**Preface**

**What Is Data Science?**

Data science comprises three distinct and overlapping areas: the skills of a statistician who knows how to model and summarize datasets (which are growing ever larger); the skills of a computer scientist who can design and use algorithms to efficiently store, process, and visualize this data; and the domain expertise—what we might think of as “classical” training in a subject—necessary both to formulate the right questions and to put their answers in context.

A diagram of data science

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**Why Python**

* NumPy for manipulation of homogeneous array-based data,
* Pandas for manipulation of heterogeneous and labeled data,
* SciPy for common scientific computing tasks,
* Matplotlib for publication-quality visualizations,
* IPython for interactive execution and sharing of code, Scikit-Learn for machine learning

**Jupyter: Beyond Normal Python**

**Getting Started in IPython and Jupyter**

* **IPython shell** for trying out short sequences of commands
* **Jupyter Notebook** for longer interactive analysis and for sharing content with others
* **Interactive development environments (IDEs)** like **Emacs** or **VSCode** for creating reusable Python packages.

**The IPython Shell**

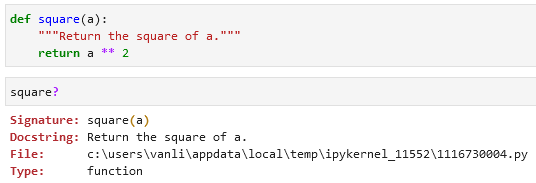
* Start the *IPython Shell* by typing ipython in the *Anaconda Prompt*.
* Launch Jupyter lab (?) $ jupyter lab

**Access documentation** with help() like help(len). The alternative is ? like len?. Get information on objects using ? like in the example below:

A screenshot of a computer

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You can also get information on functions or other objects you create like in the example below which has a docstring (a description of the function):



?? provides the source code of the object you are curious about:

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Use wildcard matching (character \*) to list every object in the namespace whose name ends with *Warning*:

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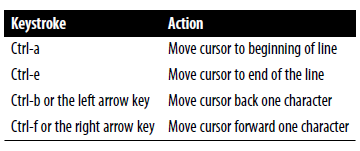
In the example below we area looking for a string method that contains the word *find* somewhere in its name:

A screenshot of a computer

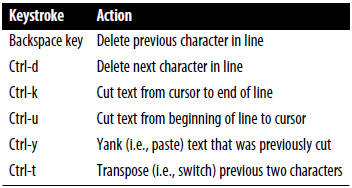
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**Keyboard Shortcuts in the IPython Shell**

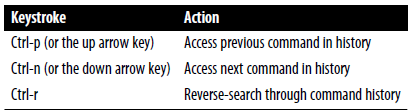
**Navigation Shortcuts**



**Text Entry Shortcuts**



**Command History Shortcuts**

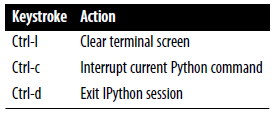


Use *Ctrl-r* to browse the search results. When you’re done press *Enter*.

A close up of text

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**Miscellaneous Shortcuts**



**Enhanced Interactive Features**

**IPython Magic Commands**

Magic commands are prefixed by the % character.

* **Line magics** are denoted by a single % prefix. They operate on a **single line of input**.
* **Cell magics** are denoted by a double %% prefix and operate on **multiple lines of input**.
* Magic commands documentation %magic.
* Quick and simple list of all available magic functions %lsmagic.

If you have a *.py* file you can execute it / run its script in IPython using %run filename.py:

A screenshot of a computer screen

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To time code execution use %timeit or %%timeit for multiple lines of code:

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You can check you input and output history using In and Out codes. You can also select specific steps like print(In[1]).

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Description automatically generated

A black text on a white background

Description automatically generated

A screenshot of a computer program

Description automatically generated

An alternative to Out[20] is \_20:



Use print(\_) to get access to the previous output:

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You can also use print(\_\_) and print(\_\_\_) to get access to the second/third-to-last outputs.

If you want to suppress you output you can do it using ; at the end of the line:

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Description automatically generated

Use %history to get an overview of your commands, use %history -n to get an numbered overview of your commands. To select a command/commands add a number like 3-5:

A black screen with white text

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Description automatically generated

Other useful commands are %rerun (re-execute some portion of the command history) and %save (saves some set of the command history to a file).

**Quick Introduction to the Shell**

Some shell commands:



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echo, pwd, ls, cd, mkdir, mv

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A screenshot of a computer program

Description automatically generated

!echo

A screenshot of a computer

Description automatically generated!pwd !cd

A screenshot of a computer program

Description automatically generated%cd mkdir ls cp rm -r

**Debugging and Profiling**

**Controlling Exceptions using %xmode**

There are 3 formats for errors: Plain, Context, and Verbose.

