Published in Better Programming

Lev Maximov Follow
Dec 21, 2020 · 19 min read ★ · Listen

NumPy Illustrated: The Visual Guide to NumPy

Brush up your NumPy or learn it from scratch

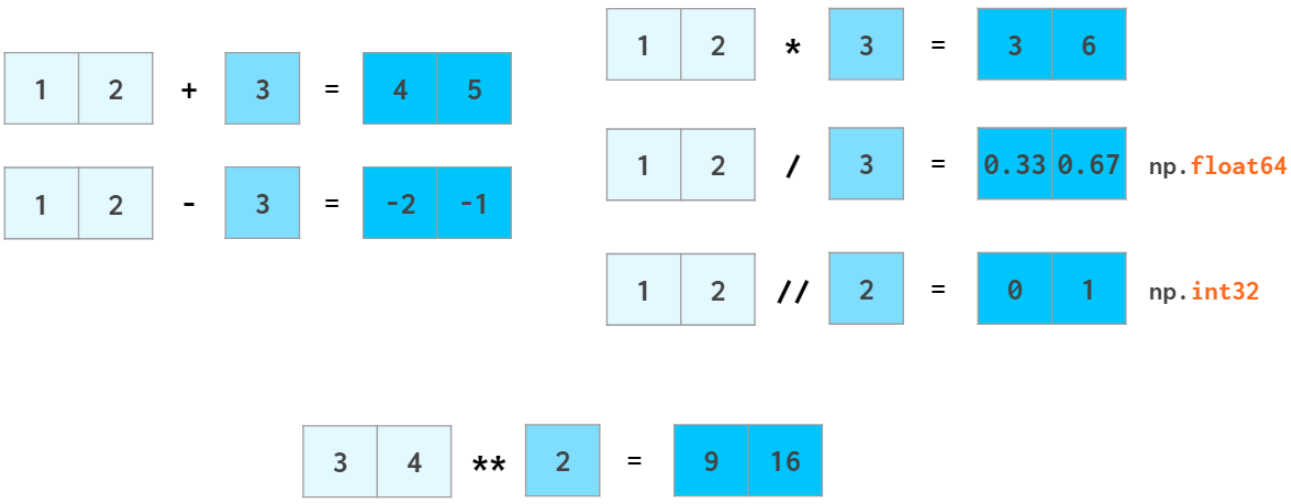


Image credit: Author

NumPy is a fundamental library that most of the widely used Python data processing libraries are built upon (pandas, OpenCV), inspired by (PyTorch), or can efficiently share data with (TensorFlow, Keras, etc). Understanding how NumPy works gives a boost to your skills in those libraries as well. It is also possible to run NumPy code with no or minimal changes on GPU[1].

The central concept of NumPy is an n-dimensional array. The beauty of it is that most operations look just the same, no matter how many dimensions an array has. But 1D

2. Matrices, the 2D Arrays
3. 3D and above

I took a great article, "A Visual Intro to NumPy" by Jay Alammar[2], as a starting point, significantly expanded its coverage, and amended a pair of nuances.

Numpy Array vs. Python List

At first glance, NumPy arrays are similar to Python lists. They both serve as containers with fast item getting and setting and somewhat slower inserts and removals of elements.

The hands-down simplest example when NumPy arrays beat lists is arithmetic:

```
In [3]: a = [1, 2, 3]
        [q*2 for q in a]
Out[3]: [2, 4, 6]
```

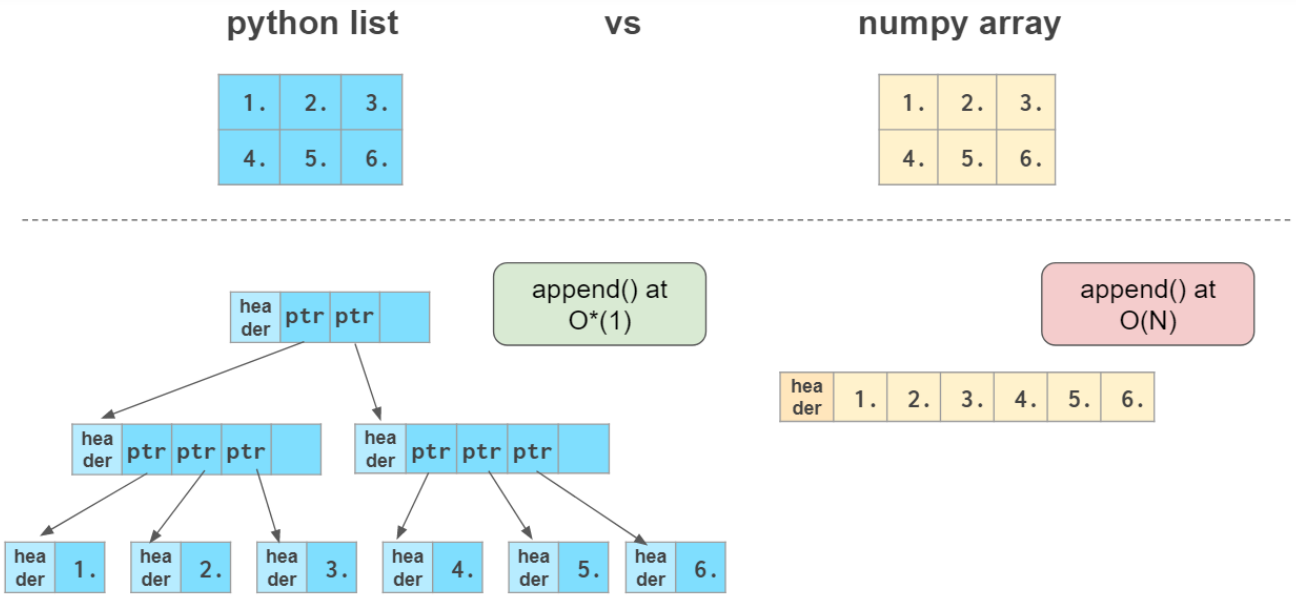
```
In [4]: a = np.array([1, 2, 3])
        a * 2
Out[4]: array([2, 4, 6])
```

```
In [1]: a = [1, 2, 3]
        b = [4, 5, 6]
        [q+r for q, r in zip(a, b)]
Out[1]: [5, 7, 9]
```

```
In [2]: a = np.array([1, 2, 3])
        b = np.array([4, 5, 6])
        a + b
Out[2]: array([5, 7, 9])
```

Other than that, NumPy arrays are:

- more compact, especially when there's more than one dimension
- faster than lists when the operation can be vectorized
- slower than lists when you append elements to the end
- usually homogeneous; can only work fast with elements of one type



Here O(N) means that the time necessary to complete the operation is proportional to the size of the array (see Big-O Cheat Sheet[3] site), and O*(1) (the so-called "amortized" O(1)) means that the time does not generally depend on the size of the array (see Python Time Complexity[4] wiki page)

1. Vectors, the 1D Arrays

Vector initialization

One way to create a NumPy array is to convert a Python list. The type will be auto-deduced from the list element types:

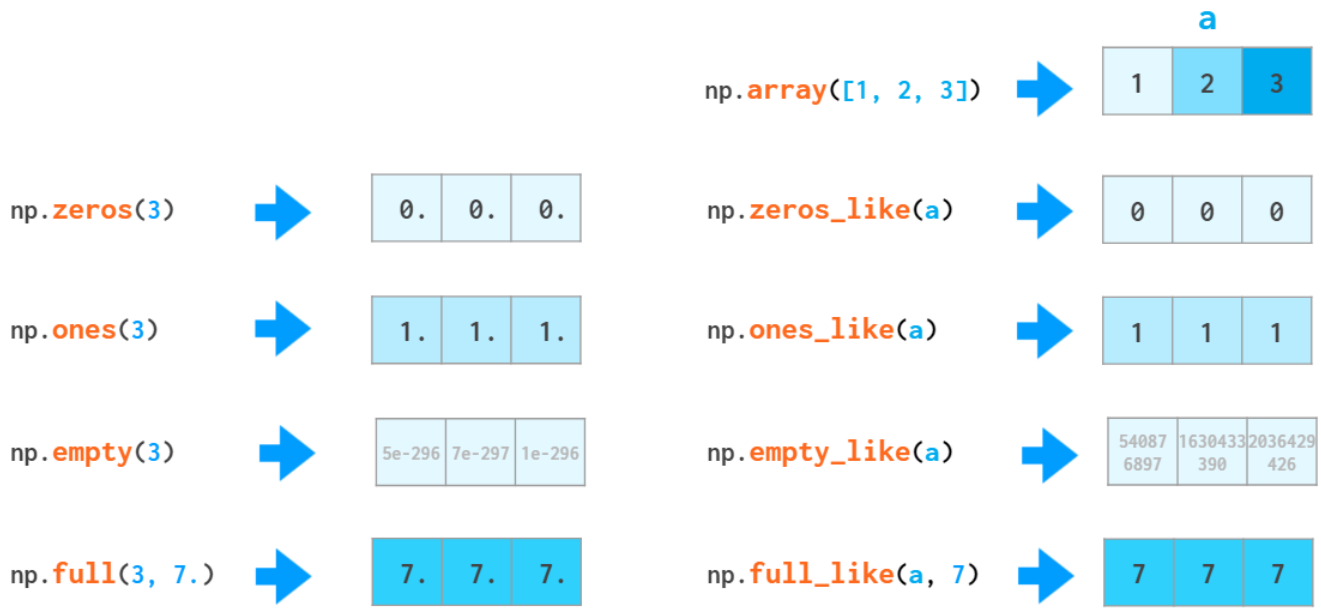
Be sure to feed in a homogeneous list, otherwise you'll end up with `dtype='object'`, which annihilates the speed and only leaves the syntactic sugar contained in NumPy.

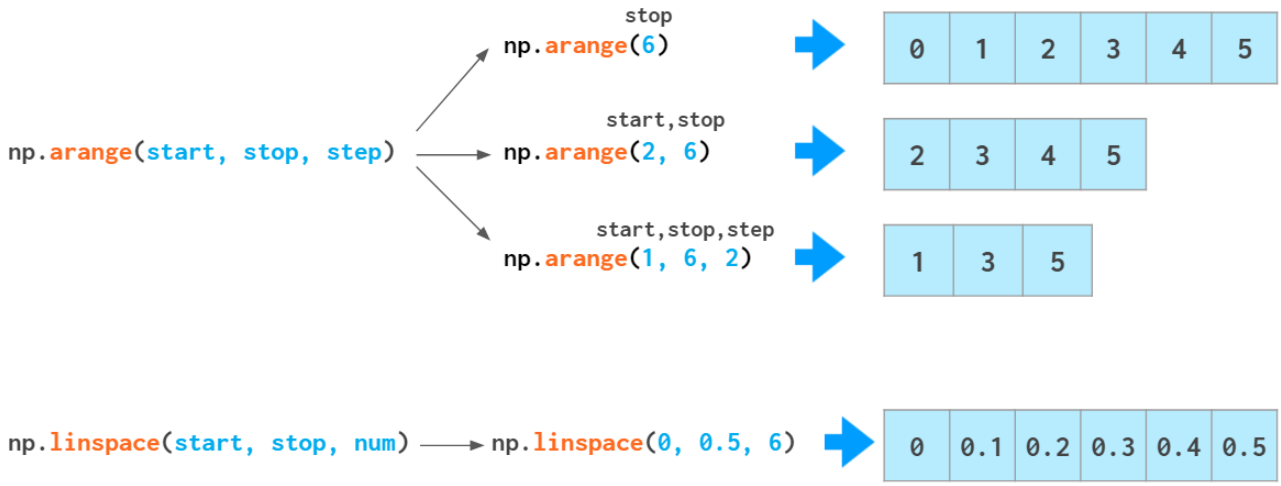
More about dtypes in my new article

NumPy arrays cannot grow the way a Python list does: No space is reserved at the end of the array to facilitate quick appends. So it is a common practice to either grow a Python list and convert it to a NumPy array when it is ready or to preallocate the necessary space with `np.zeros` or `np.empty`:

It is often necessary to create an empty array which matches the existing one by shape and elements type:

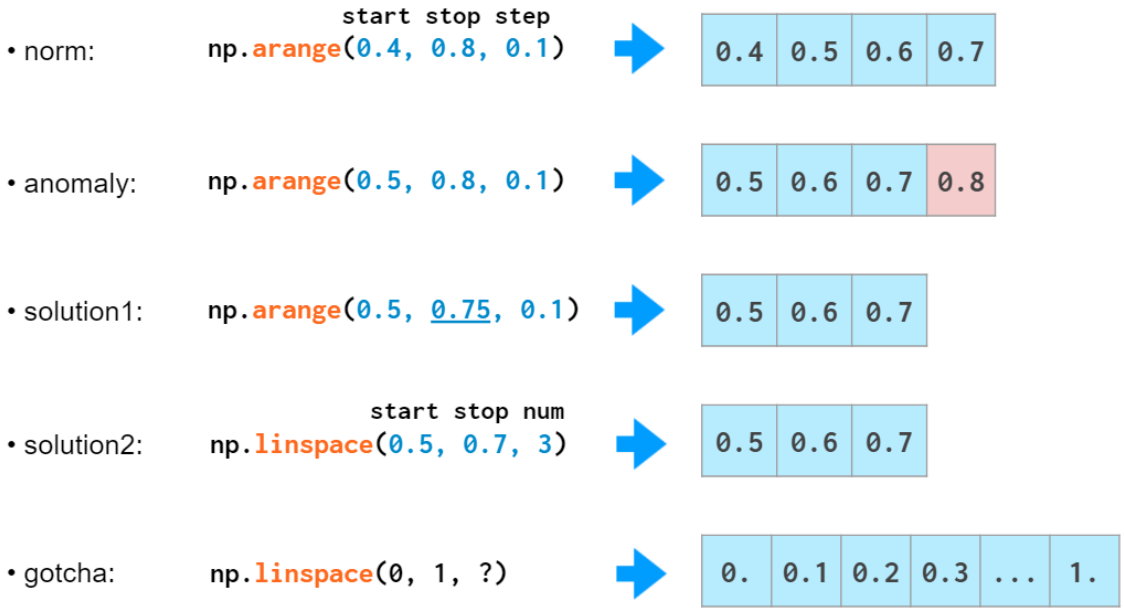
Actually, all the functions that create an array filled with a constant value have a `_like` counterpart:





If you need a similar-looking array of floats, like `[0., 1., 2.]`, you can change the type of the `arange` output: `arange(3).astype(float)`, but there's a better way. The `arange` function is type-sensitive: If you feed ints as arguments, it will generate ints, and if you feed floats (e.g., `arange(3.)`) it will generate floats.

