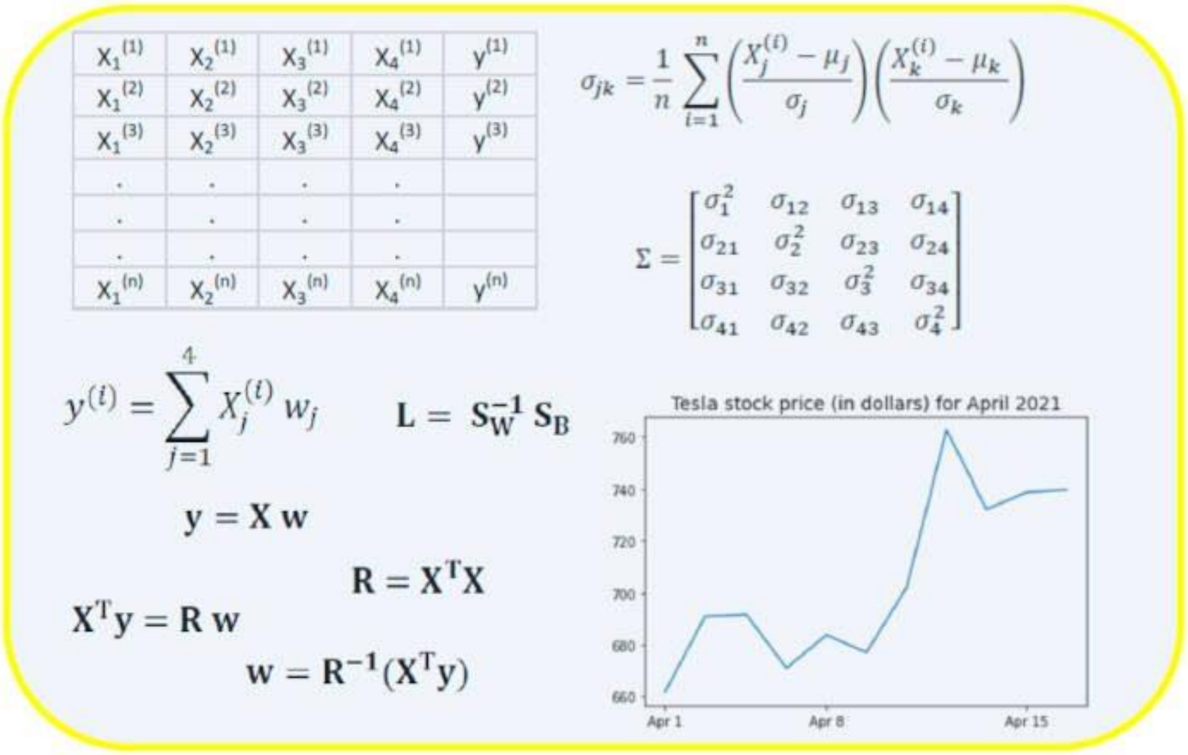
Matrices to represent relations between data, and necessary linear algebraic

Linear algebra is foundational in data science and machine learning. Beginners starting out along their learning journey in data science--as well as established practitioners--must develop a strong familiarity with the essential concepts in linear algebra.



$X_1^{(1)}$	$X_2^{(1)}$	$X_3^{(1)}$	$X_4^{(1)}$	$y^{(1)}$
$X_1^{(2)}$	$X_2^{(2)}$	$X_3^{(2)}$	$X_4^{(2)}$	$y^{(2)}$
$X_1^{(3)}$	$X_2^{(3)}$	$X_3^{(3)}$	$X_4^{(3)}$	$y^{(3)}$
.	.	.	.	
.	.	.	.	
.	.	.	.	
$X_1^{(n)}$	$X_2^{(n)}$	$X_3^{(n)}$	$X_4^{(n)}$	$y^{(n)}$

$$\sigma_{jk} = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{X_j^{(i)} - \mu_j}{\sigma_j}\right)\left(\frac{X_k^{(i)} - \mu_k}{\sigma_k}\right)$$

