1.1 Creating a Vector

Problem

You need to create a vector.

Solution

Use NumPy to create a one-dimensional array:

```
# Load library
import numpy as np

# Create a vector as a row
vector_row = np.array([1, 2, 3])

# Create a vector as a column
vector_column = np.array([[1],
                          [2],
                          [3]])
```

Discussion

NumPy's main data structure is the multidimensional array. To create a vector, we simply create a one-dimensional array. Just like vectors, these arrays can be represented horizontally (i.e., rows) or vertically (i.e., columns).

See Also

- Vectors, Math Is Fun
- Euclidean vector, Wikipedia

1.2 Creating a Matrix

Problem

You need to create a matrix.

Solution

Use NumPy to create a two-dimensional array:

```
# Load library
import numpy as np

# Create a matrix
matrix = np.array([[1, 2],
                   [1, 2],
                   [1, 2]])
```

Discussion

To create a matrix we can use a NumPy two-dimensional array. In our solution, the matrix contains three rows and two columns (a column of 1s and a column of 2s).

NumPy actually has a dedicated matrix data structure:

```
matrix_object = np.mat([[1, 2],
                        [1, 2],
                        [1, 2]])
```

```
matrix([[1, 2],
        [1, 2],
        [1, 2]])
```

However, the matrix data structure is not recommended for two reasons. First, arrays are the de facto standard data structure of NumPy. Second, the vast majority of NumPy operations return arrays, not matrix objects.

See Also

- Matrix, Wikipedia
- Matrix, Wolfram MathWorld

1.3 Creating a Sparse Matrix

Problem

Given data with very few nonzero values, you want to efficiently represent it.

Solution

Create a sparse matrix:

```
# Load libraries
import numpy as np
from scipy import sparse

# Create a matrix
matrix = np.array([[0, 0],
                   [0, 1],
                   [3, 0]])

# Create compressed sparse row (CSR) matrix
matrix_sparse = sparse.csr_matrix(matrix)
```

Discussion

A frequent situation in machine learning is having a huge amount of data; however, most of the elements in the data are zeros. For example, imagine a matrix where the columns are every movie on Netflix, the rows are every Netflix user, and the values are how many times a user has watched that particular movie. This matrix would have tens of thousands of columns and millions of rows! However, since most users do not watch most movies, the vast majority of elements would be zero.

Sparse matrices only store nonzero elements and assume

all other values will be zero, leading to significant computational savings. In our solution, we created a NumPy array with two nonzero values, then converted it into a sparse matrix. If we view the sparse matrix we can see that only the nonzero values are stored:

```
# View sparse matrix
print(matrix_sparse)
```

```
  (1, 1)    1
  (2, 0)    3
```

There are a number of types of sparse matrices. However, in *compressed sparse row* (CSR) matrices, `(1, 1)` and `(2, 0)` represent the (zero-indexed) indices of the nonzero values 1 and 3, respectively. For example, the element 1 is in the second row and second column. We can see the advantage of sparse matrices if we create a much larger matrix with many more zero elements and then compare this larger matrix with our original sparse matrix:

```
# Create larger matrix
matrix_large = np.array([[0, 0, 0, 0, 0, 0, 0,
0, 0, 0],
                         [0, 1, 0, 0, 0, 0, 0,
0, 0, 0],
```

```
                                [3, 0, 0, 0, 0, 0, 0,
0, 0, 0]])

# Create compressed sparse row (CSR) matrix
matrix_large_sparse = sparse.csr_matrix(matrix_
large)
```

```
# View original sparse matrix
print(matrix_sparse)
```

```
  (1, 1)    1
  (2, 0)    3
```

```
# View larger sparse matrix
print(matrix_large_sparse)
```

```
  (1, 1)    1
  (2, 0)    3
```

As we can see, despite the fact that we added many more zero elements in the larger matrix, its sparse representation is exactly the same as our original sparse matrix. That is, the addition of zero elements did not change the size of the sparse matrix.

As mentioned, there are many different types of sparse

matrices, such as compressed sparse column, list of lists, and dictionary of keys. While an explanation of the different types and their implications is outside the scope of this book, it is worth noting that while there is no "best" sparse matrix type, there are meaningful differences between them and we should be conscious about why we are choosing one type over another.

See Also

- Sparse matrices, SciPy documentation
- 101 Ways to Store a Sparse Matrix

1.4 Selecting Elements

Problem

You need to select one or more elements in a vector or matrix.