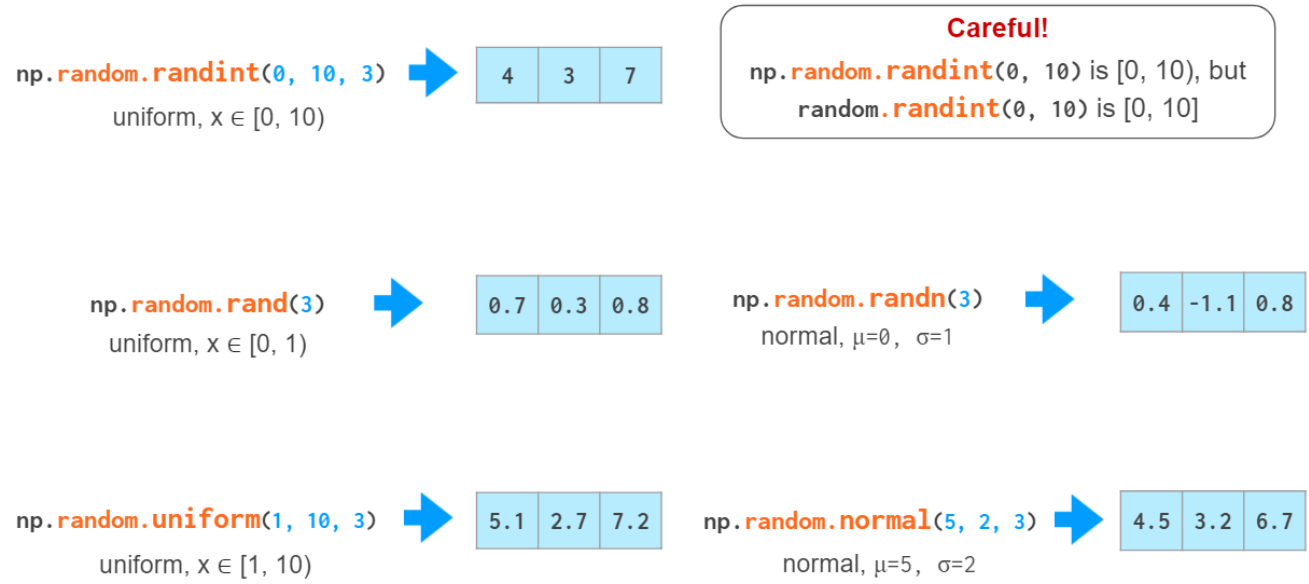
But `arange` is not especially good at handling floats:



This `0.1` looks like a finite decimal number to us but not to the computer: In binary, it is an infinite fraction and has to be rounded somewhere thus an error. That's why feeding a step with fractional part to `arange` is generally a bad idea: You might run into

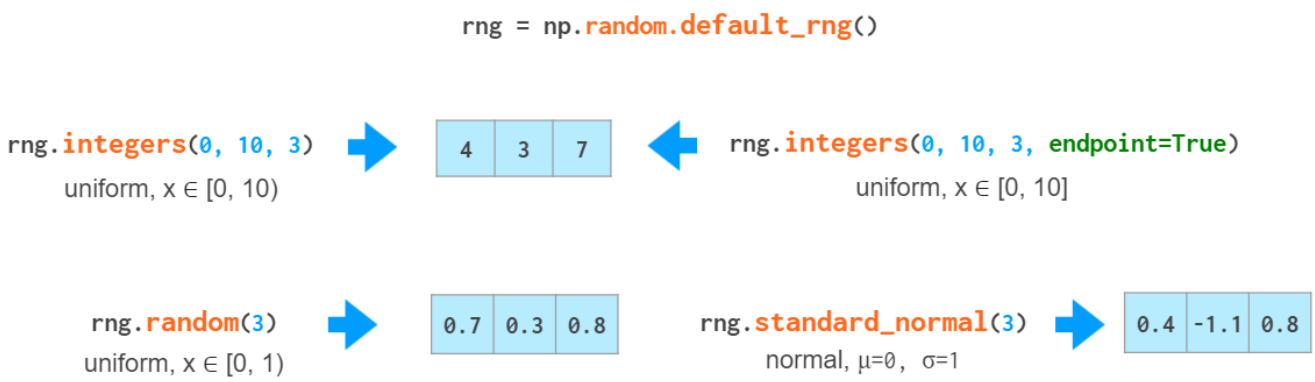
the number of elements you ask for. There's a common gotcha with `linspace`, though. It counts points, not intervals, thus the last argument is always plus one to what you would normally think of. So it is 11, not 10 in the example above.

For testing purposes it is often necessary to generate random arrays:



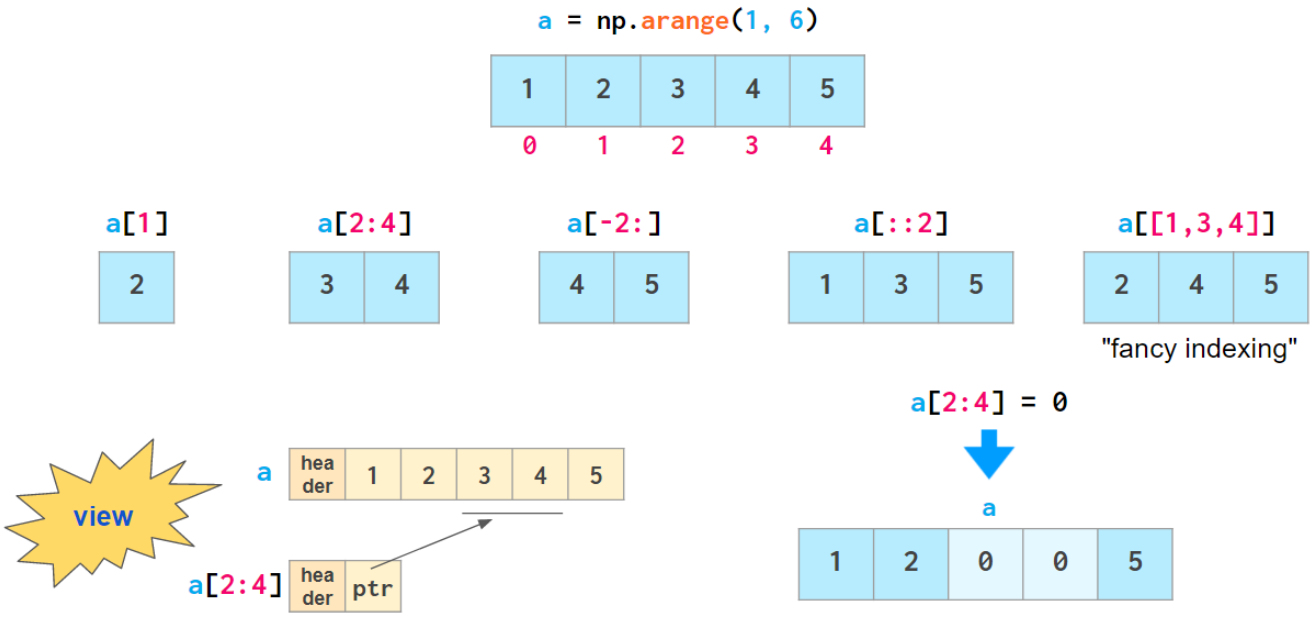
Old-style random numbers generation (deprecated)

There's also a new interface for random arrays generation. It is:
– better suited for multi-threading,
– somewhat faster,
– more configurable (you can squeeze even more speed or even more quality by choosing a non-default so-called 'bit generator'),
– able to pass two tricky synthetic tests that the old version fails.



Vector indexing

Once you have your data in the array, NumPy is brilliant at providing easy ways of giving it back:



All of the indexing methods presented above except fancy indexing are actually so-called “views”: They don’t store the data and reflect the changes in the original array if it happens to get changed after being indexed.

All of those methods including fancy indexing are mutable: They allow modification of the original array contents through assignment, as shown above. This feature breaks the habit of copying arrays by slicing them:

python list vs numpy array

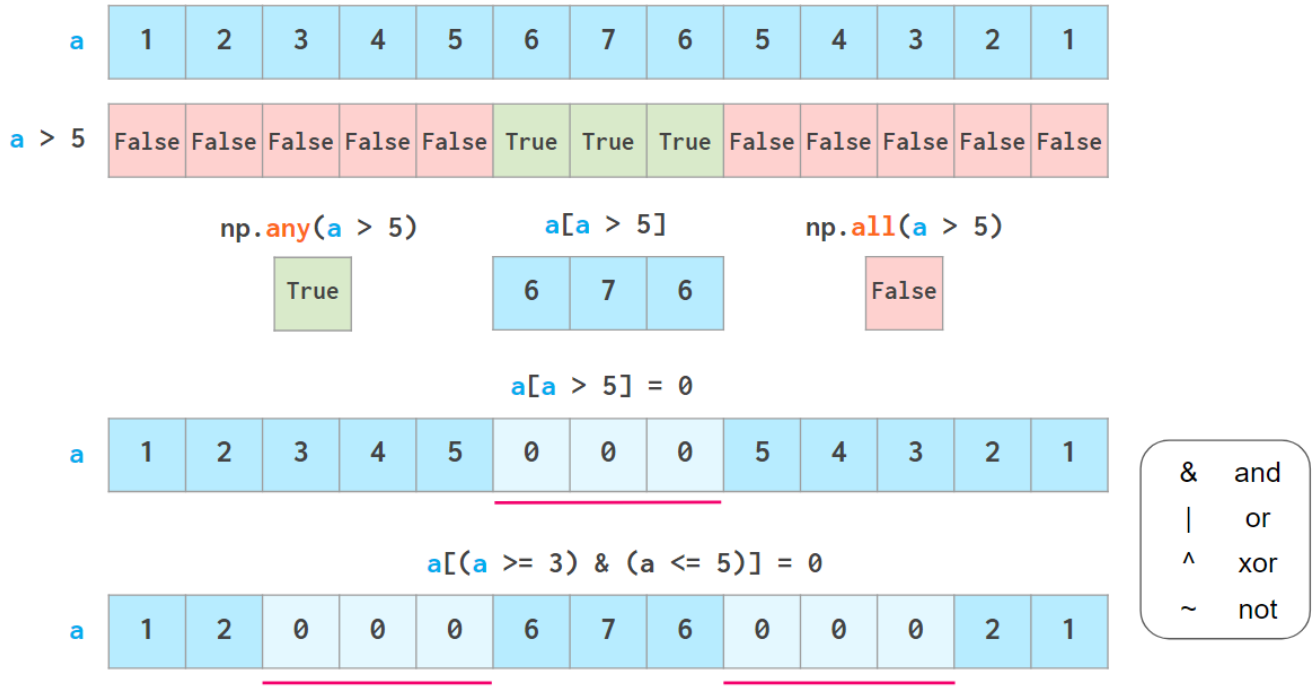
```
a = [1, 2, 3]                a = np.array([1, 2, 3])
b = a          # no copy     b = a          # no copy
c = a[:]       # copy        c = a[:]       # no copy!!!
d = a.copy() # copy          d = a.copy() # copy
```

```
a = [1, 2, 3]
a[1:2] = [5, 6]
a
```

```
[1, 5, 6, 3]
```

won't work in NumPy — use `np.insert`, `np.append`, etc. instead (described in the "2D" section below).

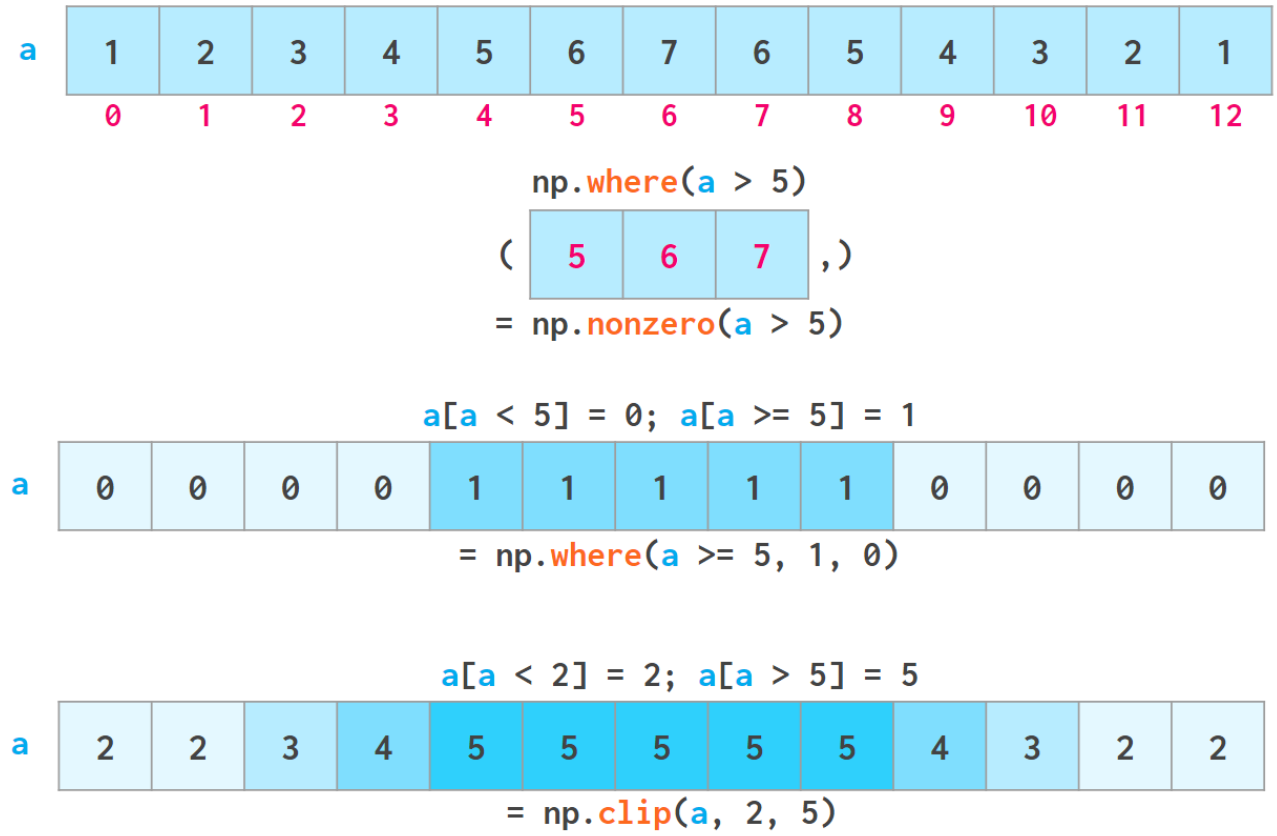
Another super-useful way of getting data from NumPy arrays is boolean indexing, which allows using all kinds of logical operators:



any and all act just like their python peers, but don't short-circuit

Careful though; Python "ternary" comparisons like `3<=a<=5` don't work here.