$$\Sigma = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \sigma_{13} & \sigma_{14} \\ \sigma_{21} & \sigma_2^2 & \sigma_{23} & \sigma_{24} \\ \sigma_{31} & \sigma_{32} & \sigma_3^2 & \sigma_{34} \\ \sigma_{41} & \sigma_{42} & \sigma_{43} & \sigma_4^2 \end{bmatrix}$$

$$y^{(i)} = \sum_{j=1}^{4} X_j^{(i)} w_j \qquad \mathbf{L} = \mathbf{S}_\mathbf{W}^{-1}\mathbf{S}_\mathbf{B}$$

$$\mathbf{y} = \mathbf{X}\,\mathbf{w}$$

$$\mathbf{R} = \mathbf{X}^\mathrm{T}\mathbf{X}$$

$$\mathbf{X}^\mathrm{T}\mathbf{y} = \mathbf{R}\,\mathbf{w}$$

$$\mathbf{w} = \mathbf{R}^{-1}(\mathbf{X}^\mathrm{T}\mathbf{y})$$

Image by Benjamin O. Tayo.

Linear Algebra is a branch of mathematics that is extremely useful in data science and machine learning. Linear algebra is the most important math skill in machine learning. Most machine learning models can be expressed in matrix form. A dataset itself is often represented as a matrix. Linear algebra is used in data preprocessing, data transformation, and model evaluation. Here are the topics you need to be familiar with:

- Vectors
- Matrices
- Transpose of a matrix
- Inverse of a matrix
- Determinant of a matrix
- Trace of a matrix
- Dot product
- Eigenvalues
- Eigenvectors

In this article, we illustrate the application of linear algebra in data science and machine learning using the tech stocks dataset, which can be found here.

1. Linear Algebra for Data Preprocessing

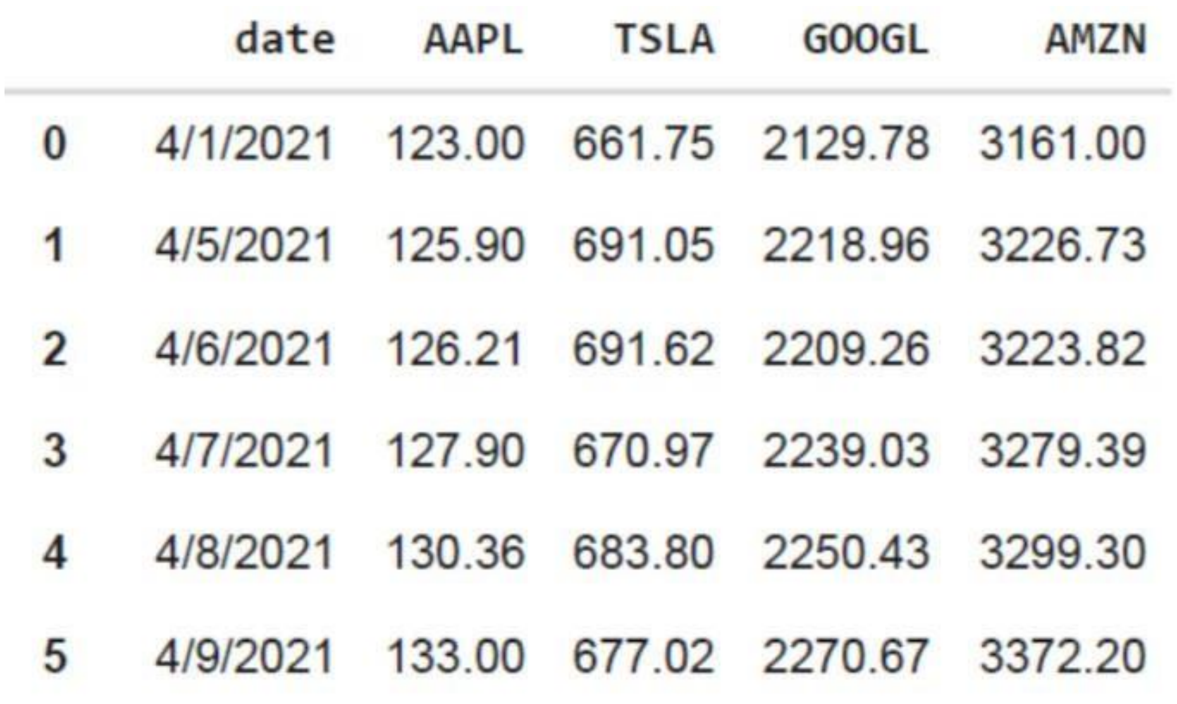
We begin by illustrating how linear algebra is used in data preprocessing.

