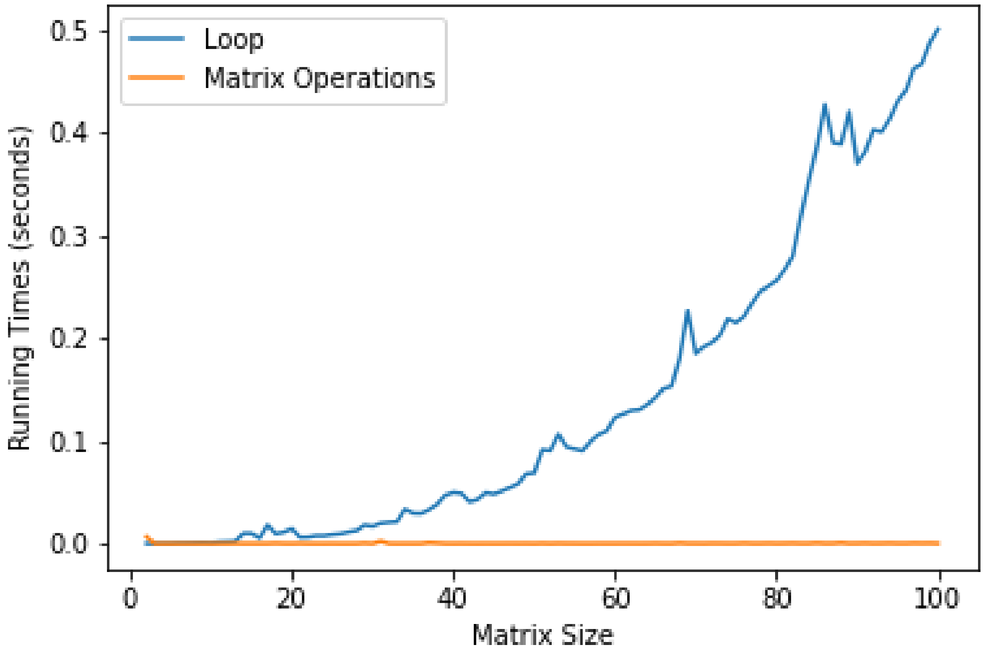
The random matrices were generated using the `numpy.random.rand` function, the functions were profiled on their running times in seconds using `timeit.timeit`, and plotted using the `matplotlib.pyplot` library.

1.2.2 2.2. Results

The plot of the running times of the pairwise distance nested loop-based function vs. pairwise distance vectorized function over square matrices of dimension 2 to 100 was plotted using `matplotlib` and looks like:

[11]:
```
from IPython.display import Image
Image(filename='comparison-problem-01.png')
```

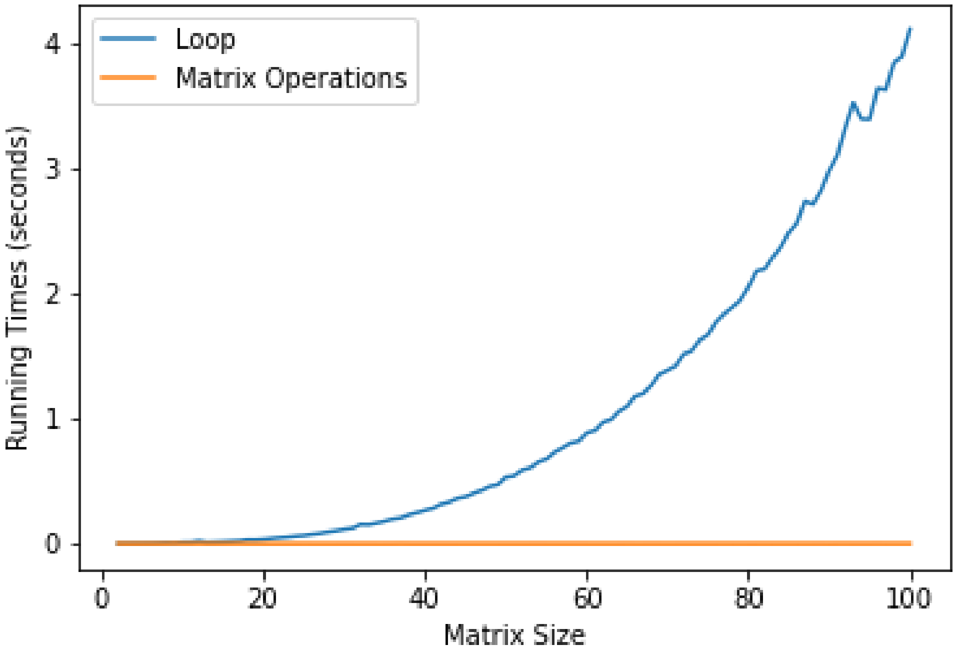
[11]:



Likewise, the running times of the correlation nested loop-based function vs. correlation vectorized function over square matrices of dimension 2 to 100 was plotted using matplotlib and looks like:

[12]:
```
Image(filename='comparison-problem-02.png')
```

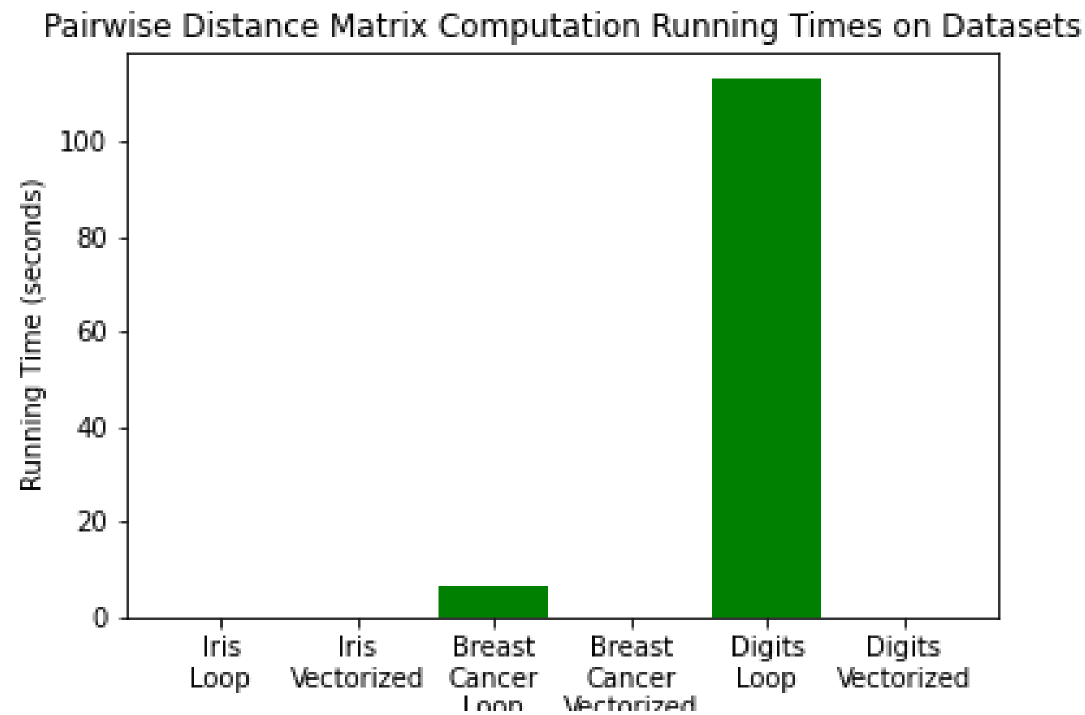
[12]:



And the bar chart for running times of the distance functions on each of the three datasets:

[13]:
```
Image(filename='datasets-distance-bar-chart.png')
```

[13]:



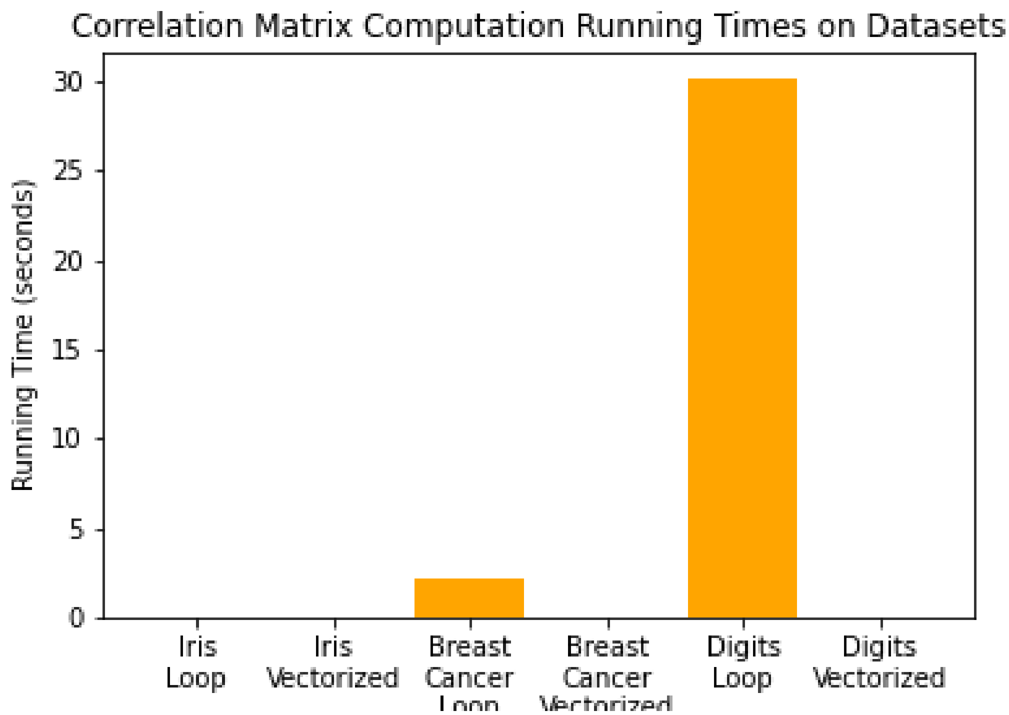
With corresponding table:

$$\begin{bmatrix} & Loop & Vectorized \\ Iris & 0.1510970079999936 & 0.0007549089999940861 \\ Breast\ Cancer & 6.3926503510000146 & 0.008255077000001165 \\ Digits & 113.27628421600002 & 0.09805695200000741 \end{bmatrix}$$

And the bar chart for the running times of the correlation functions on each of the three datasets:

[14]:
```
Image(filename='datasets-correlation-bar-chart.png')
```

[14]:



With corresponding table:

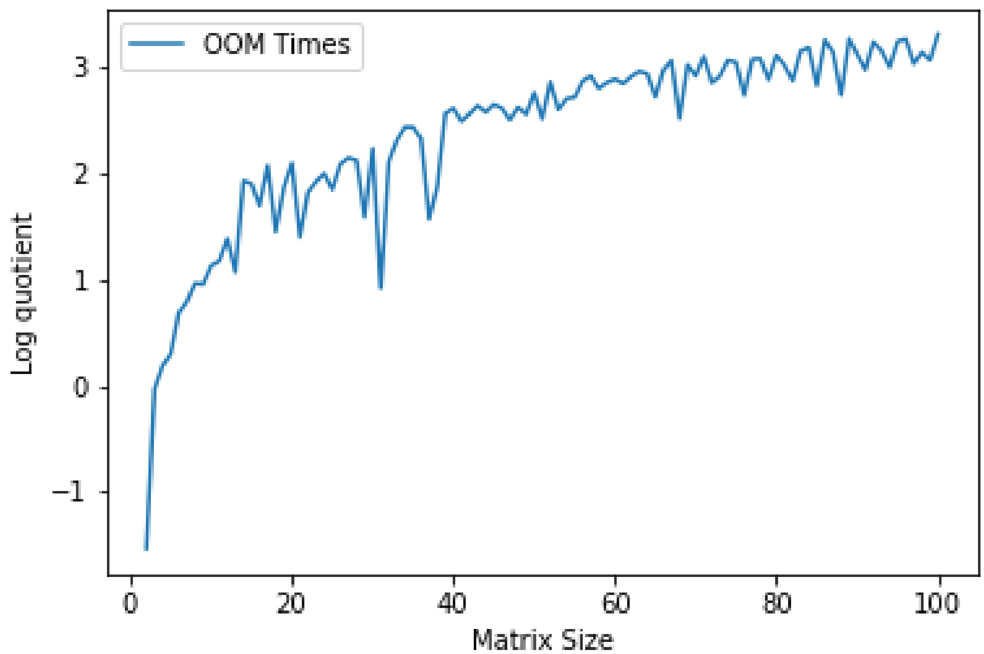
$$\begin{bmatrix} & Loop & Vectorized \\ Iris & 0.009754814000000433 & 0.0004387809999972164 \\ Breast\ \ Cancer & 2.158253350999985 & 0.0014982579999980317 \\ Digits & 30.146993707000007 & 0.011665293000021393 \end{bmatrix}$$