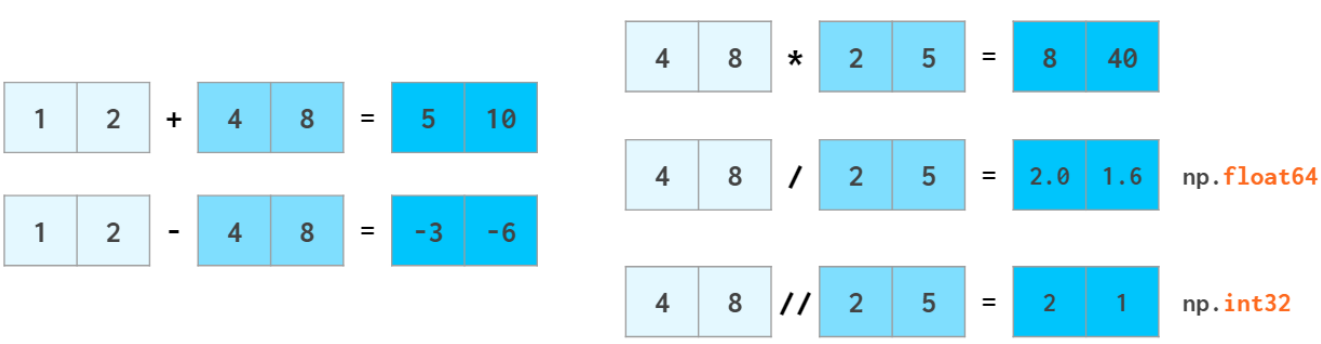
As seen above, boolean indexing is also writable. Two common use cases of it spun off as dedicated functions: the excessively overloaded `np.where` function (see both meanings below) and `np.clip`.



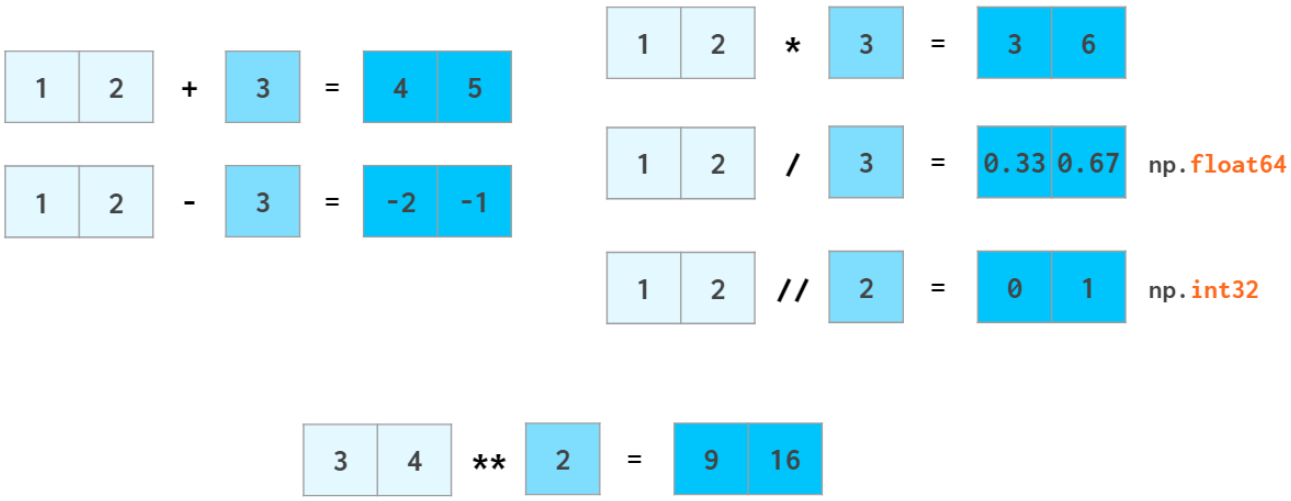
Note that `np.where` with one argument returns a tuple of arrays (1-tuple in 1D case, 2-tuple in 2D case, etc), thus you need to write `np.where(a>5)[0]` to get `np.array([5,6,7])` in the example above (same for `np.nonzero`).

Vector operations

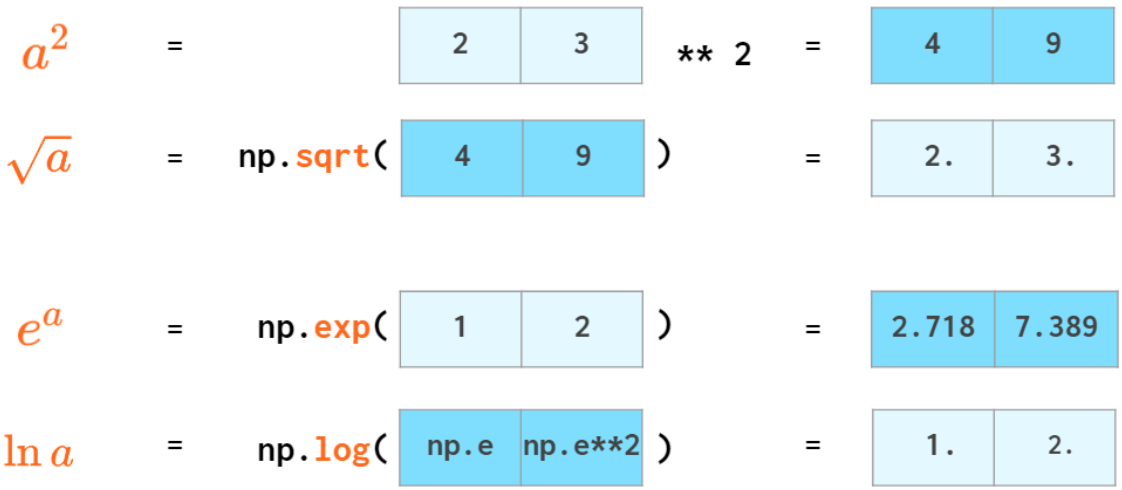
Arithmetic is one of the places where NumPy speed shines most. Vector operators are shifted to the c++ level and allow us to avoid the costs of slow Python loops. NumPy allows the manipulation of whole arrays just like ordinary numbers:



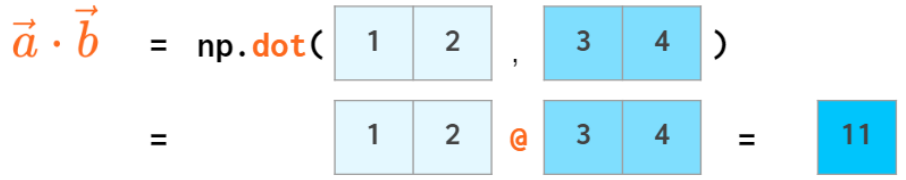
The same way ints are promoted to floats when adding or subtracting, scalars are promoted (aka *broadcasted*) to arrays:

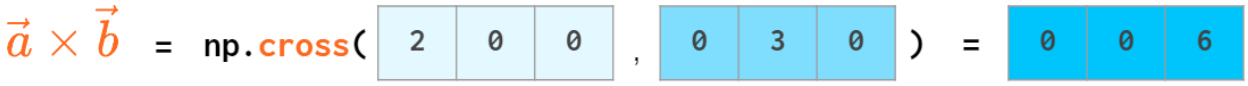


Most of the math functions have NumPy counterparts that can handle vectors:

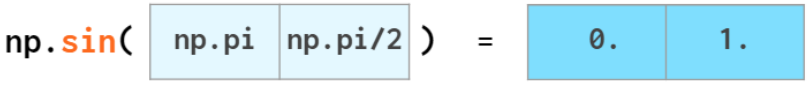


Scalar product has an operator of its own:



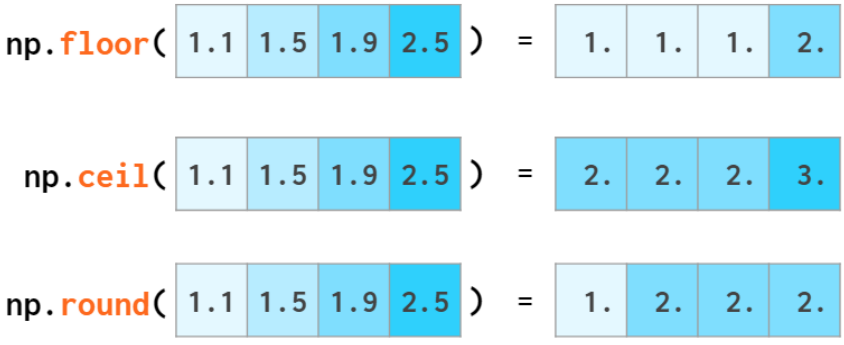


You don't need loops for trigonometry either:



sin	arcsin	sinh	arcsinh
cos	arccos	cosh	arccosh
tan	arctan	tanh	arctanh

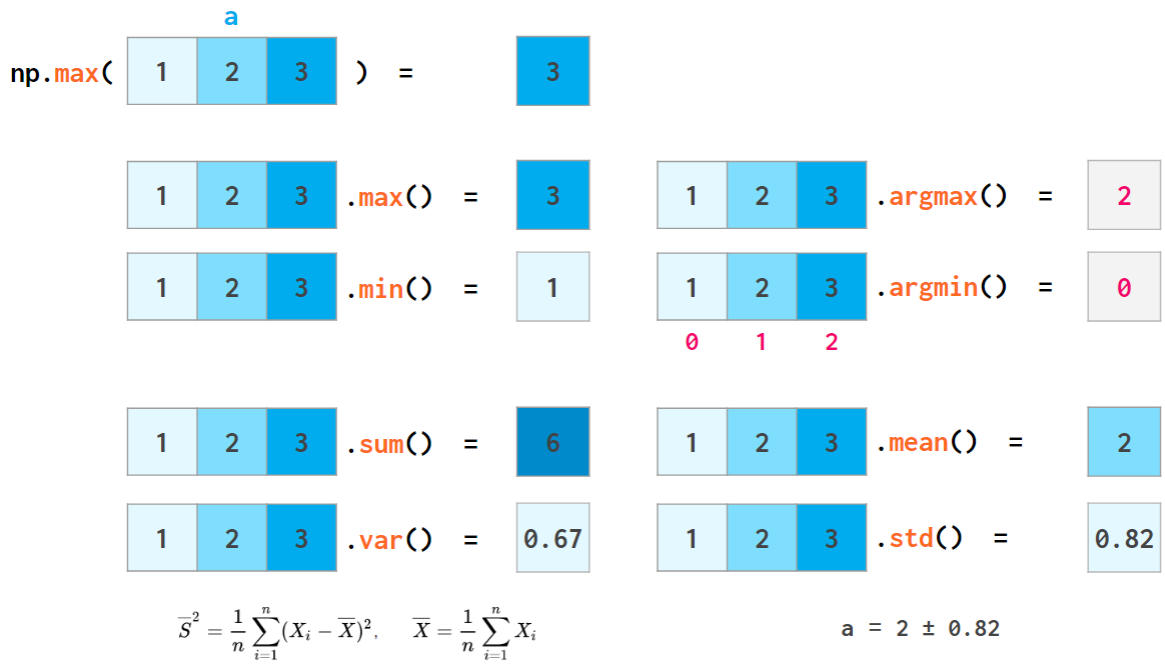
Arrays can be rounded as a whole:



`floor` rounds to -∞, `ceil` to +∞ and around — to the nearest integer (.5 to even)

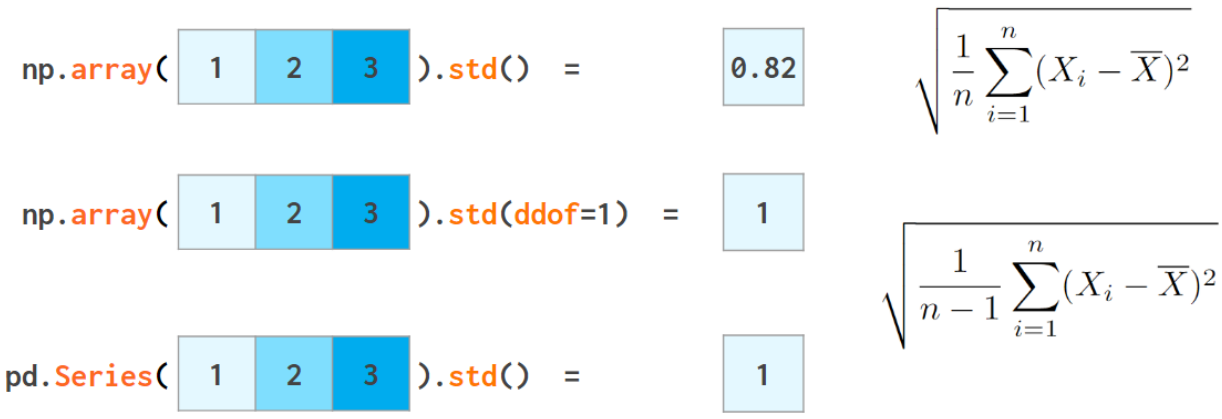
`numpy as np`). You can use `a.round()` as well.

NumPy is also capable of doing the basic stats:



Each of these functions has a nan-resistant variant: eg nansum, nanmax, etc

As you can see from the formula above, both `std` and `var` ignore Bessel's correction and give a biased result in the most typical use case of estimating std from a sample when the population mean is unknown. The standard approach to get a less biased estimation is to have `n-1` in the denominator, which is done with `ddof=1` ('delta degrees of freedom'):



Pandas std uses Bessel's correction by default

```
res1, res2, res3 = [], [], []
for i in range(10000):
    a = np.random.randn(100)
    res1.append(a.std())
    res2.append(a.std(ddof=1))
    res3.append(a.std(ddof=1.5))
```

```
np.mean(res1)                # 0.8%
```

```
0.9921820984811617
```

```
np.mean(res2)                # 0.3%
```

```
0.9971805285968072
```

```
np.mean(res3)                # 0.03%
```

```
0.9997082399489409
```

Sorting functions have fewer capabilities than their Python counterparts:

python lists	numpy arrays	
`a.sort()`	`a.sort()`	sorts in-place
`sorted(a)`	`np.sort(a)`	returns new sorted array
`a.sort(key=f)`	–	key function
`a.sort(reversed=False)`	-	ascending/descending

In the 1D case, the absence of the `reversed` keyword can be easily compensated for by reversing the result. In 2D it is somewhat trickier (feature request[5]).

