# DS-GA 1007 | Lecture 5

## Programming for Data Science

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October 10, 2023

# Array Manipulation for Scientific Computing

# DS-GA 1007 Curriculum

## Programming for Data Science:

- Introduction to Programming in Python
- Best Practice Programming and Software Engineering
- Program Efficiency
- Interacting with Programs
- **Array Manipulation for Scientific Computing**
- Data Visualization
- Advanced Data Objects ($\times 4$)
- Environments for Collaborative Programming
- Industrial Applications

# Array Manipulation for Scientific Computing

## Last week:

- Python Editors and IDEs
- Distributions, Packages and Virtual Environments
- OS Interfaces to Interact with Programs

## Today:

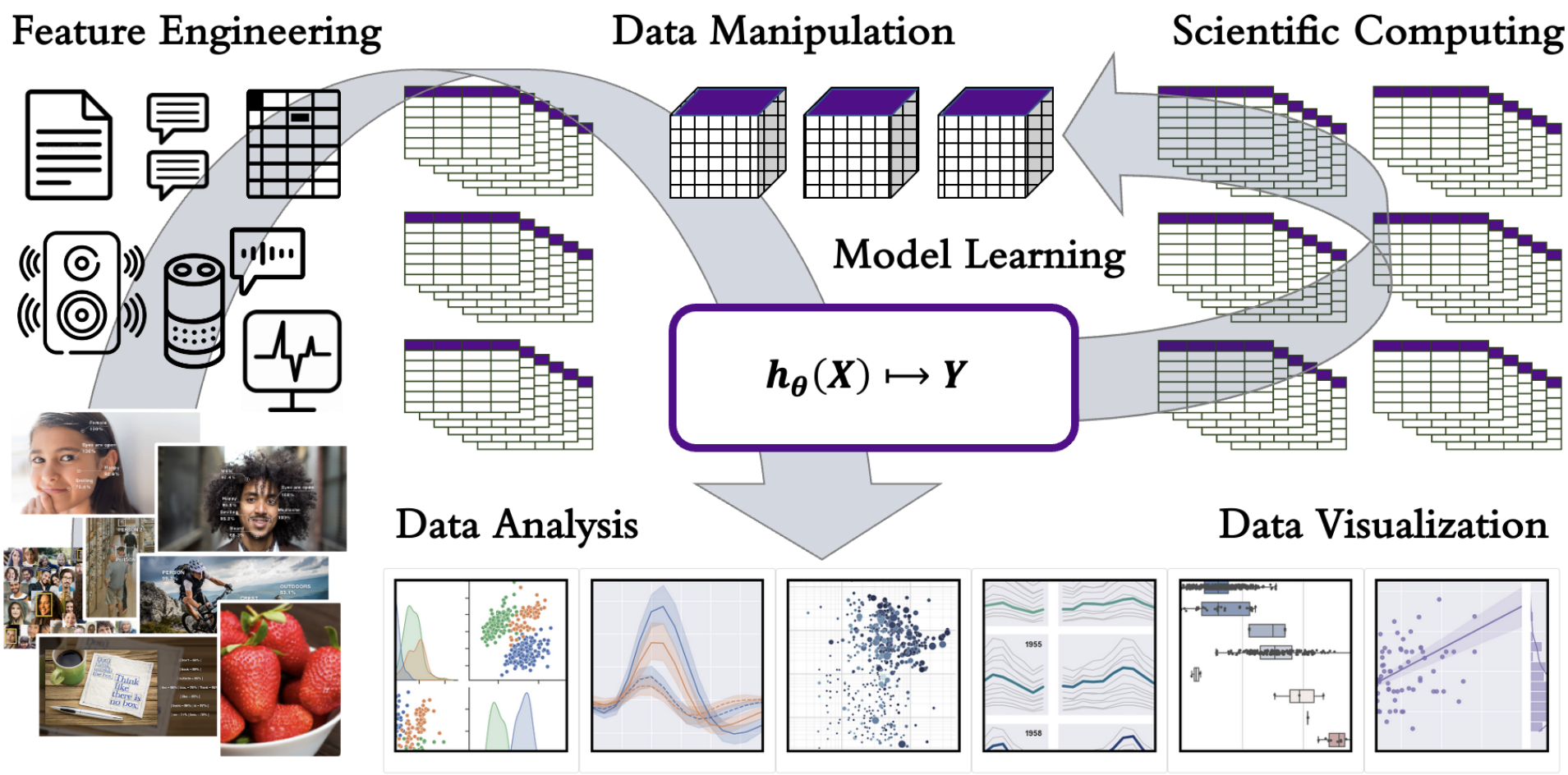
- **Array Manipulation with NumPy**
- **Mathematical Operations with NumPy**