1.1 Import necessary libraries for linear algebra

```
import numpy as np
import pandas as pd
import pylab
import matplotlib.pyplot as plt
import seaborn as sns
```

1.2 Read dataset and display features

```
data = pd.read_csv("tech-stocks-04-2021.csv")
data.head()
```



	date	AAPL	TSLA	GOOGL	AMZN
0	4/1/2021	123.00	661.75	2129.78	3161.00
1	4/5/2021	125.90	691.05	2218.96	3226.73
2	4/6/2021	126.21	691.62	2209.26	3223.82
3	4/7/2021	127.90	670.97	2239.03	3279.39
4	4/8/2021	130.36	683.80	2250.43	3299.30
5	4/9/2021	133.00	677.02	2270.67	3372.20

Table 1. *Stock prices for selected stock prices for the first 16 days in April 2021.*

```
print(data.shape)
output = (11,5)
```

The ***data.shape*** function enables us to know the size of our dataset. In this case, the dataset has 5 features (date, AAPL, TSLA, GOOGL, and AMZN), and each feature has 11 observations. *Date* refers to the trading days in April 2021 (up to April 16). AAPL, TSLA, GOOGL, and AMZN are the closing stock prices for Apple, Tesla, Google, and Amazon, respectively.

1.3 Data visualization

To perform data visualization, we would need to define ***column matrices*** for the features to be visualized:

```
x = data['date']
y = data['TSLA']
plt.plot(x,y)
plt.xticks(np.array([0,4,9]), ['Apr 1','Apr 8','Apr 15'])
plt.title('Tesla stock price (in dollars) for April 2021',size=14)
plt.show()
```