1.2.3 2.3. – Discussion

We see from the plots and tables that the vectorized method is several orders of magnitude faster than the loop-based method. From this we can tell that vectorization leads to massive performance increases when working with array data. This is even more pronounced when considering scale: the order-of-magnitude difference in performance only grows with the size of the matrix, as we can tell from the plot comparing them:

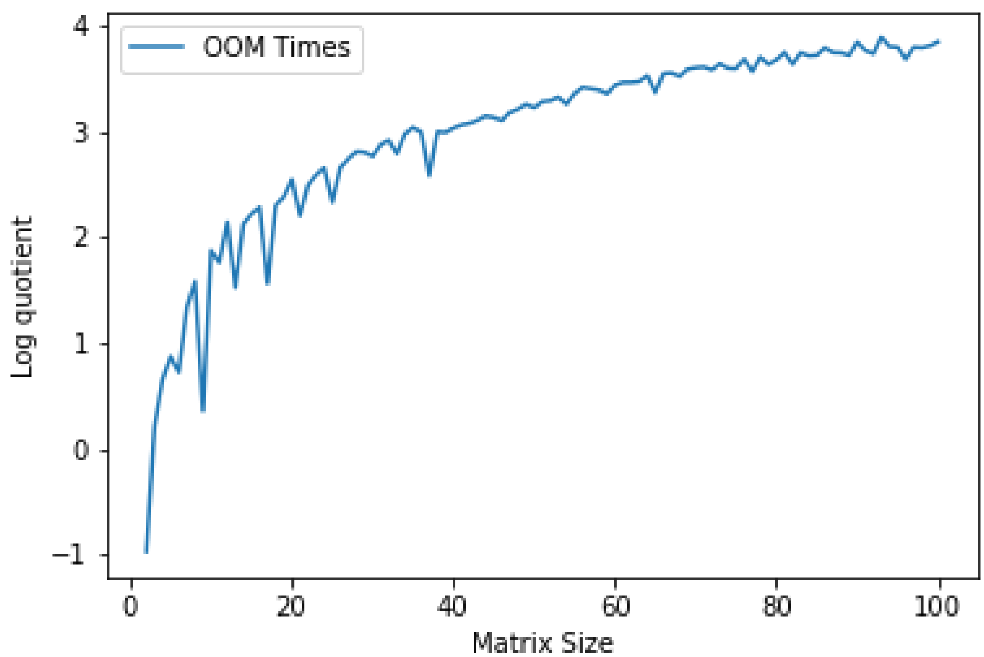
[15]:
```
Image(filename='comparison-problem-01-logs.png') # order of magnitude␣
↪difference in performance: pairwise distance matrix vectorization vs. loop
```

[15]:



[16]:
```
Image(filename='comparison-problem-02-logs.png') # order of magnitude␣
↪difference in performance: correlation matrix vectorization vs. loop
```

[16]:



It's clear that when possible, one ought to consider using vectorization instead of loop-based methods when performance is critical.