# Array Manipulation for Scientific Computing

## Do not forget:

- Today's lecture includes practice code examples in an accompanying Jupyter notebook

# Programming for Data Science



# Programming for Data Science

- Manipulation of data objects
- Scientific computing with numerical arrays
- Feature Engineering
- Mathematical operations, linear algebra
- Modeling
- Machine Learning
- Statistical analysis
- Vizualization

# Array Manipulation with NumPy

# Array Manipulation with NumPy

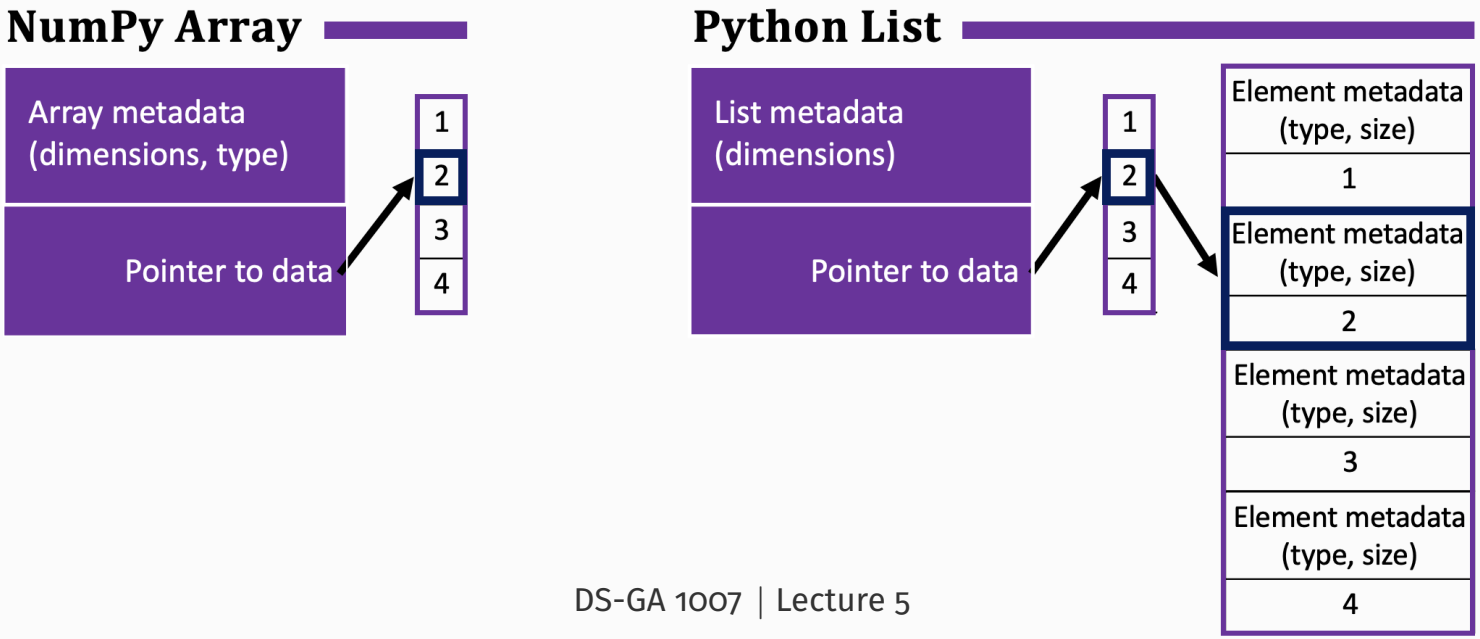
**We will cover:**

1. Arrays vs. List
2. Creating and reshaping arrays
3. Array attributes and built-in methods
4. Indexing arrays
5. Slicing arrays
6. Fancy indexing and slicing
7. Broadcasting