Searching for an element in a vector

As opposed to Python lists, a NumPy array does not have an `index` method. The corresponding feature request[6] has been hanging there for quite a while now.

Python Lists:

```
a.index(x[, i[, j]])    # first occurrence of x in a between indices i and j
```

Numpy Arrays:

```
np.where(a==x)[0][0]                                # finds all occurrences first
next(i[0] for i, v in np.ndenumerate(a) if v==x) # needs numba
np.searchsorted(a, x)                               # needs sorted array
```

The square brackets in the definition of index() mean that either j or both i and j can be omitted

- One way of finding an element is `np.where(a==x)[0][0]`, which is neither elegant nor fast as it needs to look through all elements of the array even if the item to find

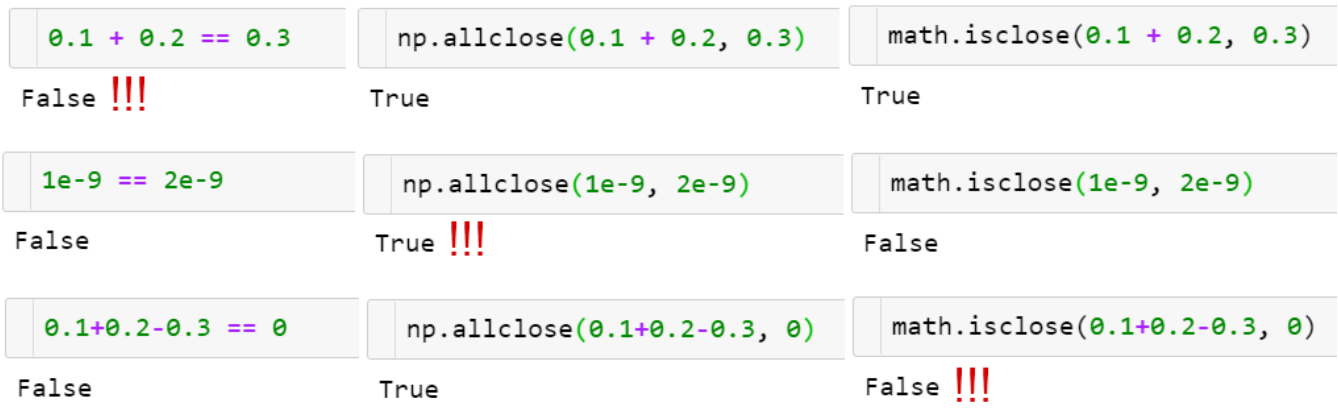
- A faster way to do it is via accelerating `next((i[0] for i, v in np.ndenumerate(a) if v==x), -1)` with Numba[7] (otherwise it's way slower in the worst case than `where`).

- Once the array is sorted though, the situation gets better: `v = np.searchsorted(a, x); return v if a[v]==x else -1` is really fast with O(log N) complexity, but it requires O(N log N) time to sort first.

Actually, it is not a problem to speed up searching by implementing it in C. The problem is float comparisons. This is a task that simply does not work out of the box for arbitrary data.

Comparing floats

The function `np.allclose(a, b)` compares arrays of floats with a given tolerance



There is no silver bullet!

- `np.allclose` assumes all the compared numbers to be of a typical scale of 1. For example, if you work with nanoseconds, you need to divide the default `atol` argument value by 1e9: `np.allclose(1e-9, 2e-9, atol=1e-17) == False`.

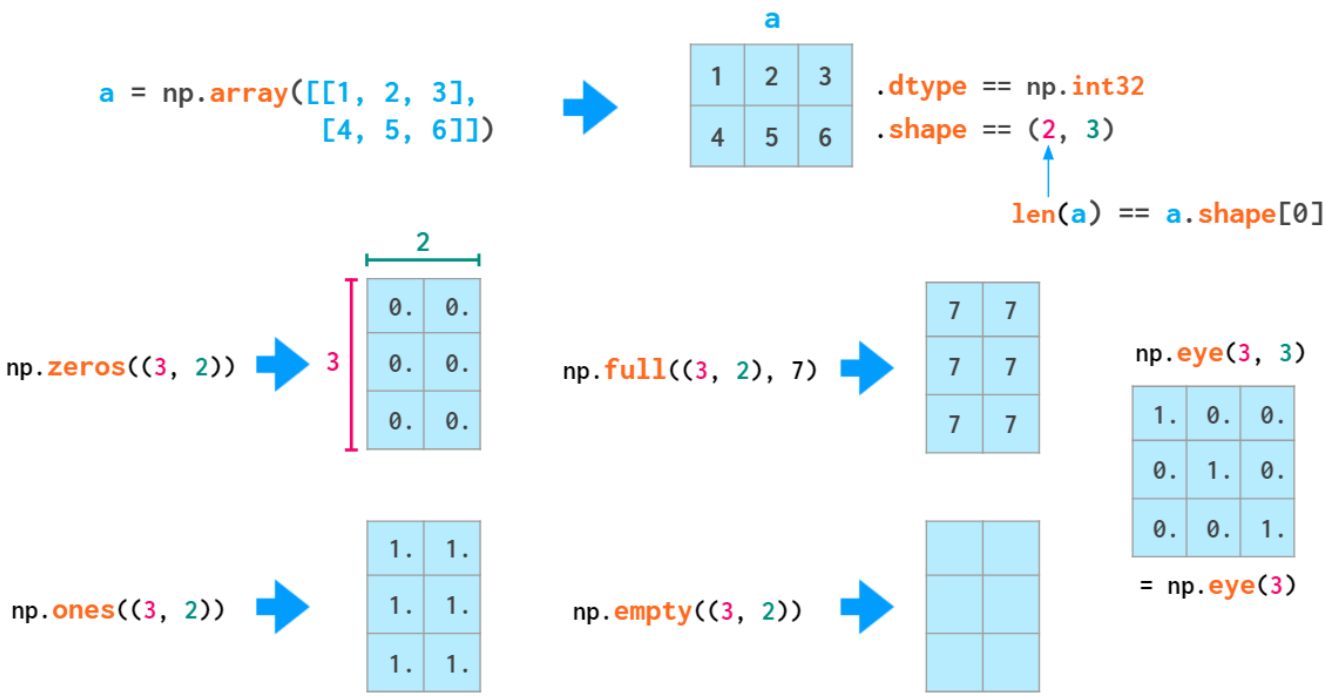
- `math.isclose` makes no assumptions about the numbers to be compared but relies on a user to give a reasonable `abs_tol` value instead (taking the default `np.allclose atol` value of 1e-8 is good enough for numbers with a typical scale of 1): `math.isclose(0.1+0.2-0.3, abs_tol=1e-8)==True`.

introduced later). To learn more on that, take a look at the excellent floating-point guide[8] and the corresponding NumPy issue[9] on GitHub.

2. Matrices, the 2D Arrays

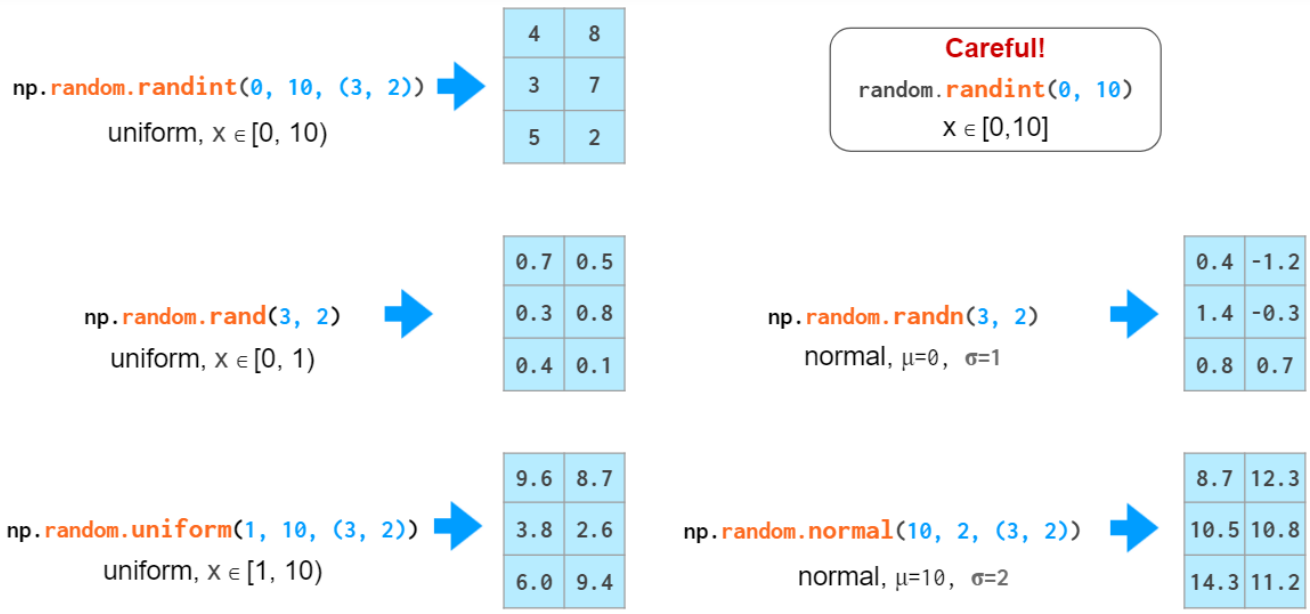
There used to be a dedicated `matrix` *class in NumPy, but it is deprecated now, so I'll use the words* matrix *and* 2D array *interchangeably.*

Matrix initialization syntax is similar to that of vectors:



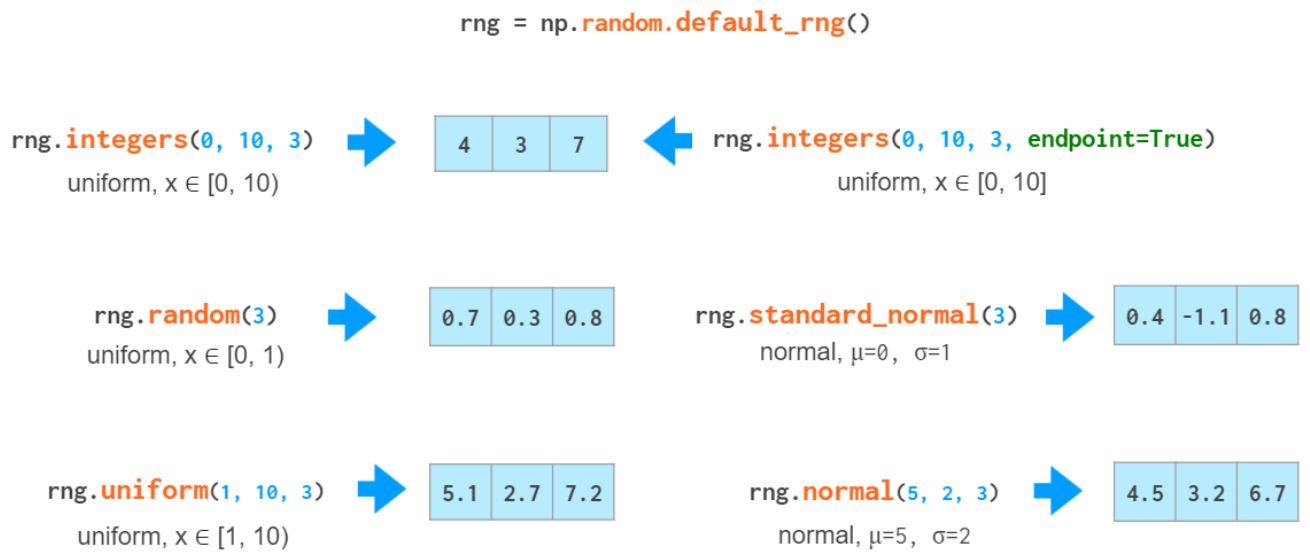
Double parentheses are necessary here because the second positional parameter is reserved for the (optional) `dtype` (which also accepts integers).

Random matrix generation is also similar to that of vectors:



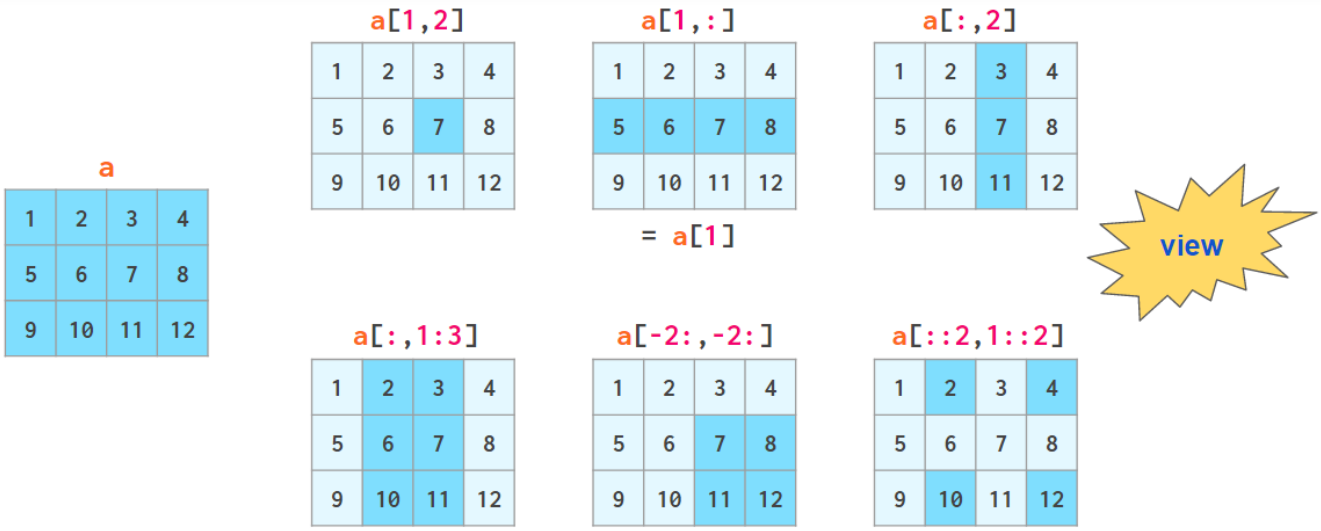
Old-style random numbers generation

The ubiquitous double parentheses found their way to the interface of the new-style (see details in the 1D section above) numbers generation routines so that as of today only in `np.eye` has beauty taken prevelence over stringency and convenience of passing shapes as is:



New-style random numbers generation

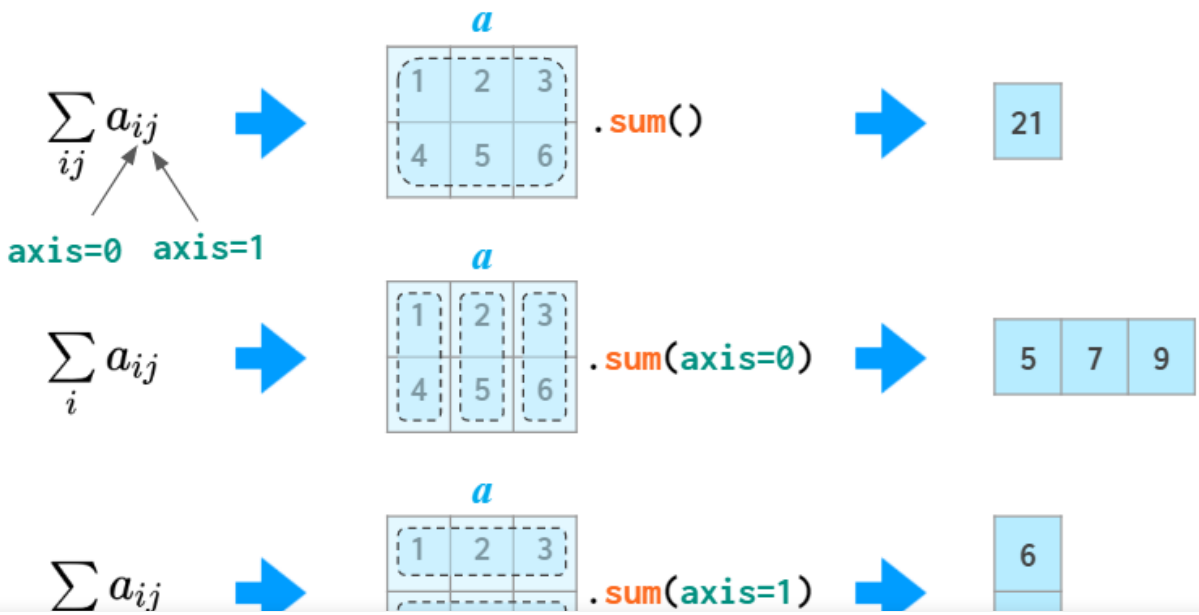
Two-dimensional indexing syntax is more convenient than that of nested lists:



The “view” sign means that no copying is actually done when slicing an array. When the array is modified, the changes are reflected in the slice as well.

The axis argument

In many operations (e.g., `sum`) you need to tell NumPy if you want to operate across rows or columns. To have a universal notation that works for an arbitrary number of dimensions, NumPy introduces a notion of axis: The value of the `axis` argument is, as a matter of fact, the number of the index in question: The first index is `axis=0`, the second one is `axis=1`, and so on. So in 2D `axis=0` is column-wise and `axis=1` means row-wise.

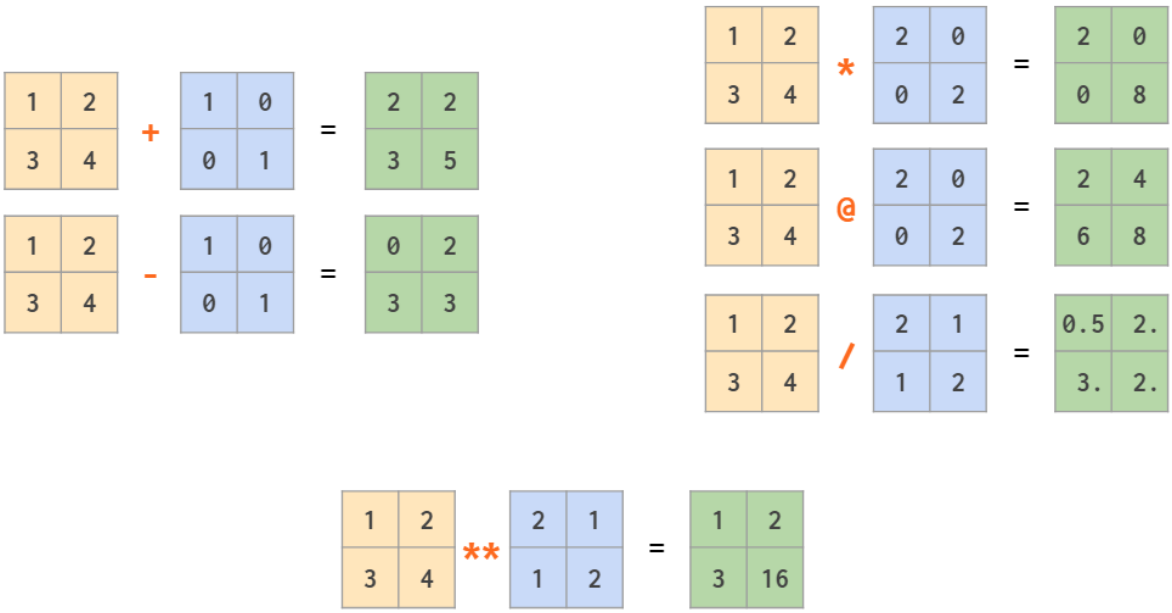


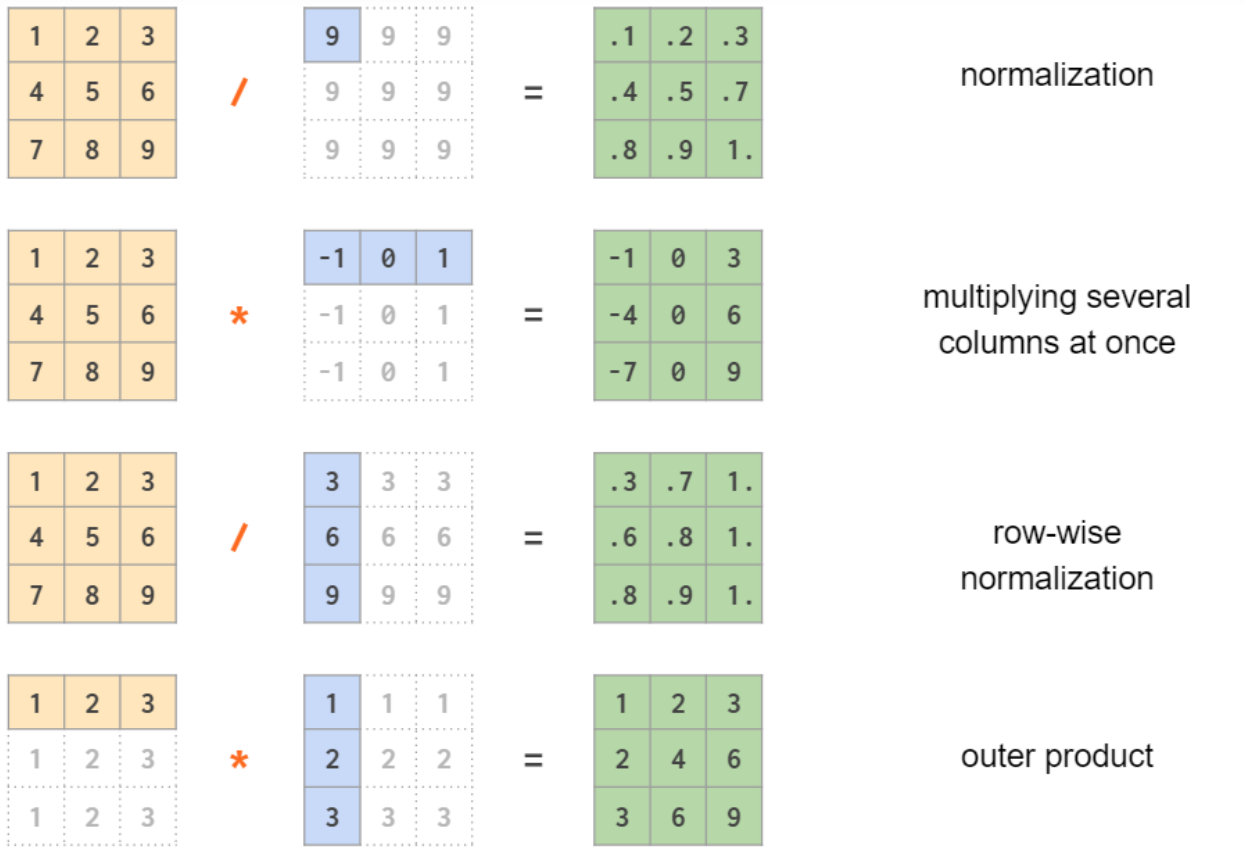
Generally speaking, the first dimension `i` (axis=0) is responsible for indexing the rows, so `sum(axis=0)` should be read like "for any given column sum over all of its rows" rather than just "column-wise". The 2D case is somewhat counter-intuitive: you need to specify the dimension *to be eliminated*, instead of the *remaining* one you would normally think about. In higher dimensional cases this is more natural, though: it'd be a burden to enumerate all the remaining dimensions if you only need to sum over a single one.

The notion of the 'axis' argument (called 'dimension' in MATLAB) is actually very simple: it is just number of the index you want the operation to carry over. It is used in many functions in NumPy so it pays off to understand it, but if for some reason it doesn't work out for you, in this particular case you can use the Einstein summation — that's a way to do the sums without 'axes': `np.einsum('ij->j', a)` is summing column-wise (same as `sum(axis=0)` in the image above) and `np.einsum('ij->i', a)` is row-wise (same as `sum(axis=1)`).

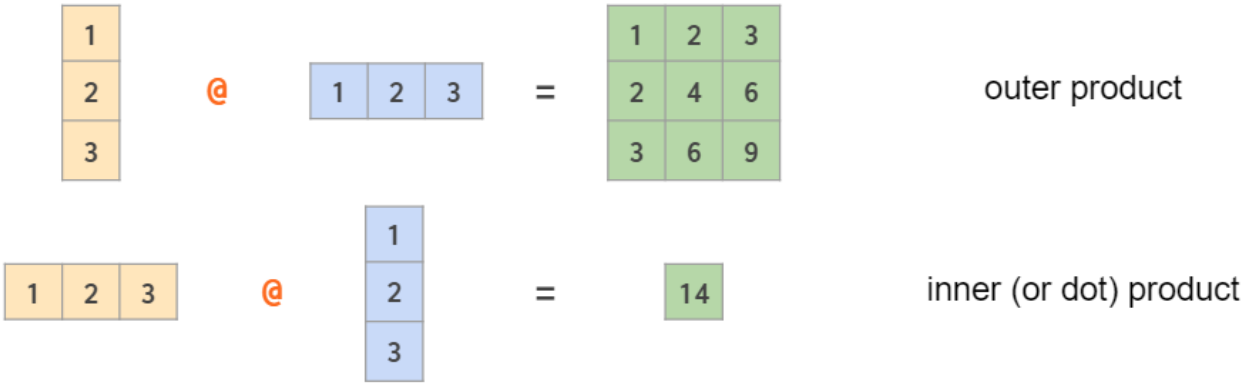
Matrix arithmetic

In addition to ordinary operators (like +,-,*,/,// and **) which work element-wise, there's a @ operator that calculates a matrix product:





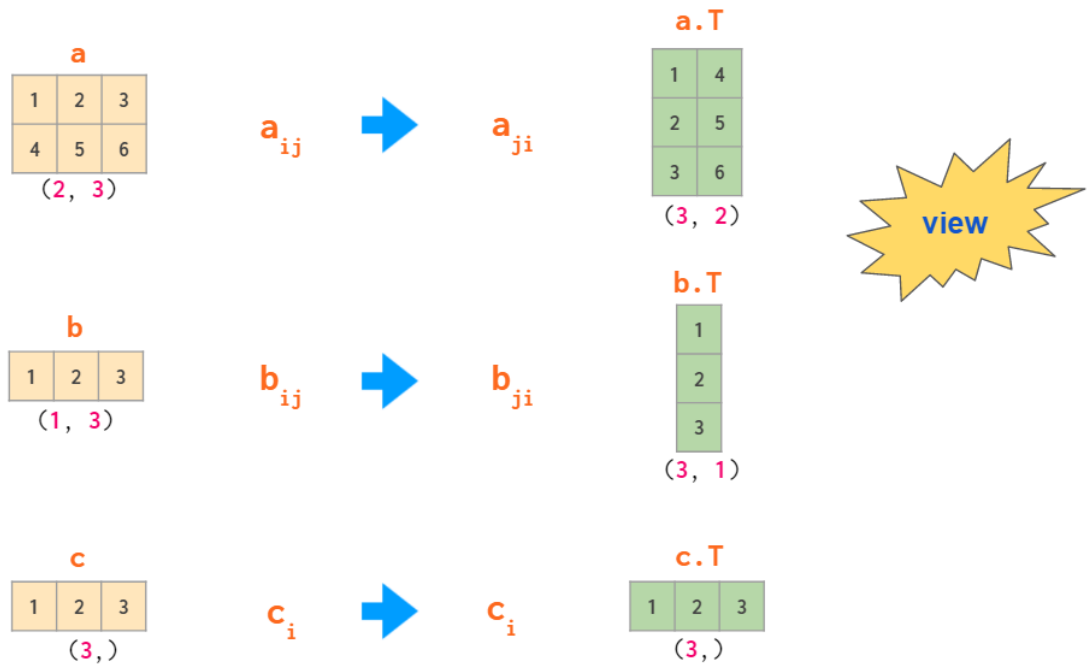
Note that in the last example it is a symmetric per-element multiplication. To calculate the outer product using an asymmetric linear algebra matrix multiplication the order of the operands should be reversed:



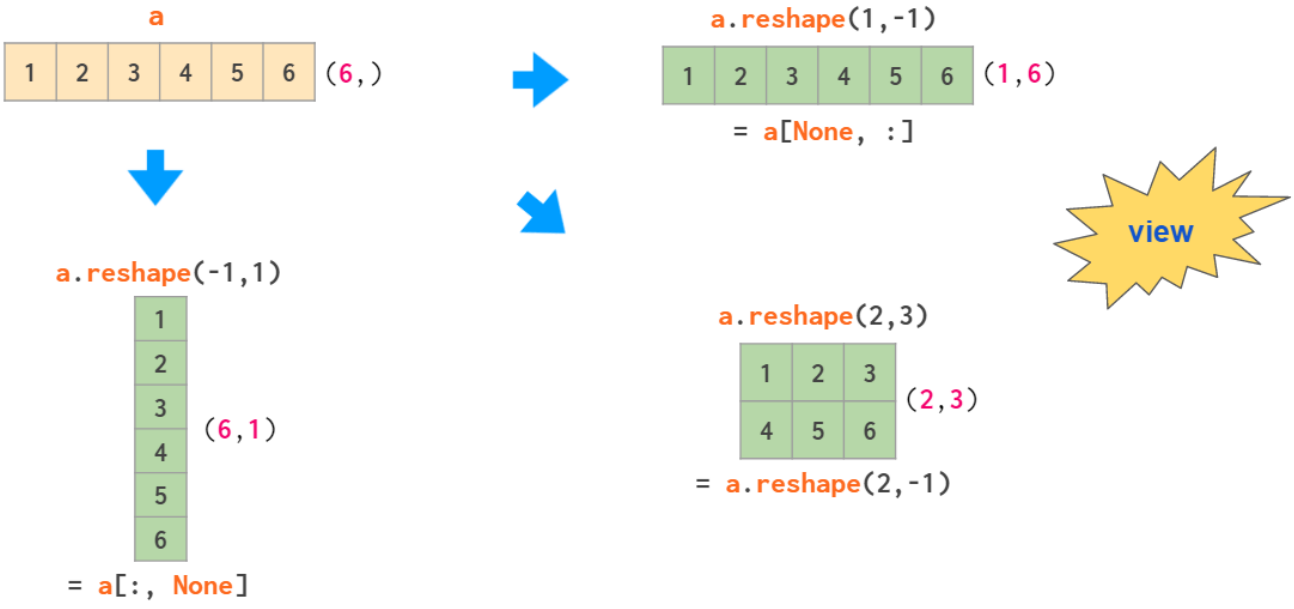
Row vectors and column vectors

As seen from the example above, in the 2D context, the row and column vectors are treated differently. This contrasts with the usual NumPy practice of having one type of 1D arrays wherever possible (e.g., `a[:,j]` — the j-th column of a 2D array `a` — is a 1D

result will be the same. If you need a column vector, there are a couple of ways to cook it from a 1D array, but surprisingly `transpose` is not one of them:

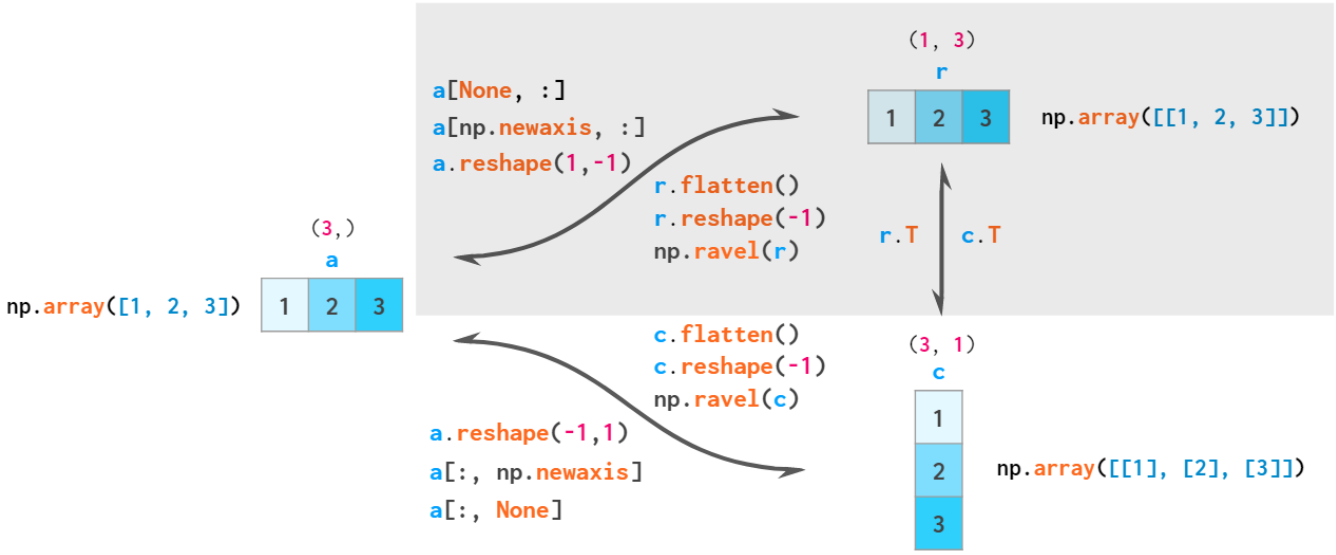


Two operations that *are* capable of making a 2D column vector out of a 1D array are reshaping and indexing with `newaxis`:



Here the -1 argument tells `reshape` to calculate one of the dimension sizes

So, there's a total of three types of vectors in NumPy: 1D arrays, 2D row vectors, and 2D column vectors. Here's a diagram of explicit conversions between those:



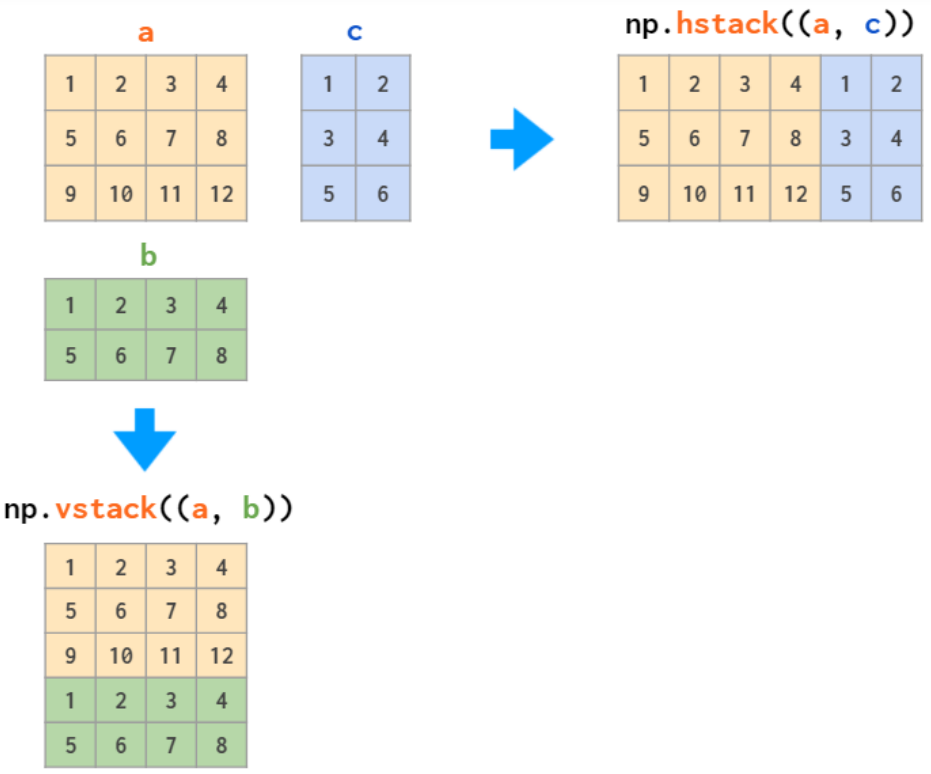
flatten is always a copy, reshape(-1) is always a view, ravel is a view when possible

By the rules of broadcasting, 1D arrays are implicitly interpreted as 2D row vectors, so it is generally not necessary to convert between those two — thus the corresponding area is shaded.

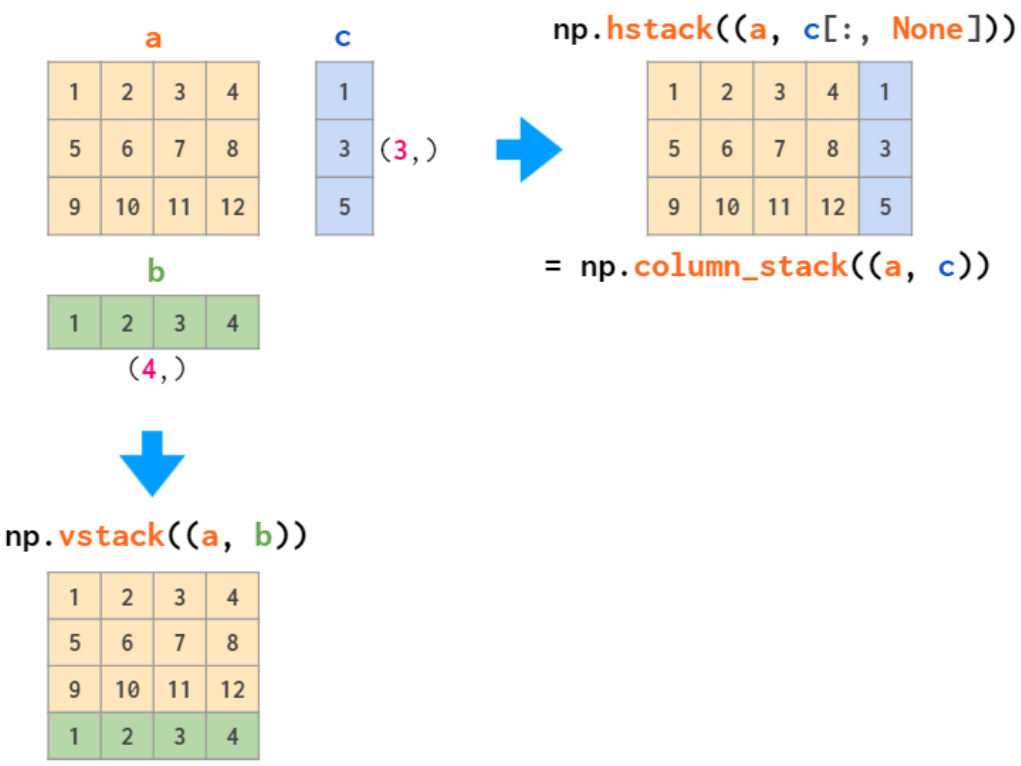
Strictly speaking, any array, all but one dimensions of which are single-sized, is a vector (eg. `a.shape==[1,1,1,5,1,1]` *), so there's an infinite number of vector types in numpy, but only these three are commonly used. You can use* `np.reshape` *to convert a 'normal' 1D vector to this form and* `np.squeeze` *to get it back. Both functions act as views.*

Matrix manipulations

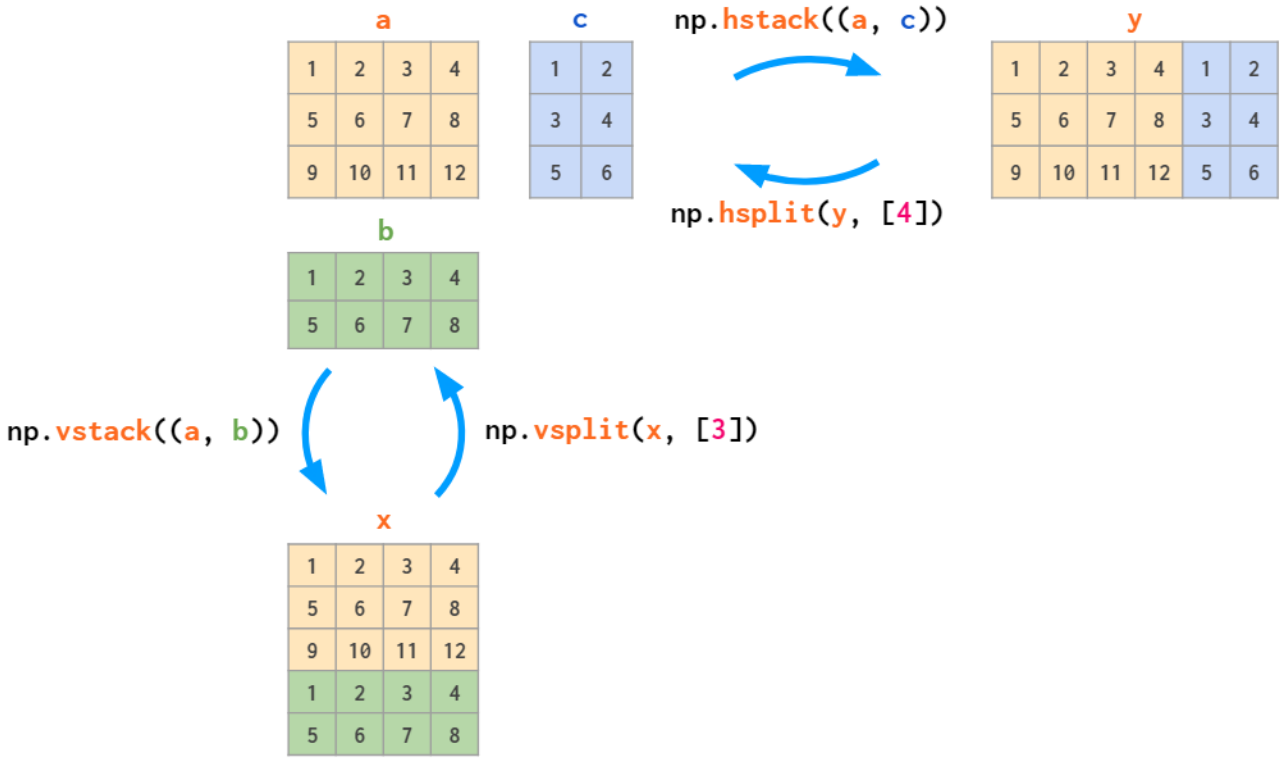
There are two main functions for joining the arrays:

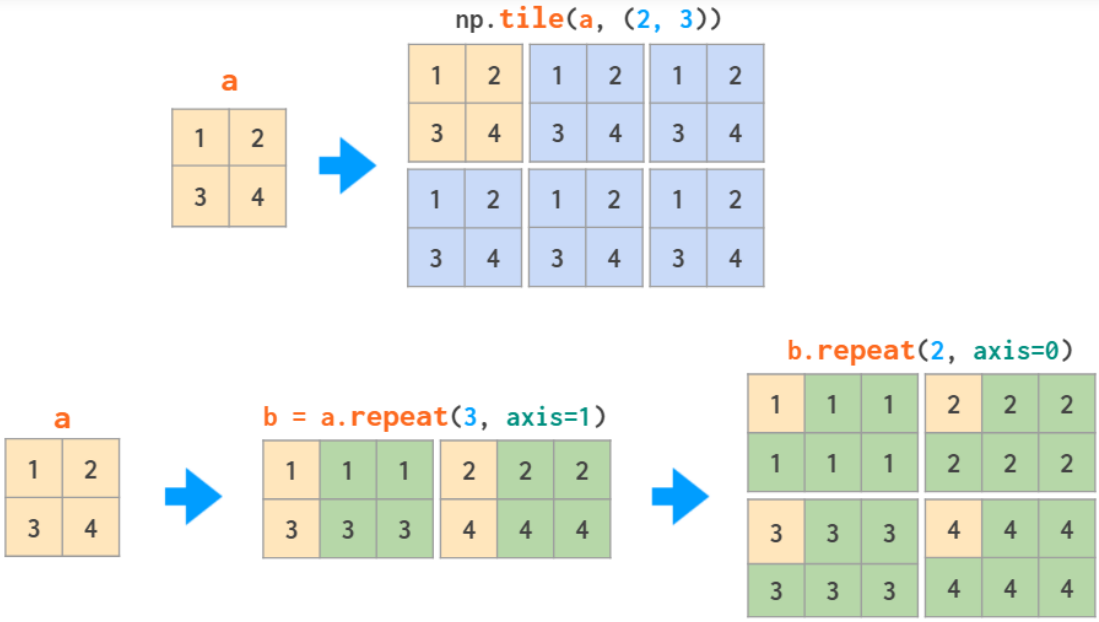


Those two work fine with stacking matrices only or vectors only, but when it comes to mixed stacking of 1D arrays and matrices, only the `vstack` works as expected: The `hstack` generates a dimensions-mismatch error because as described above, the 1D array is interpreted as a row vector, not a column vector. The workaround is either to convert it to a row vector or to use a specialized `column_stack` function which does it automatically:

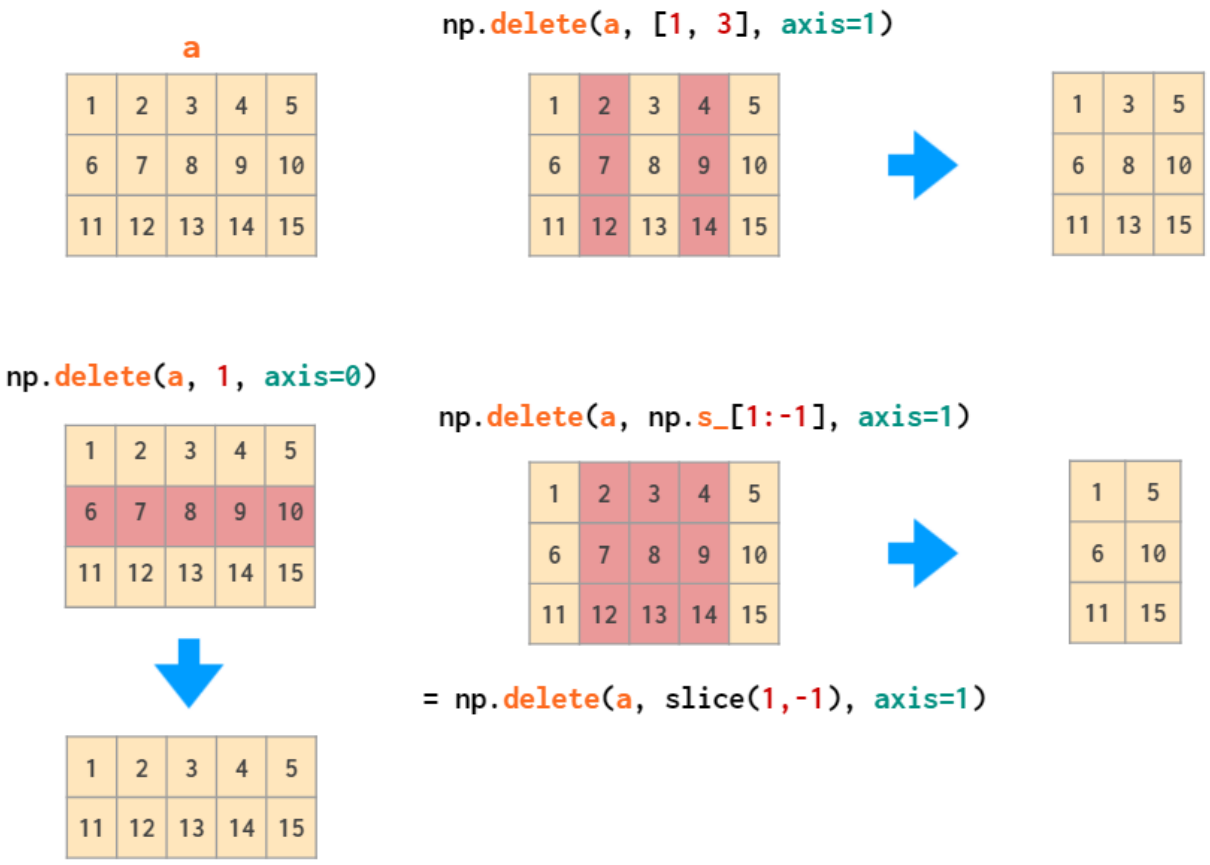


The inverse of stacking is splitting:

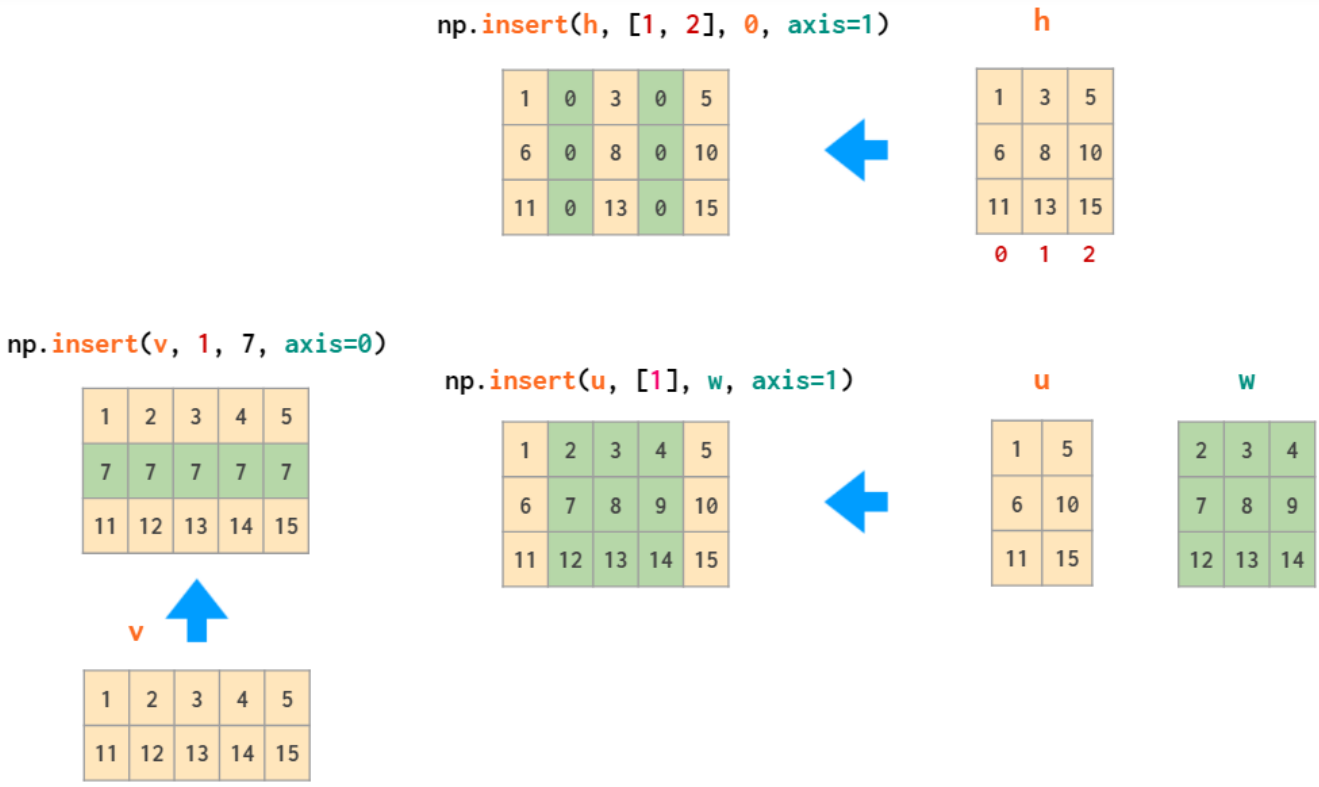




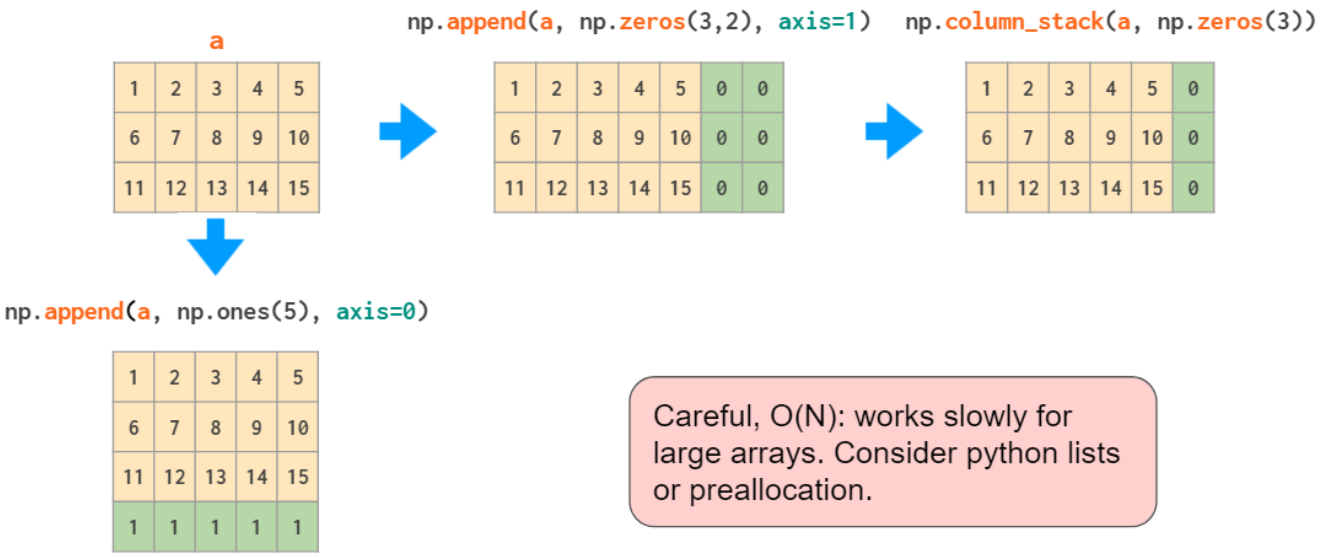
Specific columns and rows can be `delete` d like that:



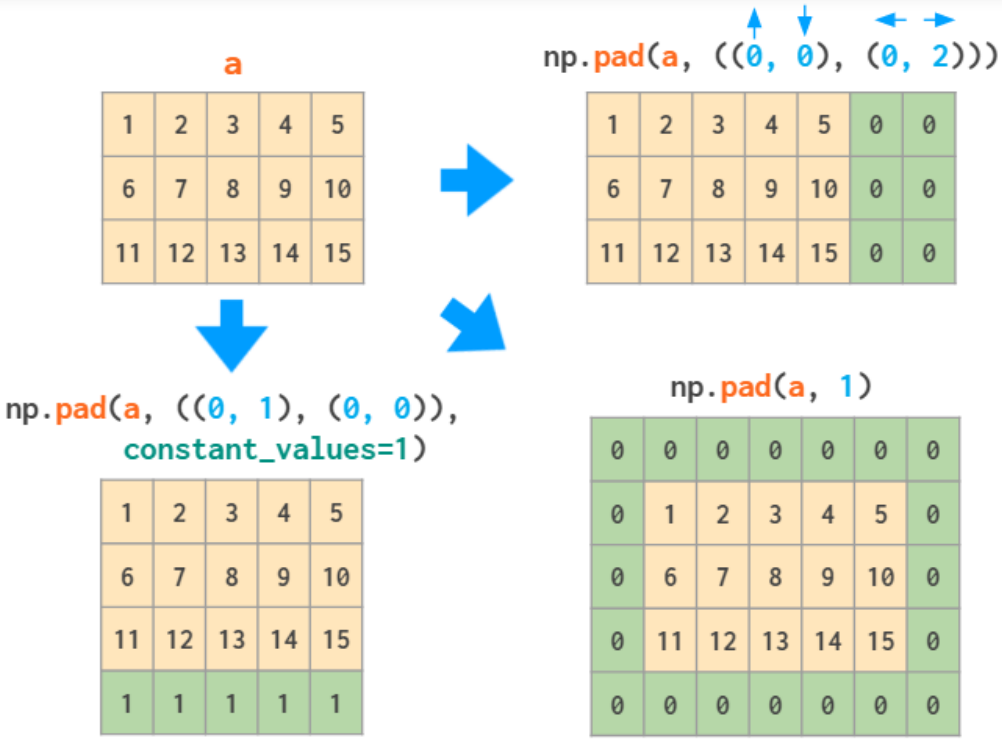
The inverse operation is `insert` :



The `append` function, just like `hstack`, is unable to automatically transpose 1D arrays, so once again, either the vector needs to be reshaped or a dimension added, or `column_stack` needs to be used instead:



Actually, if all you need to do is add constant values to the border(s) of the array, the



Meshgrids

The broadcasting rules make it simpler to work with meshgrids. Suppose, you need the following matrix (but of a very large size):

$$A_{ij} = j - i$$

0	1	2
-1	0	1

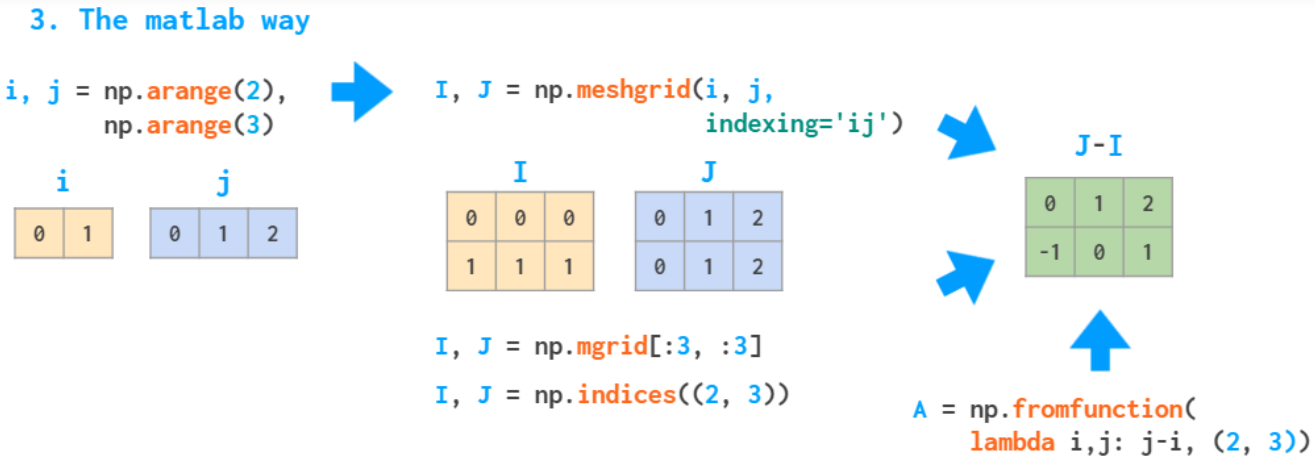
1. The c way

```
a = np.empty((2, 3))
for i in range(2):
    for j in range(3):
        a[i, j] = j - i
```