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The last provides the most information but can be bulky.

**To launch a debugger** write %debug.

**Launch the Sdebugger automatically** whenever an exception is raised using

%xmode Plain

%pdb on

A computer code with text

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**Partial list of debugging commands:**

A screenshot of a computer program

Description automatically generatedl(ist) h(elp) q(uit) c(ontinue) n(ext) <enter> p(rint) s(tep) r(eturn)

**Profiling and Timing Code**

%time Time the execution of a single statement

%timeit Time repeated execution of a single statement for more accuracy

%prun Run code with the profiler

%lprun Run code with the line-by-line profiler

%memit Measure the memory use of a single statement

%mprun Run code with the line-by-line memory profiler

%timeit

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%time

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%prun

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A close up of text

Description automatically generated

%lprun

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Description automatically generated%load\_ext line\_profiler %lprun -f

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%memit (is a memory-measuring equivalent of %timeit) and %mprun (memory-measuring equivalent of %lprun)

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Description automatically generated pip install memory\_profiler

A white rectangular object with black text

Description automatically generated%load\_ext memory\_profiler

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Description automatically generated with medium confidence %memit

A close-up of a text

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A screenshot of a computer program

Description automatically generated%%file %mprun -f

**NumPy**

In some ways, NumPy arrays are like Python’s built-in *list* type, but NumPy arrays provide much more efficient storage and data operations as the arrays grow larger in size.

Check NumPy version: numpy.\_\_version\_\_

**Fixed-Type Arrays in Python**

Example of an array in Python:

A screenshot of a computer code

Description automatically generatedimport array, array.array



Python arrays objects provide efficient storage. NumPy adds to this efficient operations on that data.

**Creating Arrays from Python Lists**

NumPy arrays can only contain data of the same type. This is unlike Python lists.

NumPy arrays can be multidimensional. Python lists are always one-dimensional sequences.

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**Creating Arrays from Scratch**

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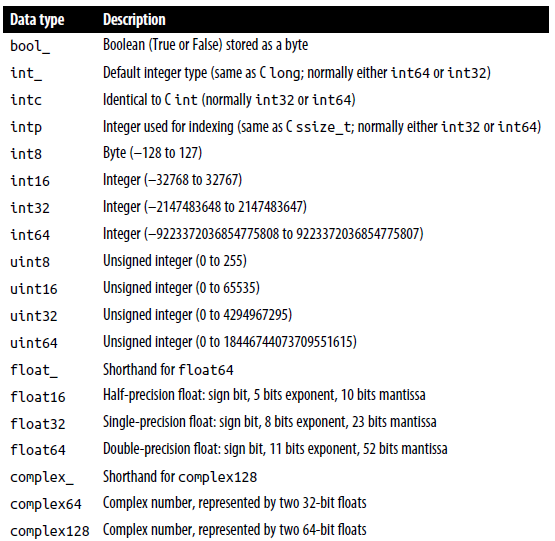
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**Specify data type when creating an array using dtype=’int16’ or dtype=np.int16:**

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**Standard NumPy data types:**



**NumPy Array Attributes**

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ndim, shape, size, dtype, default\_rng(seed= integers

**Array Slicing: Accessing Subarrays**

Follow this logic to access a slice of an array x:

x[start:stop:step]

If any of these are unspecified, they default to the values start=0, stop=<size of dimension>, step=1.



A screenshot of a computer code

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A white background with black text

Description automatically generatedreverse an array [::-1]

A white background with numbers and symbols

Description automatically generatedreverse a multiarray [::-1, ::-1]

 first column of a multiarray [0, :]

 first row of a multiarray [0] or [0, :]



**Subarrays as no-copy views**

Unlike Python list slices, NumPy array slices are returned as views rather than copies of the array data.

In the example below if we modify the subarray *x2\_sub* the original array *x2* will also change.

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It can be advantageous when working with large datasets. We can access and process pieces of these datasets without the need to copy the underlying data buffer.

If you want to create a copy that can be changed without affecting the original data use the .copy() code:

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**Reshaping of arrays**

Use .reshape() to put if you want to put e.g. numbers from 1 to 9 in a 3 × 3 grid:

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Note that the size of the array should match the size of the reshaped array.

You can also use .reshape() to convert a one-dimensional array into…

…a two-dimensional row matrix: …or a column matrix:

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You can achieve the same using np.newaxis in the slicing index:

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**Array concatenation (combine multiple arrays into one)**

Use np.concatenate, np.vstack, and np.hstack to join two arrays.