# What are NumPy Arrays?

## NumPy Array vs. Python List

- Both are multi-element, mutable containers for data
- List elements are complete Python objects allowing for flexibility of heterogenous types
- Array elements are of fixed type allowing for more efficient storage and operations



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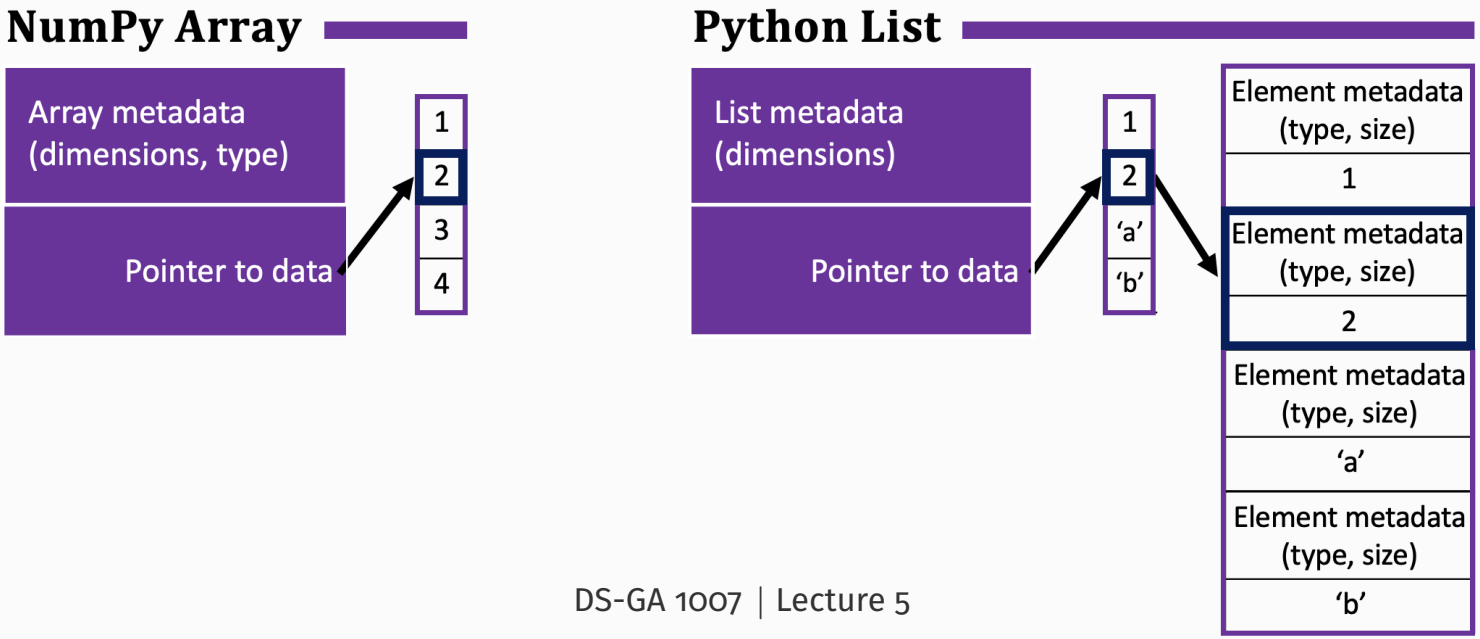


# Creating NumPy Arrays

**There are many ways to create NumPy arrays:**

```
l = [1,2,3,4,5]
np.array(l)
np.arange(0,10)
np.arange(0,10,2)
np.linspace(0,10,3)
np.zeros(5)
np.arange(0,25).reshape(5,5)
np.random.rand(5,5)
np.zeros((5,5))
np.ones((5,5))
np.eye(5)
```