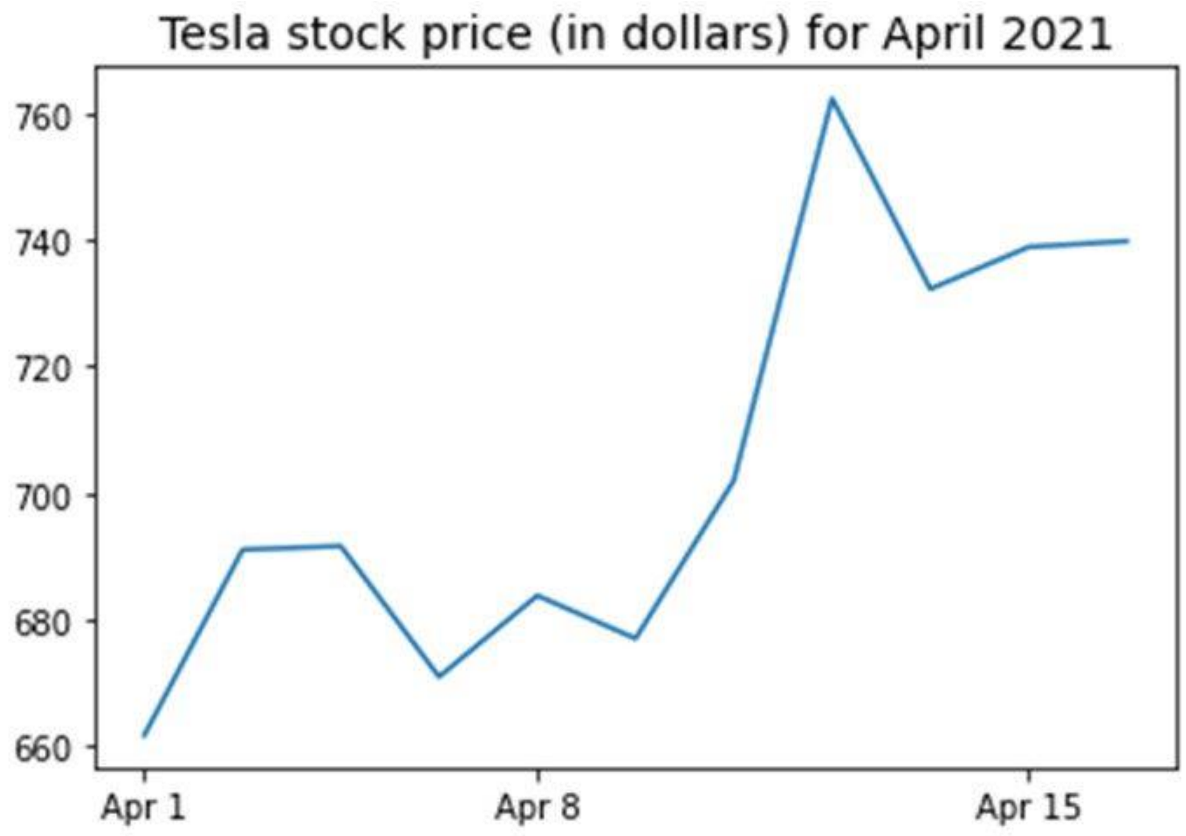
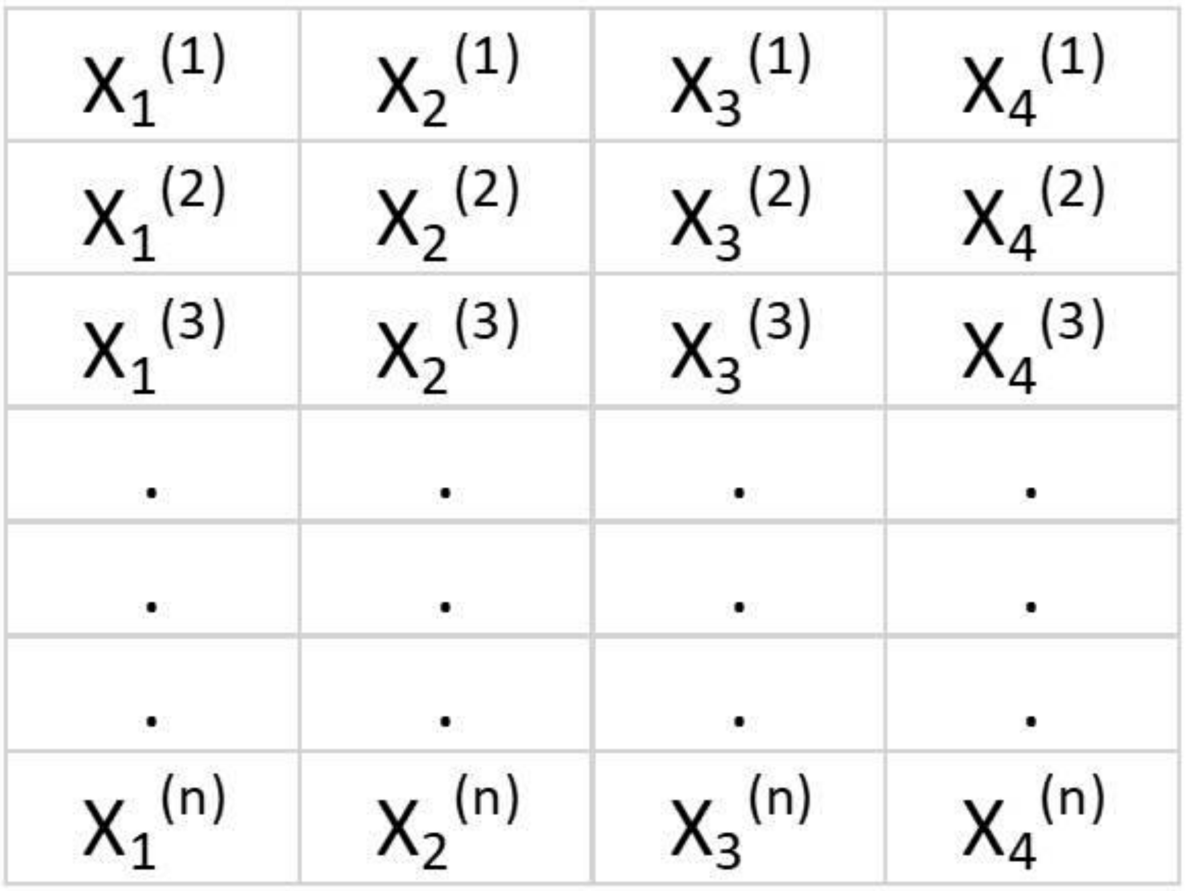