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Concatenate a two-dimensional array along the first axis: …and among the second axis:

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When you have arrays of mixed dimensions you can use np.vstack and np.hstack:

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For higher-dimensional arrays np.dstack will stack arrays along the third axis.

**Array splitting (split a single array into multiple arrays)**

To split arrays use functions np.split, np.hsplit, np.vsplit.

Using np.split(array\_name, [splitting\_location(s)]):

A screenshot of a math problem

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Splitting using np.hsplit and np.vsplit:

A screenshot of a computer program

Description automatically generated

For higher-dimensional arrays np.dsplit will split arrays along the third axis.

**NumPy universal functions (ufuncs)**

To make computation on NumPy arrays fast use vectorized operations that are generally implemented through *universal functions (ufuncs)*.

There are *two types of ufuncs:*

* *Unary ufuncs* operate on a single input
* *Binary ufuncs* operate on two inputs.

**Arithmetic operators examples in NumPy:**

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Description automatically generated

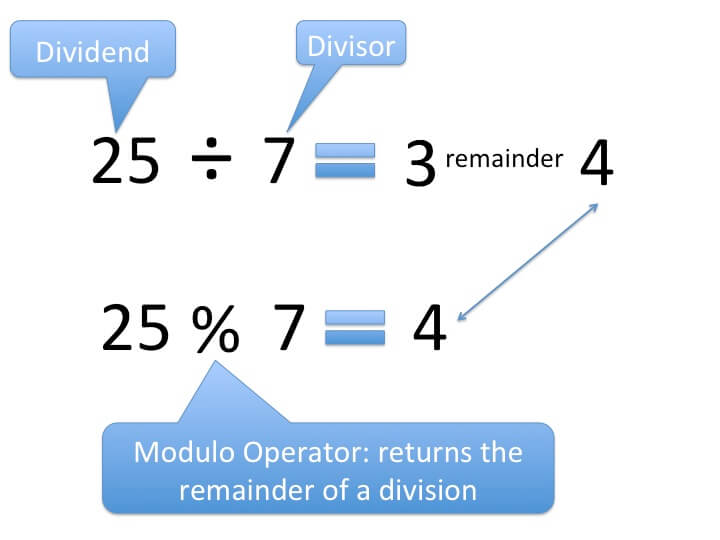
- is negation (turn *1* into *-1*), % is an operator for *modulus \**.

These arithmetic operations are convenient wrappers around specific ufuncs built into NumPy. For example, the + operator is a wrapper for the np.add() ufunc:

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*\* Modulus:*



**Arithmetic operators implemented in NumPy:**

|  |  |  |
| --- | --- | --- |
| **Operator** | **Equivalent ufunc** | **Description** |
| + | np.add | Addition (e.g., 1 + 1 = 2) |
| - | np.subtract | Subtraction (e.g., 3 - 2 = 1) |
| - | np.negative | Unary negation (e.g., -2) |
| \* | np.multiply | Multiplication (e.g., 2 \* 3 = 6) |
| / | np.divide | Division (e.g., 3 / 2 = 1.5) |
| // | np.floor\_divide | Floor division (e.g., 3 // 2 = 1) |
| \*\* | np.power | Exponentiation (e.g., 2 \*\* 3 = 8) |
| % | np.mod | Modulus/remainder (e.g., 9 % 4 = 1) |

To make values absolute (e.g. from -2 to 2) use abs(name), np.absolute(name) or np.abs(name):

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**Trigonometric functions**

Functions like np.sin, np.cos, np.tan:

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Inverse trigonometric functions like np.arcsin, np.arccos, np.arctan:

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**Exponents and logarithms**

Exponentials in NumPy like np.exp, np.exp2, np.power:

A screenshot of a math program

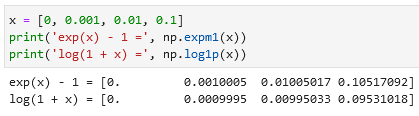
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Inverse of the exponentials or the logarithms are computed using np.log (natural logarithm), np.log2 (base-2 logarithm), and np.log10 (base-10 logarithm):

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Specialized versions useful for maintaining precision with very small input (np.expm1 and np.log1p). When x is very small, these functions give more precise values than if the raw np.log or np.exp were to be used.