# Array Attributes and Methods

## There are key attributes of NumPy arrays

```
x.ndim   # Number of dimensions
x.shape  # Size of each dimension
x.size   # Total size of the array
x.dtype  # Data type of the array
```

## ...and many, many built-in methods such as:

```
x.max()  # or np.max(a)
x.min()  # or np.min(a)
x.mean() # or np.mean(a)
x.std()  # or np.std(a)
```

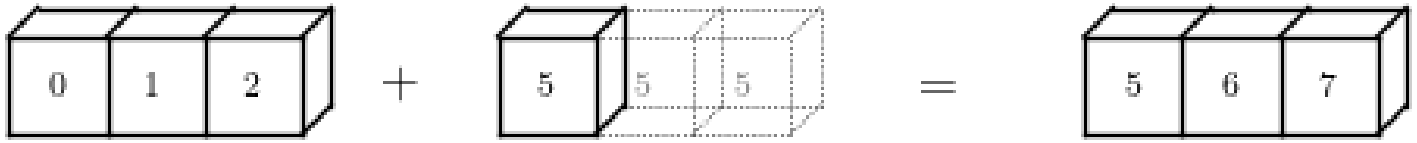
# Array Indexing and Selection

## Indexing, Slicing, Broadcasting, and Fancy Indexing...

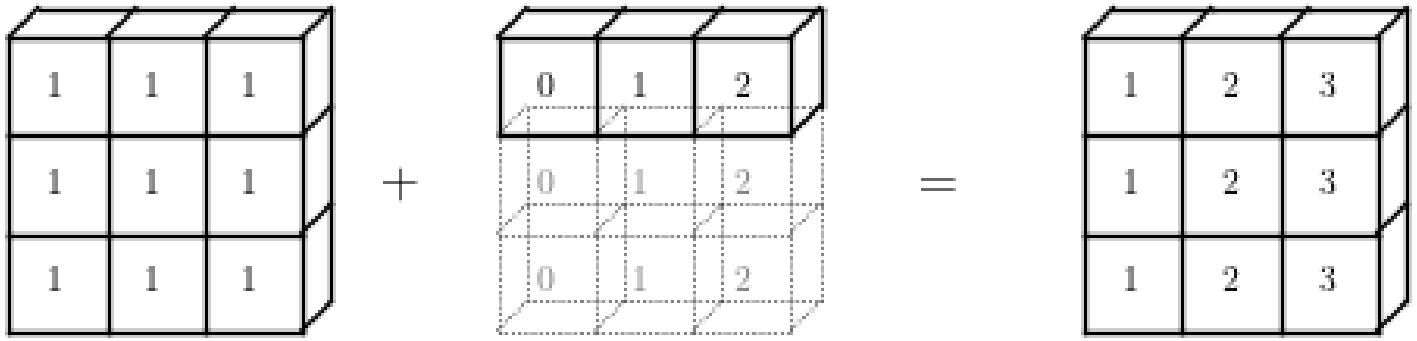
```
a = np.arange(0,9)
a[5]     # Simple indexing
a[2:5]   # Slicing (view to access subarray, data not copied)
a[0:5]=100 # Scalar broadcasting
np.ones((3,3)) + np.arange(3) # Array broadcasting

a2 = a.reshape(3,3)
a2[1,0]        # or a2[1][0] but not recommended
a2[1:,:]       # Slicing in 2D
a2[[2,0]]      # Fancy: Select entire rows out of order
a2[:,[2,0,2]] # Fancy: Select entire columns out of order
a[a>5]         # Fancy: a > 5 is itself a Boolean array...
```