***Figure 1**. Tesla stock price for first 16 days in April 2021.*

2. Covariance Matrix

The ***covariance matrix*** is one of the most important matrices in data science and machine learning. It provides information about co-movement (correlation) between features. Suppose we have a features matrix with *4* features and *n* observations as shown in **Table 2**:



$X_1^{(1)}$	$X_2^{(1)}$	$X_3^{(1)}$	$X_4^{(1)}$
$X_1^{(2)}$	$X_2^{(2)}$	$X_3^{(2)}$	$X_4^{(2)}$
$X_1^{(3)}$	$X_2^{(3)}$	$X_3^{(3)}$	$X_4^{(3)}$
.	.	.	.
.	.	.	.
.	.	.	.
$X_1^{(n)}$	$X_2^{(n)}$	$X_3^{(n)}$	$X_4^{(n)}$

Table 2. *Features matrix with 4 variables and n observations.*

To visualize the correlations between the features, we can generate a scatter pairplot:

```
cols=data.columns[1:5]
print(cols)
output = Index(['AAPL', 'TSLA', 'GOOGL', 'AMZN'], dtype='object')
sns.pairplot(data[cols], height=3.0)
```

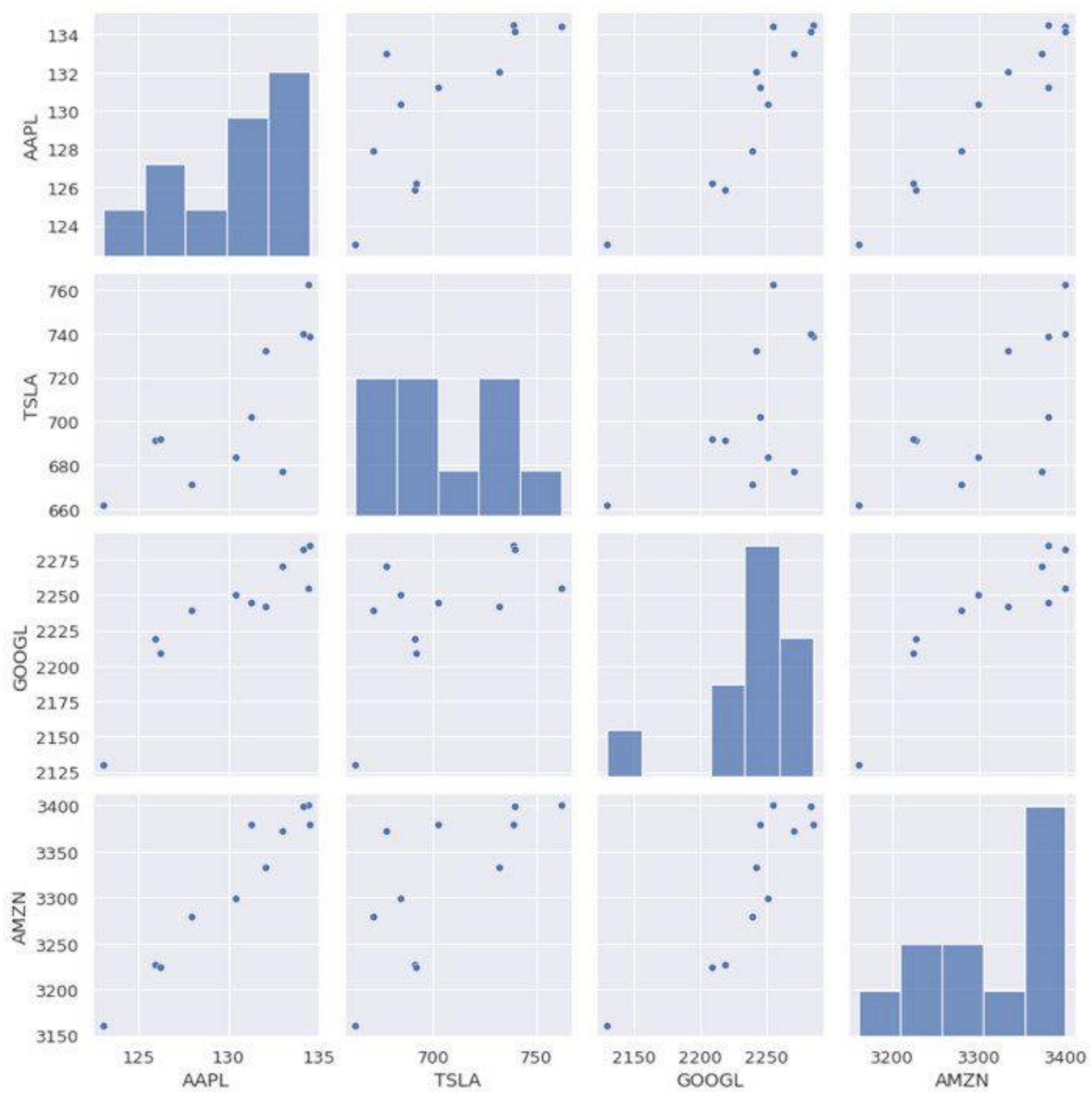


Figure 2. *Scatter pairplot for selected tech stocks.*

To quantify the degree of correlation between features (multicollinearity), we can compute the covariance matrix using this equation:

$$\sigma_{jk} = \frac{1}{n} \sum_{i=1}^{n} \left(\frac{X_j^{(i)} - \mu_j}{\sigma_j} \right) \left(\frac{X_k^{(i)} - \mu_k}{\sigma_k} \right)$$

where and are the mean and standard deviation of feature , respectively. This equation indicates that when features are standardized, the covariance matrix is simply the ***dot product*** between features.

In matrix form, the covariance matrix can be expressed as a 4 x 4 real and symmetric matrix:

$$\Sigma = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \sigma_{13} & \sigma_{14} \\ \sigma_{21} & \sigma_2^2 & \sigma_{23} & \sigma_{24} \\ \sigma_{31} & \sigma_{32} & \sigma_3^2 & \sigma_{34} \\ \sigma_{41} & \sigma_{42} & \sigma_{43} & \sigma_4^2 \end{bmatrix}$$

This matrix can be diagonalized by performing a ***unitary transformation***, also referred to as Principal Component Analysis (PCA) transformation, to obtain the following:

$$\tilde{\Sigma} = \begin{bmatrix} \lambda_1 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 \\ 0 & 0 & \lambda_3 & 0 \\ 0 & 0 & 0 & \lambda_4 \end{bmatrix}$$

Since the ***trace of a matrix*** remains invariant under a unitary transformation, we observe that the sum of the eigenvalues of the diagonal matrix is equal to the total variance contained in features X_1, X_2, X_3, and X_4.

2.1 Computing the covariance matrix for tech stocks

```
from sklearn.preprocessing import StandardScaler
stdsc = StandardScaler()
X_std = stdsc.fit_transform(data[cols].iloc[:,range(0,4)].values)
```

```
cov_mat = np.cov(X_std.T, bias= True)
```

Note that this uses the ***transpose*** of the standardized matrix.

2.2 Visualization of covariance matrix

```
plt.figure(figsize=(8,8))
sns.set(font_scale=1.2)
hm = sns.heatmap(cov_mat,
                 cbar=True,
                 annot=True,
                 square=True,
                 fmt='.2f',
                 annot_kws={'size': 12},
                 yticklabels=cols,
                 xticklabels=cols)
plt.title('Covariance matrix showing correlation coefficients')
plt.tight_layout()
plt.show()
```

