NumPy

Intro to NumPy: Arrays

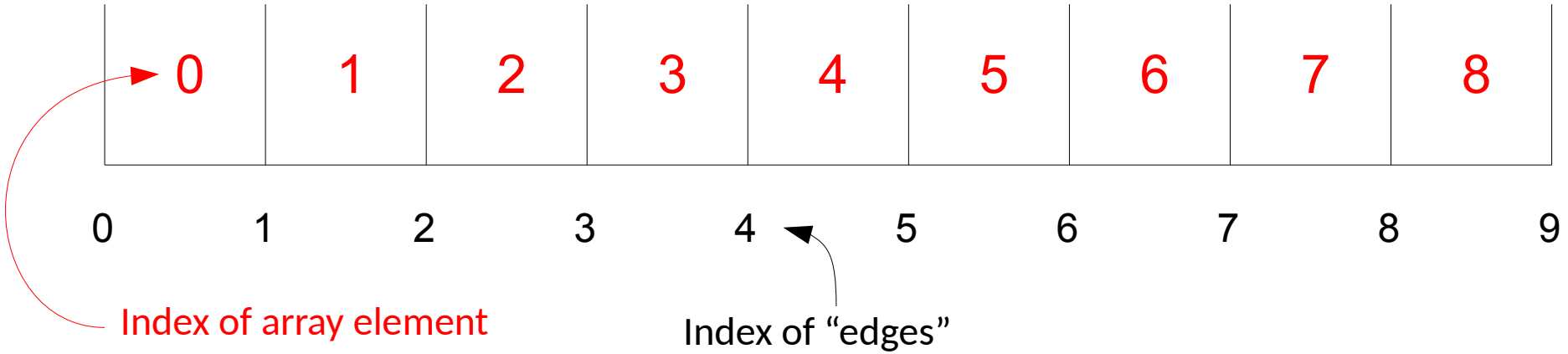
- NumPy provides a multidimensional array
  - All elements must be the same data type
  - Many different datatypes supported
  - Size is fixed (memory is allocated for the size specified)
- Arithmetic operations work on arrays
- Provides MANY functions that operate on whole arrays
  - These operations are written in a compiled language, and run fast
  - Generally speaking, you want to avoid loops to get the best performance.
    - Can sometimes make code unreadable
- Lots of ways to create arrays

Intro to NumPy: Array Operations

- Arithmetic operator (+, —, /, *) work elementwise
  - `A * B` is not a matrix product, but instead multiples the corresponding elements in each array together
  - `dot(A,B)` does a dot product
- Universal functions (`sin`, `cos`, `exp`, ...) work elementwise
- New @ operator
  - Accepted for python 3.5, the "@" will be a new operator in python available for overloading. NumPy will implement it as matrix multiplication
    - http://legacy.python.org/dev/peps/pep-0465/
    - `A @ B` will be equivalent to `np.dot(A,B)`
- Array creation and operations examples...

Intro to NumPy: Array Indexing/Slicing

- Biggest source of confusion: selecting a range is best thought of as referring to the "edges" of the array locations
  - Differs from Fortran, IDL

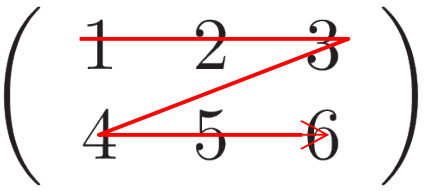


  - For the array above:
    - `A[2] = 2`
    - `A[2:3] = [2]`
    - `A[2:4] = [2 3]`
  - Note also: zero-based indexing

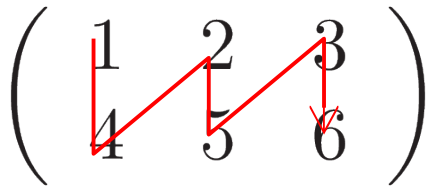
Note: this same behavior applies to Python lists and strings when slicing

Arrays

- Building block of many numerical methods
- Row vs. Column major: A(m,n)
  - First index is called the row
  - Second index is called the column
  - Multi-dimensional arrays are flattened into a one-dimensional sequence for storage
  - Row-major (C, python): rows are stored one after the other
  - Column-major (Fortran, matlab): columns are stored one after the other
- Ordering matters for:
  - Passing arrays between languages
  - Deciding which index to loop over first



Row major



Column major

Arrays

- This is why in Fortran, you want to loop as:

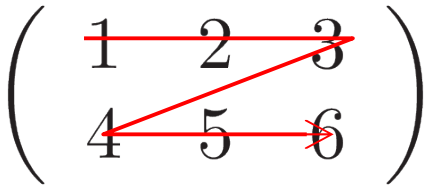
```
double precision :: A(M,N)
do j = 1, N
   do i = 1, M
      A(i,j) = …
   enddo
enddo
```

- And in C:

```
double A[M][N];
for (i = 0; i < M; i++) {
   for (j = 0; j < N; j++) {
      A[i][j] = …
   }
}
```

Intro to NumPy: Array Indexing/Slicing

- Remember, multi-dimensional arrays are stored in row-major fashion
  - Rows are stored one after the other, within a row, the column data is closest to one another



  - You see this when you print an array:
    - `a = numpy.arange(15).reshape(3,5)`
    - `print a`

```
[[ 0  1  2  3  4]
 [ 5  6  7  8  9]
 [10 11 12 13 14]]
```

3 rows,
5 columns

Note that the braces [ ] show that the columns are together

- Some slicing examples…

Intro to NumPy: Array Views/Copies

- When "copying", need to understand if two arrays, A and B, point to:
  - the same array (including shape and data/memory space)
  - the same data/memory space (but perhaps different shapes)
  - a separate copy of the data (i.e. stored separately in memory)
- `B = A` (assignment)
  - No copy is made. A and B point to the same data in memory and share the same shape, etc.
- `B = A[:]` (view or shallow copy)
  - The shape info for A and B are stored independently, but both point to the same memory location for the data
- `B = A.copy()` (deep copy)
  - The data in B is stored completely separately in memory from A
- Copying examples…

Intro to NumPy: Boolean Indexing

- Many fancy ways to index arrays
- `A[A > 4] = 0`
  - Boolean indexing
  - Similar to IDL's where command
- Boolean indexing example…

Avoiding Loops

- Slicing (and using boolean indexing) can be used to avoid loops

More NumPy

- See the tutorial for some other features:
  - Shape manipulation
  - Merging/splitting arrays
  - Fancier indexing
  - Other numpy functions/methods
- NumPy functions page…