Using the NumPy Package

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Outline

Intro to NumPy

NumPy arrays

Linear algebra with NumPy

Broadcasting and efficient operations

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 Depending on how you are interacting with Python, may have to install the numpy package before the first use. Open a command terminal (Ctrl+`, in VSCode on Windows) and type the appropriate command below:

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py -m pip install numpy (Windows)
python3-m pip install numpy (macOS)
sudo pip install numpy (Linux based)
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When installing other packages, replace numpy with the package name.

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Basic NumPy arrays

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Example:

```
v = np.array([-1, 1, 1])
w = np.array([0.5, 0, 1.1])
# print the (vector) sum: [-0.5 1. 2.1]
print(v + w)
# prints [1.0, 0.0, 2.2]
print(2*w)
```

More than 1d

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A 2-dimensional array, or tensor of order 2, is like a matrix. You construct it with np.array() from a list of lists – each of the same length.

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A = np.array([[1, 2, 3], [4, 5, 6]])
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Every array in NumPy has an attribute shape.

- Previous slide: v = np.array([-1,1,1]) has v.shape = (3,).
- The matrix here: A.shape is equal to (2, 3).

Operations on arrays

Multiplying two arrays: most recent version of Python uses the a symbol. 1

When the arrays are both matrices, it computes their matrix product; when one is a vector, it computes the matrix-vector product; when both are vectors, it computes the dot product.

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For example, say that A is the matrix $\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$ from before, v is the vector (-1, 1, 1), and let B and u be the matrix and vector defined in the code below.

```
B = np.array([[1, 0], [1, -1], [1, 1]])
u = np.array([1, 1, 0])
(A @ B, A @ v, v @ u)
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1 | B = np.array([[1, 0], [1, -1], [1, 1]])
2 | u = np.array([1, 1, 0])
3 | (A \( \text{0} \) B, A \( \text{0} \) v, v \( \text{0} \) u)
```

Output: (array([[6, 1], [15, 1]]), array([4, 7]), 0).

 $^{^1\}mbox{In older versions, matrix multiplication is } \mbox{np.matmul()}$ and dot product is $\mbox{np.dot()}.$

Items in 1d array are accessed the same way as in a list e.g., v[0] is first item in v, at index o.

For a 2d array, say the matrix A, we can access the item in the row i and column j by A[i, j].

²The colon here says to take all indices in that position.

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With arrays (not lists), can even use non-consecutive indices; e.g.,

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Identity matrix: The command np.identity(n) constructs the $n \times n$ identity matrix (and np.eye(n) does also).

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- For example, for the determinant of a square matrix M, you type
 np.linalg.det(M)
- Many other linear algebra functions in this package (see the docs here).

Some are only implemented with square matrices (and perhaps only invertible ones), even though it would make sense to implement them in more general settings – for example, np.linalg.solve(A,b) only solves the system of equations Ax=b if A is a square matrix.

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Efficient way in NumPy is called broadcasting. If v is the array, type

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| sqrt_v = np.sqrt(v)
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The function np.sqrt() takes the square root of each entry in v; you don't need to write a for loop.⁴

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```
np.abs(), np.sum(), np.maximum(), np.minimum(), np.exp(),
np.log().
```

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Many basic operations with NumPy arrays also use broadcasting. Here are a few examples with an array v.

- 1. To add a number, say 1.2, to every array entry: type v+1.2.
- 2. To multiply every entry by 1.2: type 1.2*v.

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Exercise. Use broadcasting to create a 100 \times 100 matrix with all non-diagonal entries equal to -1 and diagonal entries equal to $\sqrt{2} - 1$.

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To check the efficiency of broadcasting, use the time package. Beforehand, make sure that you imported both numpy and time (see slide in first section).

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First, we use a for loop. Run the code below in your Jupyter notebook.

```
id_matrix = np.eye(1000)
exp_matrix = np.zeros((1000, 1000))
start = time.time()
for i in range(1000):
    for j in range(1000):
        exp_matrix[i,j] = np.exp(id_matrix[i,j])
end = time.time()
print(f"Seconds taken: {end-start}.")
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The output gives the number of seconds to run the computation. The exact time will vary based on your computer. Mine took around 0.55 seconds.

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Run the following code in your Jupyter notebook.

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print(f"Seconds taken: {end-start}.")
```

Again, the output is the number of seconds of runtime. For this approach with np.exp(), my computer took around 0.0045 seconds. That is over 100 times faster than using the loop!