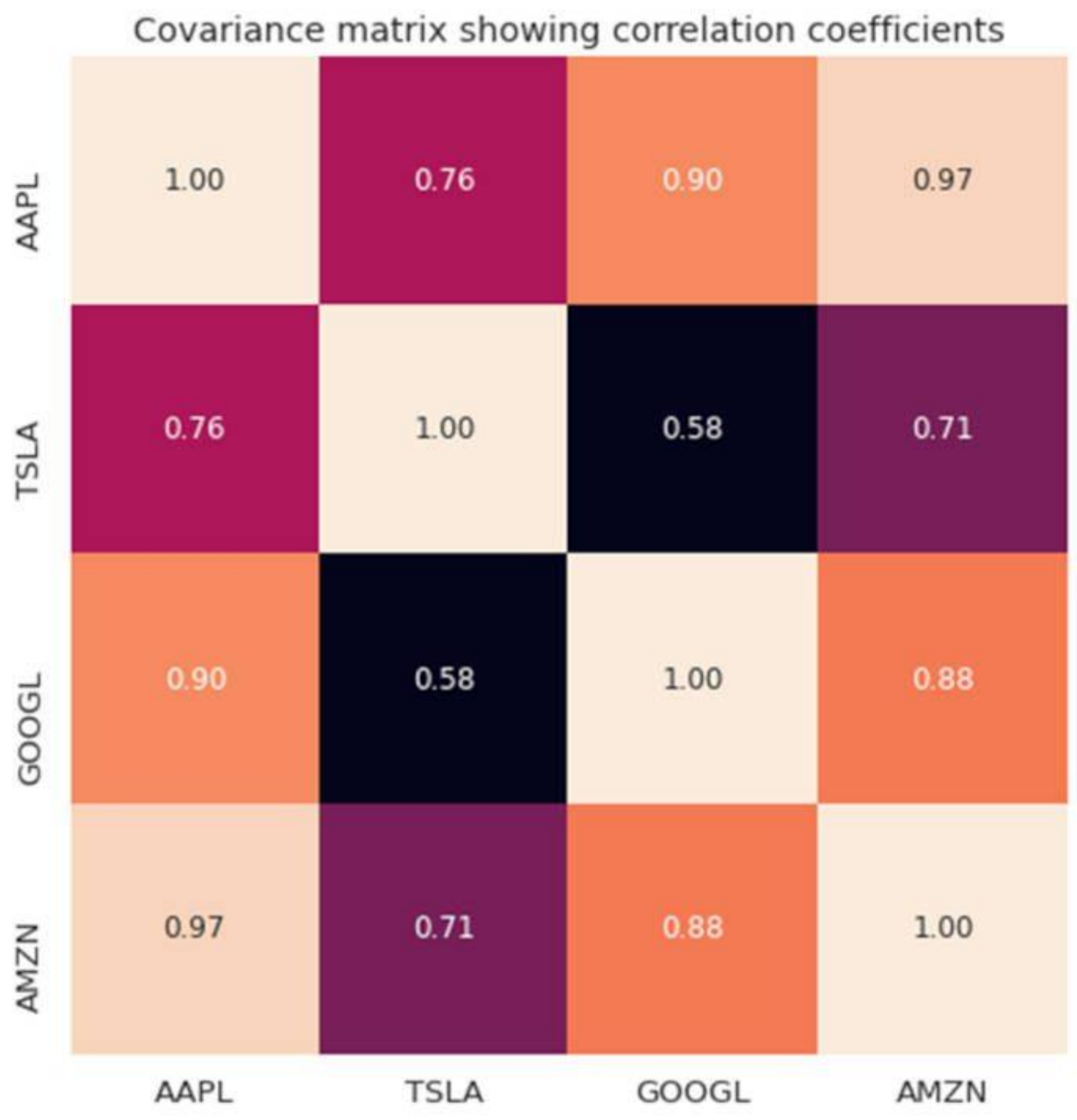


Figure 3. *Covariance matrix plot for selected tech stocks.*

We observe from Figure 3 that AAPL correlates strongly with GOOGL and AMZN, and weakly with TSLA. TSLA correlates generally weakly with AAPL, GOOGL and AMZN, while AAPL, GOOGL, and AMZN correlate strongly among each other.

2.3 Compute eigenvalues of the covariance matrix

```
np.linalg.eigvals(cov_mat)
output = array([3.41582227, 0.4527295 , 0.02045092, 0.11099732])
np.sum(np.linalg.eigvals(cov_mat))
output = 4.000000000000006
```

```
np.trace(cov_mat)
output = 4.000000000000001
```

We observe that the trace of the covariance matrix is equal to the sum of the eigenvalues as expected.