**Specialized ufuncs**

You can use scipy special for specialized functions. For example gamma functions (generalized factorials) and related functions (special.gamma, special.gammaln, special.beta):

A screenshot of a computer

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Error functions (integral of Gaussian), its complement, and its inverse (special.erf, special.erfc, special.erfinv):

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**Specifying output of an array**

For large calculations, it is sometimes useful to be able to specify the array where the result of the calculation will be stored. For all ufuncs, this can be done using the out argument of the function:

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This can even be used with *array views*. For example, we can write the results of a computation to every other element of a specified array (in the example below every second):

A screenshot of a math equation

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If we had instead written y[::2] = 2 \*\* x, this would have resulted in the creation of a temporary array to hold the results of 2 \*\* x, followed by a second operation copying those values into the y array. This doesn’t make much of a difference for such a small computation, but **for very large arrays the** **memory savings from careful use of the out argument can be significant**.

**Aggregations**

Use the reduce function to reduce an array with a particular operation.

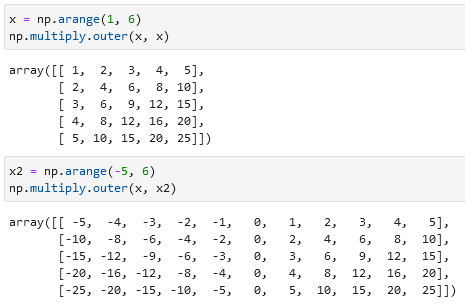
You can use np.add.reduce, np.multiply.reduce to sum or multiply an array. If you want to store intermediate results use np.add.accumulate or np.multiply.accumulate.

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**Outer products**

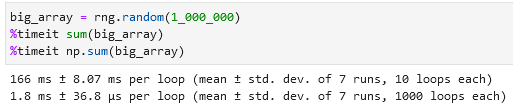
Compute the output of all pairs of two inputs using np.multiply.output(input\_1, input\_2):



**Aggregations in NumPy: min, max, and everything in between**

**Summing the Values in an Array**

You can sum using Python like sum(x) or you can use NumPy’s np.sum(x). Because NumPy executes the operation in a compiled code, **NumPy’s version of the operation is computed much more quickly**:



However, sum(x) and np.sum(x) are not identical. Their optional arguments have different meanings. Python’s *sum(x, 1)* initializes the sum at *1* (meaning that if your sum(x) is equal to *5*, your sum(x, 1 or 10) will be equal to *5 + 1 or 10 = 6 or 15*), while np.sum(x, 1) sums along *axis 1*.Also, np.sum is aware of multiple array dimensions.

**Minimum and maximum (min, max)**

Same as with summing you can use Python’s min(x) or NumPy’s np.min(x) or max(x) / np.max(x). An alternative is x.min() / x.max() / x.sum(). Same as with summing, **NumPy’s version is faster**.

**Multidimensional Aggregates**

Finding the minimum value within each column/row by specifying axis=0 / axis=1:

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The axis keyword specifies the dimension of the array that will be *collapsed*, rather than the dimension that will be returned. So, specifying axis=0 means that axis 0 will be collapsed: for two-dimensional arrays, values within each column will be aggregated.

**Other aggregation functions**

Most additional aggregation functions have a NaN-safe counterpart that computes the result while ignoring missing values.

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np.sum, np.prod, np.mean, np.std, np.var, np.min, np.max, np.argmin, np.argmax, np.median, np.percentile, np.any, np.all



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**Broadcasting**

Broadcasting allows these types of binary operations to be performed on arrays of different sizes—for example, we can just as easily add a scalar (think of it as a zerodimensional array) to an array:

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We can think of this as an operation that stretches or duplicates the value 5 into the array [5, 5, 5], and adds the results.

**Broadcasting is stretching an array** across a (in the example below) second dimension:



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You can also stretch or broadcast both arrays to match a common shape:

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**Visualization of broadcasting:**

A group of cubes with numbers

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**Rules of broadcasting**

1. If the two arrays differ in their number of dimensions, the shape of the one with fewer dimensions is padded with ones on its leading (left) side.
2. If the shape of the two arrays does not match in any dimension, the array with shape equal to 1 in that dimension is stretched to match the other shape.
3. If in any dimension the sizes disagree and neither is equal to 1, an error is raised.

Rule 1 example: Rule 2 example:

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**Using broadcasting for centering an array**

You can subtract from an array the mean of that array.

|  |  |
| --- | --- |
| **Array:** | **Centered (difference to mean):** |
| 34 | -4 |
| 65 | 27 |
| 23 | -15 |
| 76 | 38 |
| 22 | -16 |
| 43 | 5 |
| 63 | 25 |
| 32 | -6 |
| 23 | -15 |
| 27 | -11 |
| 5 | -33 |
|  |  |
| **Mean:** |  |
| 38 |  |

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**Comparisons, Masks, and Boolean Logic**

**Comparison Operators as Ufuncs**

As in the case of arithmetic operators, the comparison operators are implemented as ufuncs in NumPy; for example, when you write x < 3, internally NumPy uses np.less(x, 3). These operators will work on arrays of any size and shape.