# NumPy Rules of Broadcasting

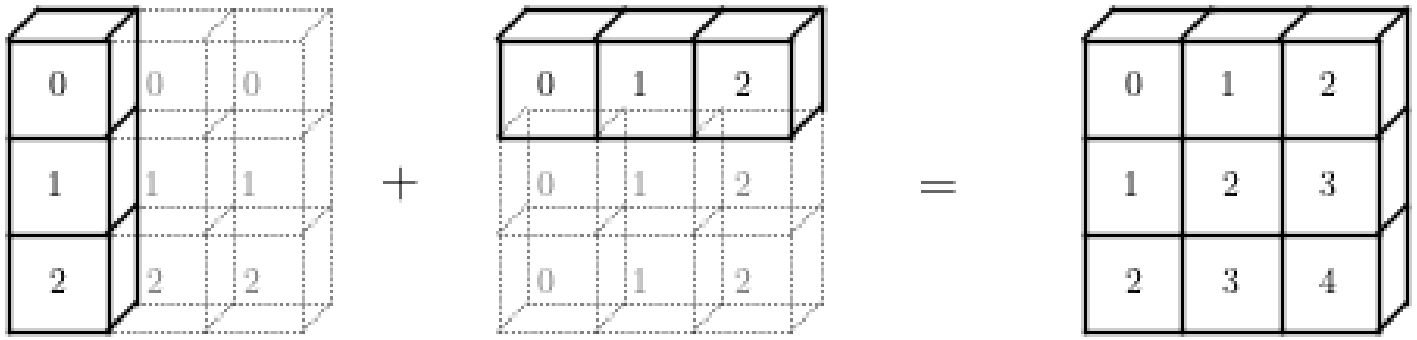
`np.arange(3) + 5`




`np.ones((3, 3)) + np.arange(3)`




`np.arange(3).reshape((3, 1)) + np.arange(3)`



# Mathematical Operations with Numpy

# Mathematical Operations on Arrays

## NumPy Functions perform Vectorized Operations

- Arithmetic, trigonometric, and common mathematic functions

| Arithmetic | | Trigonometric | | Exp/Log/Abs | |
|---|---|---|---|---|---|
| $+$ | Addition | np.sin(x) | Sine | np.exp(x) | $e^x$ |
| $-$ | Substraction | np.cos(x) | Cosine | np.exp2(x) | $2^x$ |
| $*$ | Multiplication | np.tan(x) | Tangent | np.power(3,x) | $3^x$ |
| $/$ | Division | | | np.log(x) | $ln(x)$ |
| $//$ | Floor division | | | np.log2(x) | $log2(x)$ |
| $\%$ | Modulus | | | np.log10(x) | $log10(x)$ |
| $**$ | Exponentiation | | | np.abs(x) | $\|x\|$ |

# Mathematical Operations on Arrays

## NumPy Functions perform Vectorized Operations

- Basic statistics, aggregation, and comparison functions

| Basic Statistics | | Aggregation | | Comparison | |
|---|---|---|---|---|---|
| np.mean | Mean | np.sum | Sum | == | Equality |
| np.std | Std Dev | np.prod | Product | != | Inequality |
| np.var | Variance | np.min | Min value | > | More than |
| np.median | Median | np.max | Max value | >= | More or equal |
| np.percentile | Rank-statistics | np.argmin | Index min | < | Less than |
| | | np.argmax | Index max | <= | Less or equal |

# Linear Algebra in NumPy

## A NumPy Array can be used as a Matrix

| Matrix and Vector Product | | Other Matrix Operations* | |
|---|---|---|---|
| @ | Matrix product | np.corrcoef | Correlation matrix |
| np.matmul | Matrix product | linalg.inv | Inverse matrix |
| np.dot | Dot product | linalg.norm | Norm |
| np.innner | Inner product | linalg.det | Determinant |
| np.outer | Outer product | linalg.eig | Eigenvalues |

* More Linear Algebra Numpy methods are available, see link below:

`https://numpy.org/doc/stable/reference/routines.linalg.html`

# A refresh in Linear Algebra

## Matrix Form of a Linear Regression Model $Ax = y$

$$\begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \cdots & a_{mn} \end{bmatrix} \times \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}$$

$$(m \times n) \quad \times \quad (n \times 1) \quad = \quad (m \times 1)$$

**Example: m = 100 observations, n = 10 features:**

$$\begin{bmatrix} a_{1,1} & \cdots & a_{1,10} \\ \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots \\ a_{100,1} & \cdots & a_{100,10} \end{bmatrix} \times \begin{bmatrix} x_1 \\ \vdots \\ x_{10} \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ \vdots \\ y_{100} \end{bmatrix}$$

# Now let’s practice!