2.4 Compute the cumulative variance

Since the trace of a matrix remains invariant under a unitary transformation, we observe that the sum of the eigenvalues of the diagonal matrix is equal to the total variance contained in features X_1, X_2, X_3, and X_4. Hence, we can define the following quantities:

Notice that when $p = 4$, the cumulative variance becomes equal to 1 as expected.

```
eigen = np.linalg.eigvals(cov_mat)
cum_var = eigen/np.sum(eigen)
print(cum_var)
output = [0.85395557 0.11318237 0.00511273 0.02774933]

print(np.sum(cum_var))
output = 1.0
```

We observe from the cumulative variance (***cum_var***) that 85% of the variance is contained in the first eigenvalue and 11% in the second. This means when PCA is implemented, only the first two principal components could be used, as 97% of the total variance is contributed by these 2 components. This can essentially reduce the dimensionally of the feature space from 4 to 2 when PCA is implemented.

3. Linear Regression Matrix

Suppose we have a dataset that has 4 predictor features and *n* observations, as shown below.

***Table 3**. Features matrix with 4 variables and n observations. Column 5 is the target variable (y).*

We would like to build a multi-regression model for predicting the *y* values (column 5). Our model can thus be expressed in the form

$$y^{(i)} = \sum_{j=1}^{4} X_j^{(i)} \, w_j$$

In matrix form, this equation can be written as

$$\mathbf{y} = \mathbf{X}\,\mathbf{w}$$

where **X** is the (n x 4) features matrix, **w** is the (4 x 1) matrix representing the regression coefficients to be determined, and **y** is the (n x 1) matrix containing the n observations of the target variable y.

Note that **X** is a rectangular matrix, so we can't solve the equation above by taking the inverse of **X**.

To convert **X** into a square matrix, we multiple the left-hand side and right-hand side of our equation by the ***transpose*** of **X**, that is

$$\mathbf{X}^{\mathrm{T}}\mathbf{y} = \mathbf{X}^{\mathrm{T}}\mathbf{X}\,\mathbf{w}$$

This equation can also be expressed as

$$\mathbf{X}^{\mathrm{T}}\mathbf{y} = \mathbf{R}\,\mathbf{w}$$

where

$$\mathbf{R} = \mathbf{X}^{\mathrm{T}}\mathbf{X}$$

is the (4×4) regression matrix. Clearly, we observe that **R** is a real and symmetric matrix. Note that in linear algebra, the transpose of the product of two matrices obeys the following relationship

$$(\mathbf{AB})^{\mathrm{T}} = \mathbf{B}^{\mathrm{T}}\mathbf{A}^{\mathrm{T}}$$

Now that we've reduced our regression problem and expressed it in terms of the (4×4) real, symmetric, and invertible regression matrix **R**, it is straightforward to show that the exact solution of the regression equation is then

$$\mathbf{w} = \mathbf{R}^{-1}(\mathbf{X}^{\mathrm{T}}\mathbf{y})$$

4. Linear Discriminant Analysis Matrix

Another example of a real and symmetric matrix in data science is the Linear Discriminant Analysis (LDA) matrix. This matrix can be expressed in the form:

$$\mathbf{L} = \mathbf{S}_{\mathbf{W}}^{-1}\,\mathbf{S}_{\mathbf{B}}$$

where $\mathbf{S}_{\mathbf{W}}$ is the within-feature scatter matrix, and $\mathbf{S}_{\mathbf{B}}$ is the between-feature scatter matrix. Since both matrices $\mathbf{S}_{\mathbf{W}}$ and $\mathbf{S}_{\mathbf{B}}$ are real and symmetric, it follows that **L** is also real and symmetric. The diagonalization of **L** produces a feature subspace that optimizes class separability and reduces dimensionality. Hence LDA is a supervised algorithm, while PCA is not.

For more details about the implementation of LDA, please see the following references:

Machine Learning: Dimensionality Reduction via Linear Discriminant Analysis

GitHub repository for LDA implementation using Iris dataset