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Description automatically generatednp.equal, np.less, np.greater, np.not\_equal, np.less\_equal, np.greater\_equal

Example:

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In each case, the result is a Boolean array, and NumPy provides a number of straight-forward patterns for working with these Boolean results.

**Working with Boolean Arrays**

**Counting Entries**

To count the number of True entries you can use np.count\_nonzero:

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**Alternatively you can use np.sum (*False* is *0* and *True* is *1*).** With np.sum you can sum along rows or columns.

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Description automatically generated ← e.g. in row 1 there are 3 values below 6, in row 2 2 values, in row 3 3.

If you want to count the number of True entries that fulfill multiple conditions like *x > 10 AND x < 20* you can use symbols like &, |, ^, and ~:

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Description automatically generated ← same result in a different manner

Note that parentheses are important. Without them this code with result in an error.

**If you want to check if an array has values that fulfill a specific condition you can use np.any or np.all.**

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You can also use np.any and np.all along a particular axis:

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Description automatically generated

**Boolean operators and their equivalent ufuncs**

|  |  |
| --- | --- |
| **Operator** | **Equivalent ufunc** |
| & | np.bitwise\_and |
| ^ | np.bitwise\_xor |
| | | np.bitwise\_or |
| ~ | np.bitwise\_not |

Examples:

A screenshot of a computer

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**Boolean arrays as masks**

Selecting values from an array using Boolean operators is called a masking operation. Example:

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Description automatically generated

A one-dimensional array is returned with all the values that meet this condition.

**Examples of Boolean arrays as masks:**

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**Comment on using and/or instead of &/|**

The difference is this: and and or operate on the object as a whole, while & and | operate on the elements within the object.

and and or perform a single Boolean evaluation on an entire object, while & and | perform multiple Boolean evaluations on the content (the individual bits or bytes) of an object. **For Boolean NumPy arrays, the latter (& and |) is nearly always the desired operation.**

Using and and or instead of &/| will simply result in an error:

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**Fancy indexing / vectorized indexing**

To access values with specific indexes you can use this:

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When using arrays of indices, the shape of the result reflects the shape of the index arrays rather than the shape of the array being indexed. In the example below x[ind] returns the same form as of *ind* but instead of index coordinates (*3, 7,* etc.) it returns values from *x*.

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**Combined indexing**

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A screenshot of a computer code

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**Modifying values with fancy indexing**

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An alternative to np.add.at is reduceat.

**Example: Binning data**

You could use these ideas to efficiently do custom binned computations on data. For example, imagine we have 100 values and would like to quickly find where they fall within an array of bins. We could compute this using ufunc.at like this:

A screen shot of a graph

Description automatically generated

Alternatively using Matplotlib:

A graph on a grid

Description automatically generated

The difference between these two options is in the processing speed. Matplotlib is slower than the custom version for a small dataset and faster for a larger.

**Sorting arrays**

**In Python**

Python’s built-in functions to sort lists and other iterable objects: sorted(x) (returns a copy) and x.sort() (acts in-place). Two examples:

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Description automatically generated



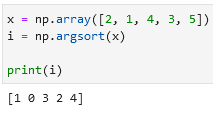
**In NumPy**

The np.sort function is analogous to sorted(). It will return a sorted copy of an array. Example:

A screenshot of a computer

Description automatically generated

np.argsort() returns the indices of the sorted elements:



You can then use these indices to construct the sorted array using fancy indexing:

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Sorting along rows or columns is possible by adding axis=0 for sorting columns or axis=1 for sorting rows. Note that this operation will treat each row or column as an independent array and any relationship between the row or column values will be lost.

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**You can also find e.g. 3 smallest values in an array using np.partition.** It will return these smallest values in arbitrary order followed by other values also in arbitrary order.

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**Checking the diagonal of a matrix**

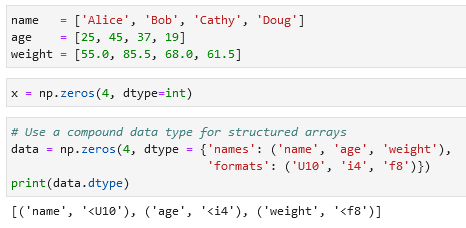
You can check the diagonal values of a matrix using x.diagonal():

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**NumPy’s structured arrays and record arrays**

Creating an empty container array:



* U10 = Unicode string of maximum length 10
* i4 = 4-byte (i.e. 32-bit) integer
* f8 = 8-byte (i.e. 64-bit) float

Filling the empty array with data in a one structured array:

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Filtering the data:

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