Solution

NumPy's arrays make that easy:

```
# Load library
import numpy as np

# Create row vector
```

```
vector = np.array([1, 2, 3, 4, 5, 6])

# Create matrix
matrix = np.array([[1, 2, 3],
                   [4, 5, 6],
                   [7, 8, 9]])

# Select third element of vector
vector[2]
```

```
3
```

```
# Select second row, second column
matrix[1,1]
```

```
5
```

Discussion

Like most things in Python, NumPy arrays are zero-indexed, meaning that the index of the first element is 0, not 1. With that caveat, NumPy offers a wide variety of methods for selecting (i.e., indexing and slicing) elements or groups of elements in arrays:

```
# Select all elements of a vector
vector[:]
```

```
array([1, 2, 3, 4, 5, 6])
```

```
# Select everything up to and including the thi
rd element
vector[:3]
```

```
array([1, 2, 3])
```

```
# Select everything after the third element
vector[3:]
```

```
array([4, 5, 6])
```

```
# Select the last element
vector[-1]
```

```
6
```

```
# Select the first two rows and all columns of
a matrix
matrix[:2,:]
```

```
array([[1, 2, 3],
       [4, 5, 6]])
```

```
# Select all rows and the second column
matrix[:,1:2]
```

```
array([[2],
       [5],
       [8]])
```

1.5 Describing a Matrix

Problem

You want to describe the shape, size, and dimensions of the matrix.

Solution

Use `shape`, `size`, and `ndim`:

```
# Load library
import numpy as np

# Create matrix
matrix = np.array([[1, 2, 3, 4],
                   [5, 6, 7, 8],
```

```
                    [9, 10, 11, 12]])
```

```
# View number of rows and columns
matrix.shape
```

```
(3, 4)
```

```
# View number of elements (rows * columns)
matrix.size
```

```
12
```

```
# View number of dimensions
matrix.ndim
```

```
2
```

Discussion

This might seem basic (and it is); however, time and again it will be valuable to check the shape and size of an array both for further calculations and simply as a gut check after some operation.

1.6 Applying Operations to Elements

Problem

You want to apply some function to multiple elements in an array.

Solution

Use NumPy's `vectorize`:

```
# Load library
import numpy as np

# Create matrix
matrix = np.array([[1, 2, 3],
                   [4, 5, 6],
                   [7, 8, 9]])

# Create function that adds 100 to something
add_100 = lambda i: i + 100

# Create vectorized function
vectorized_add_100 = np.vectorize(add_100)

# Apply function to all elements in matrix
vectorized_add_100(matrix)
```

```
array([[101, 102, 103],
       [104, 105, 106],
```

```
       [107, 108, 109]])
```

Discussion

NumPy's `vectorize` class converts a function into a function that can apply to all elements in an array or slice of an array. It's worth noting that `vectorize` is essentially a `for` loop over the elements and does not increase performance. Furthermore, NumPy arrays allow us to perform operations between arrays even if their dimensions are not the same (a process called *broadcasting*). For example, we can create a much simpler version of our solution using broadcasting:

```
# Add 100 to all elements
matrix + 100
```

```
array([[101, 102, 103],
       [104, 105, 106],
       [107, 108, 109]])
```

1.7 Finding the Maximum and Minimum Values

Problem

You need to find the maximum or minimum value in an array.

Solution

Use NumPy's `max` and `min`:

```
# Load library
import numpy as np

# Create matrix
matrix = np.array([[1, 2, 3],
                   [4, 5, 6],
                   [7, 8, 9]])

# Return maximum element
np.max(matrix)
```

```
9
```

```
# Return minimum element
np.min(matrix)
```

```
1
```

Discussion

Often we want to know the maximum and minimum value in an array or subset of an array. This can be accomplished with the `max` and `min` methods. Using the `axis` parameter we can also apply the operation along a certain axis:

```
# Find maximum element in each column
np.max(matrix, axis=0)
```

```
array([7, 8, 9])
```

```
# Find maximum element in each row
np.max(matrix, axis=1)
```

```
array([3, 6, 9])
```

1.8 Calculating the Average, Variance, and Standard Deviation

Problem

You want to calculate some descriptive statistics about an array.

Solution

Use NumPy's `mean`, `var`, and `std`:

```
# Load library
import numpy as np

# Create matrix
matrix = np.array([[1, 2, 3],
                   [4, 5, 6],
                   [7, 8, 9]])

# Return mean
np.mean(matrix)
```

```
5.0
```

```
# Return variance
np.var(matrix)
```

```
6.666666666666667
```

```
# Return standard deviation
np.std(matrix)
```

```
2.5819888974716112
```

Discussion

Just like with `max` and `min`, we can easily get descriptive statistics about the whole matrix or do calculations along a single axis:

```
# Find the mean value in each column
np.mean(matrix, axis=0)
```

```
array([ 4.,  5.,  6.])
```

1.9 Reshaping Arrays

Problem

You want to change the shape (number of rows and columns) of an array without changing the element values.

Solution

Use NumPy's `reshape`:

```
# Load library
import numpy as np

# Create 4x3 matrix
```

```
matrix = np.array([[1, 2, 3],
                   [4, 5, 6],
                   [7, 8, 9],
                   [10, 11, 12]])

# Reshape matrix into 2x6 matrix
matrix.reshape(2, 6)
```

```
array([[ 1,  2,  3,  4,  5,  6],
       [ 7,  8,  9, 10, 11, 12]])
```

Discussion

`reshape` allows us to restructure an array so that we maintain the same data but it is organized as a different number of rows and columns. The only requirement is that the shape of the original and new matrix contain the same number of elements (i.e., the same size). We can see the size of a matrix using `size`:

```
matrix.size
```

```
12
```

One useful argument in `reshape` is `-1`, which effectively means "as many as needed," so `reshape(-1, 1)` means

one row and as many columns as needed:

```
matrix.reshape(1, -1)
```

```
array([[ 1,  2,  3,  4,  5,  6,  7,  8,  9, 10, 11,
```

Finally, if we provide one integer, `reshape` will return a 1D array of that length:

```
matrix.reshape(12)
```

```
array([ 1,  2,  3,  4,  5,  6,  7,  8,  9, 10, 11,
```

1.10 Transposing a Vector or Matrix

Problem

You need to transpose a vector or matrix.

Solution

Use the T method:

```
# Load library
```

```
import numpy as np

# Create matrix
matrix = np.array([[1, 2, 3],
                   [4, 5, 6],
                   [7, 8, 9]])

# Transpose matrix
matrix.T
```

```
array([[1, 4, 7],
       [2, 5, 8],
       [3, 6, 9]])
```

Discussion

Transposing is a common operation in linear algebra where the column and row indices of each element are swapped. One nuanced point that is typically overlooked outside of a linear algebra class is that, technically, a vector cannot be transposed because it is just a collection of values:

```
# Transpose vector
np.array([1, 2, 3, 4, 5, 6]).T
```

```
array([1, 2, 3, 4, 5, 6])
```

However, it is common to refer to transposing a vector as converting a row vector to a column vector (notice the second pair of brackets) or vice versa:

```
# Tranpose row vector
np.array([[1, 2, 3, 4, 5, 6]]).T
```

```
array([[1],
       [2],
       [3],
       [4],
       [5],
       [6]])
```

1.11 Flattening a Matrix

Problem

You need to transform a matrix into a one-dimensional array.

Solution

Use `flatten`:

```
# Load library
import numpy as np
```

```
# Create matrix
matrix = np.array([[1, 2, 3],
                   [4, 5, 6],
                   [7, 8, 9]])

# Flatten matrix
matrix.flatten()
```

```
array([1, 2, 3, 4, 5, 6, 7, 8, 9])
```

Discussion

`flatten` is a simple method to transform a matrix into a one-dimensional array. Alternatively, we can use `reshape` to create a row vector:

```
matrix.reshape(1, -1)
```

```
array([[1, 2, 3, 4, 5, 6, 7, 8, 9]])
```

1.12 Finding the Rank of a Matrix

Problem

You need to know the rank of a matrix.

Solution

Use NumPy's linear algebra method `matrix_rank`:

```
# Load library
import numpy as np

# Create matrix
matrix = np.array([[1, 1, 1],
                   [1, 1, 10],
                   [1, 1, 15]])

# Return matrix rank
np.linalg.matrix_rank(matrix)
```

```
2
```

Discussion

The rank of a matrix is the dimensions of the vector space spanned by its columns or rows. Finding the rank of a matrix is easy in NumPy thanks to `matrix_rank`.

See Also

- The Rank of a Matrix, CliffsNotes

1.13 Calculating the Determinant

Problem

You need to know the determinant of a matrix.

Solution

Use NumPy's linear algebra method `det`:

```
# Load library
import numpy as np

# Create matrix
matrix = np.array([[1, 2, 3],
                   [2, 4, 6],
                   [3, 8, 9]])

# Return determinant of matrix
np.linalg.det(matrix)
```

```
0.0
```

Discussion

It can sometimes be useful to calculate the determinant of a matrix. NumPy makes this easy with `det`.

See Also

- The determinant | Essence of linear algebra, chapter 5,

3Blue1Brown

- Determinant, Wolfram MathWorld

1.14 Getting the Diagonal of a Matrix

Problem

You need to get the diagonal elements of a matrix.

Solution

Use `diagonal`:

```
# Load library
import numpy as np

# Create matrix
matrix = np.array([[1, 2, 3],
                   [2, 4, 6],
                   [3, 8, 9]])

# Return diagonal elements
matrix.diagonal()
```

```
array([1, 4, 9])
```

Discussion

NumPy makes getting the diagonal elements of a matrix easy with `diagonal`. It is also possible to get a diagonal off from the main diagonal by using the `offset` parameter:

```
# Return diagonal one above the main diagonal
matrix.diagonal(offset=1)
```

```
array([2, 6])
```

```
# Return diagonal one below the main diagonal
matrix.diagonal(offset=-1)
```

```
array([2, 8])
```

1.15 Calculating the Trace of a Matrix

Problem

You need to calculate the trace of a matrix.

Solution

Use `trace`:

```
# Load library
import numpy as np

# Create matrix
matrix = np.array([[1, 2, 3],
                   [2, 4, 6],
                   [3, 8, 9]])

# Return trace
matrix.trace()
```

```
14
```

Discussion

The trace of a matrix is the sum of the diagonal elements and is often used under the hood in machine learning methods. Given a NumPy multidimensional array, we can calculate the trace using `trace`. We can also return the diagonal of a matrix and calculate its sum:

```
# Return diagonal and sum elements
sum(matrix.diagonal())
```

```
14
```

See Also

- The Trace of a Square Matrix

1.16 Finding Eigenvalues and Eigenvectors

Problem

You need to find the eigenvalues and eigenvectors of a square matrix.

Solution

Use NumPy's `linalg.eig`:

```
# Load library
import numpy as np

# Create matrix
matrix = np.array([[1, -1, 3],
                   [1, 1, 6],
                   [3, 8, 9]])

# Calculate eigenvalues and eigenvectors
eigenvalues, eigenvectors = np.linalg.eig(matri
x)
```

```
# View eigenvalues
eigenvalues
```

```
array([ 13.55075847,   0.74003145,  -3.29078992])
```

```
# View eigenvectors
eigenvectors
```

```
array([[-0.17622017, -0.96677403, -0.53373322],
       [-0.435951  ,  0.2053623 , -0.64324848],
       [-0.88254925,  0.15223105,  0.54896288]])
```

Discussion

Eigenvectors are widely used in machine learning libraries. Intuitively, given a linear transformation represented by a matrix, *A*, eigenvectors are vectors that, when that transformation is applied, change only in scale (not direction). More formally:

$$A\mathbf{v} = \lambda\mathbf{v}$$

where *A* is a square matrix, λ contains the eigenvalues and *v* contains the eigenvectors. In NumPy's linear algebra toolset, `eig` lets us calculate the eigenvalues, and eigenvectors of any square matrix.

See Also

- Eigenvectors and Eigenvalues Explained Visually, Setosa.io
- Eigenvectors and eigenvalues | Essence of linear algebra, Chapter 10, 3Blue1Brown

1.17 Calculating Dot Products

Problem

You need to calculate the dot product of two vectors.

Solution

Use NumPy's `dot`:

```
# Load library
import numpy as np

# Create two vectors
vector_a = np.array([1,2,3])
vector_b = np.array([4,5,6])

# Calculate dot product
np.dot(vector_a, vector_b)
```

```
32
```

Discussion

The dot product of two vectors, *a* and *b*, is defined as:

$$\sum_{i=1}^{n} a_i \, b_i$$

where a_i is the *i*th element of vector *a*. We can use NumPy's `dot` class to calculate the dot product. Alternatively, in Python 3.5+ we can use the new `@` operator:

```
# Calculate dot product
vector_a @ vector_b
```

```
32
```

See Also

- Vector dot product and vector length, Khan Academy
- Dot Product, Paul's Online Math Notes

1.18 Adding and Subtracting Matrices

Problem

You want to add or subtract two matrices.

Solution

Use NumPy's add and `subtract`:

```
# Load library
import numpy as np

# Create matrix
matrix_a = np.array([[1, 1, 1],
                     [1, 1, 1],
                     [1, 1, 2]])

# Create matrix
matrix_b = np.array([[1, 3, 1],
                     [1, 3, 1],
                     [1, 3, 8]])

# Add two matrices
np.add(matrix_a, matrix_b)
```

```
array([[ 2,  4,  2],
       [ 2,  4,  2],
       [ 2,  4, 10]])
```

```
# Subtract two matrices
np.subtract(matrix_a, matrix_b)
```

```
array([[ 0, -2,  0],
       [ 0, -2,  0],
```

```
       [ 0, -2, -6]])
```

Discussion

Alternatively, we can simply use the + and – operators:

```
# Add two matrices
matrix_a + matrix_b
```

```
array([[ 2,  4,  2],
       [ 2,  4,  2],
       [ 2,  4, 10]])
```

1.19 Multiplying Matrices

Problem

You want to multiply two matrices.

Solution

Use NumPy's `dot`:

```
# Load library
import numpy as np

# Create matrix
```

```
matrix_a = np.array([[1, 1],
                     [1, 2]])

# Create matrix
matrix_b = np.array([[1, 3],
                     [1, 2]])

# Multiply two matrices
np.dot(matrix_a, matrix_b)
```

```
array([[2, 5],
       [3, 7]])
```

Discussion

Alternatively, in Python 3.5+ we can use the @ operator:

```
# Multiply two matrices
matrix_a @ matrix_b
```

```
array([[2, 5],
       [3, 7]])
```

If we want to do element-wise multiplication, we can use the $*$ operator:

```
# Multiply two matrices element-wise
```

```
matrix_a * matrix_b
```

```
array([[1, 3],
       [1, 4]])
```

See Also

- Array vs. Matrix Operations, MathWorks

1.20 Inverting a Matrix

Problem

You want to calculate the inverse of a square matrix.

Solution

Use NumPy's linear algebra `inv` method:

```
# Load library
import numpy as np

# Create matrix
matrix = np.array([[1, 4],
                   [2, 5]])

# Calculate inverse of matrix
np.linalg.inv(matrix)
```

```
array([[-1.66666667,  1.33333333],
       [ 0.66666667, -0.33333333]])
```

Discussion

The inverse of a square matrix, **A**, is a second matrix $\mathbf{A}^{-1}$, such that:

$$\mathbf{A}\mathbf{A}^{-1} = \mathbf{I}$$

where **I** is the identity matrix. In NumPy we can use `linalg.inv` to calculate $\mathbf{A}^{-1}$ if it exists. To see this in action, we can multiply a matrix by its inverse and the result is the identity matrix:

```
# Multiply matrix and its inverse
matrix @ np.linalg.inv(matrix)
```

```
array([[ 1.,  0.],
       [ 0.,  1.]])
```

See Also

- Inverse of a Matrix

1.21 Generating Random Values

Problem

You want to generate pseudorandom values.

Solution

Use NumPy's `random`:

```
# Load library
import numpy as np

# Set seed
np.random.seed(0)

# Generate three random floats between 0.0 and
1.0
np.random.random(3)
```

```
array([ 0.5488135 ,  0.71518937,  0.60276338])
```

Discussion

NumPy offers a wide variety of means to generate random numbers, many more than can be covered here. In our solution we generated floats; however, it is also common to generate integers:

```
# Generate three random integers between 1 and
10
```

```
np.random.randint(0, 11, 3)
```

```
array([3, 7, 9])
```

Alternatively, we can generate numbers by drawing them from a distribution:

```
# Draw three numbers from a normal distribution
 with mean 0.0
# and standard deviation of 1.0
np.random.normal(0.0, 1.0, 3)
```

```
array([-1.42232584,  1.52006949, -0.29139398])
```

```
# Draw three numbers from a logistic distributi
on with mean 0.0 and scale of 1.0
np.random.logistic(0.0, 1.0, 3)
```

```
array([-0.98118713, -0.08939902,  1.46416405])
```

```
# Draw three numbers greater than or equal to 1
.0 and less than 2.0
np.random.uniform(1.0, 2.0, 3)
```