2. The python way

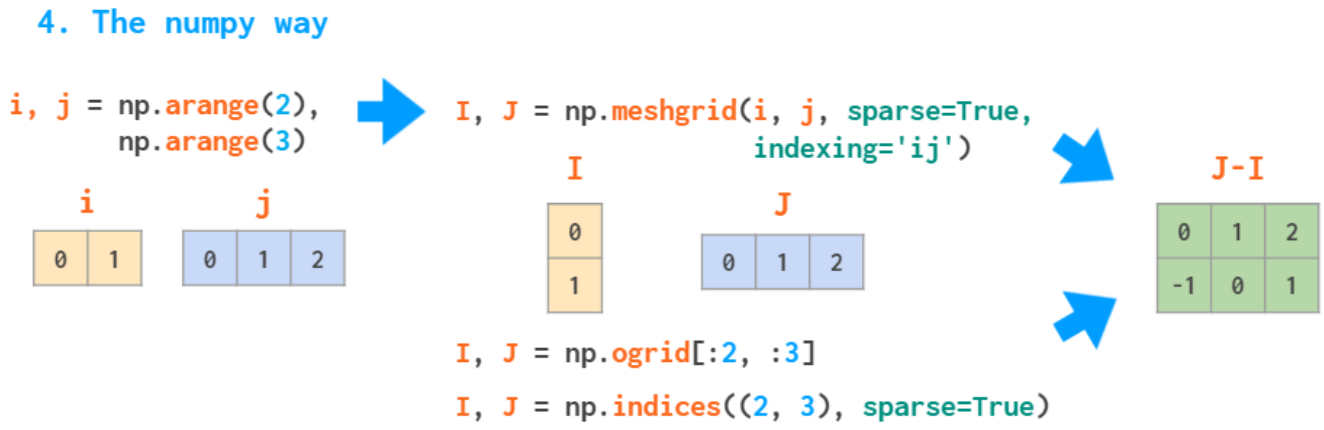
```
c = [[(j-i) for j in range(3)] for i in range(2)]
a = np.array(c)
```

Two obvious approaches are slow, as they use Python loops. The MATLAB way of dealing with such problems is to create a meshgrid:



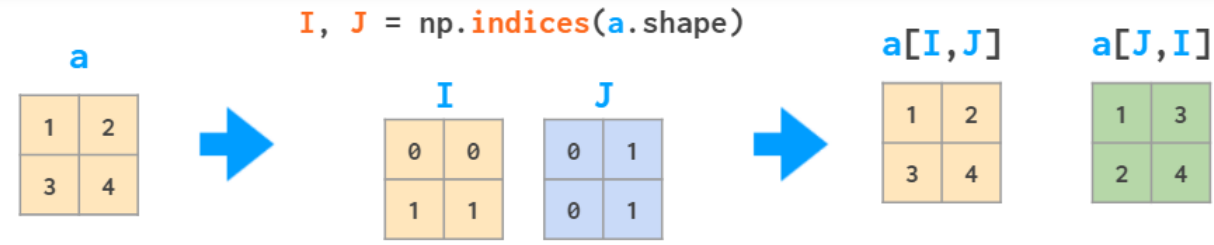
The `meshgrid` function accepts an arbitrary set of indices, `mgrid` — just slices and `indices` can only generate the complete index ranges. `fromfunction` calls the provided function just once, with the I and J argument as described above.

But actually, there is a better way to do it in NumPy. There's no need to spend memory on the whole I and J matrices (even though `meshgrid` is smart enough to only store references to the original vectors if possible). It is sufficient to store only vectors of the correct shape, and the broadcasting rules take care of the rest:



Without the `indexing='ij'` argument, `meshgrid` will change the order of the arguments: `J, I= np.meshgrid(j, i)` — it is an 'xy' mode, useful for visualizing 3D plots (see the example from the docs).

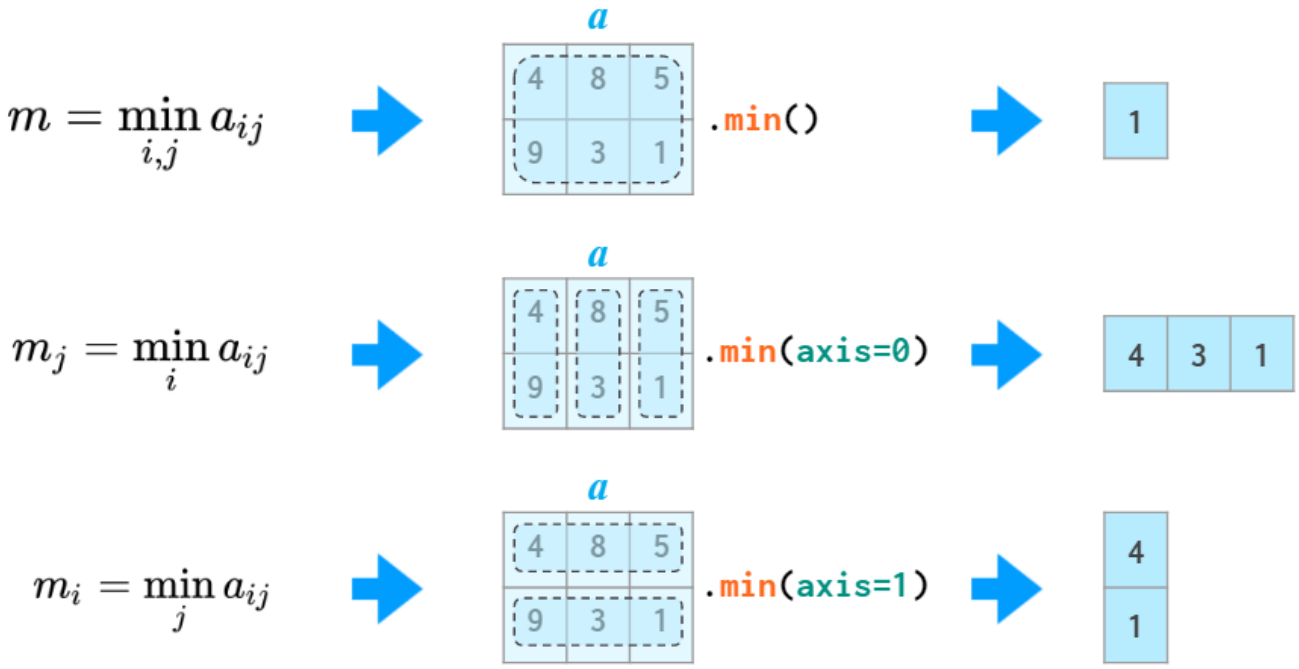
Aside from initializing functions over a two- or three-dimensional grid, the meshes can be useful for indexing arrays:



Works with sparse meshgrids, too

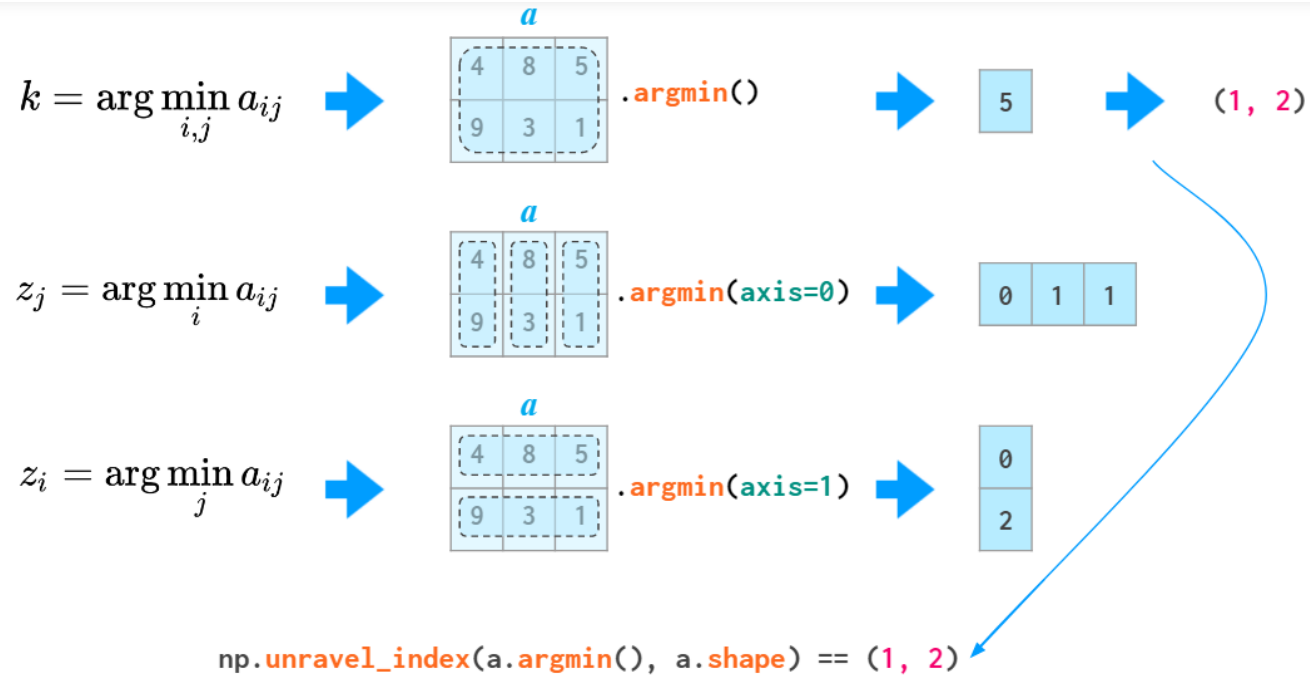
Matrix statistics

Just like `sum`, all the other stats functions (`min`/`max`, `argmin`/`argmax`, `mean`/`median`/`percentile`, `std`/`var`) accept the `axis` parameter and act accordingly:

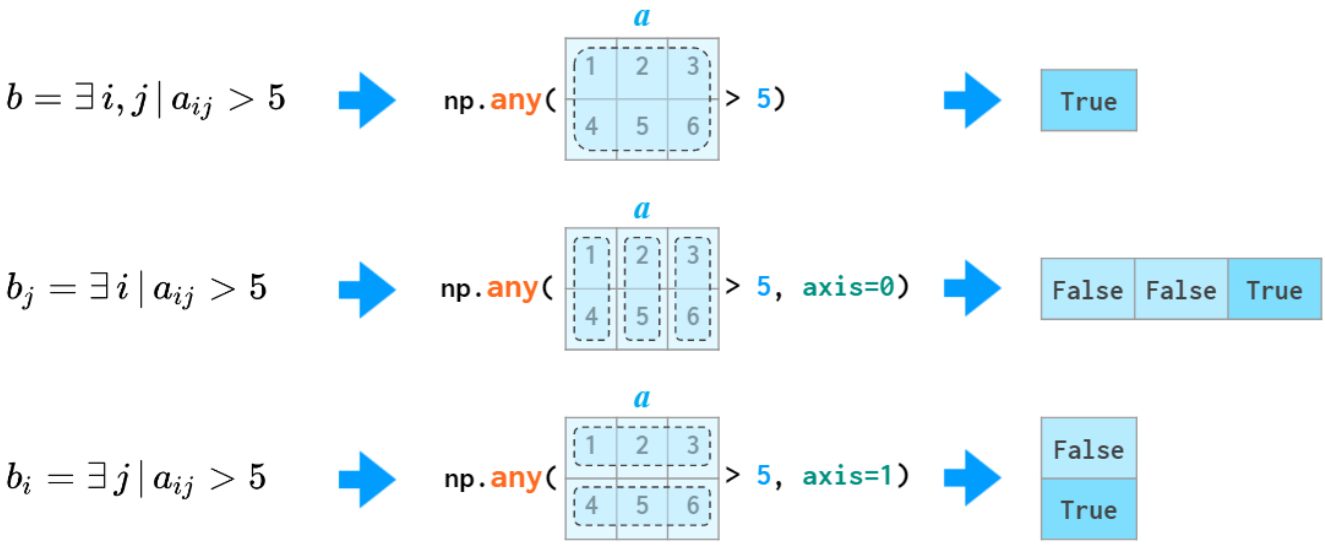


np.amin is just an alias of np.min to avoid shadowing the Python min when you write '`from numpy import *`'

The `argmin` and `argmax` functions in 2D and above have an annoyance of returning the flattened index (of the first instance of the min and max value). To convert it to two coordinates, an `unravel_index` function is required:



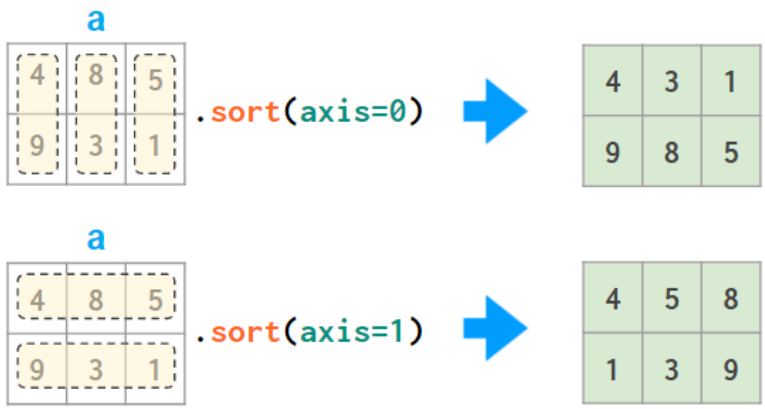
The quantifiers `all` and `any` are also aware of the `axis` argument:



Matrix sorting

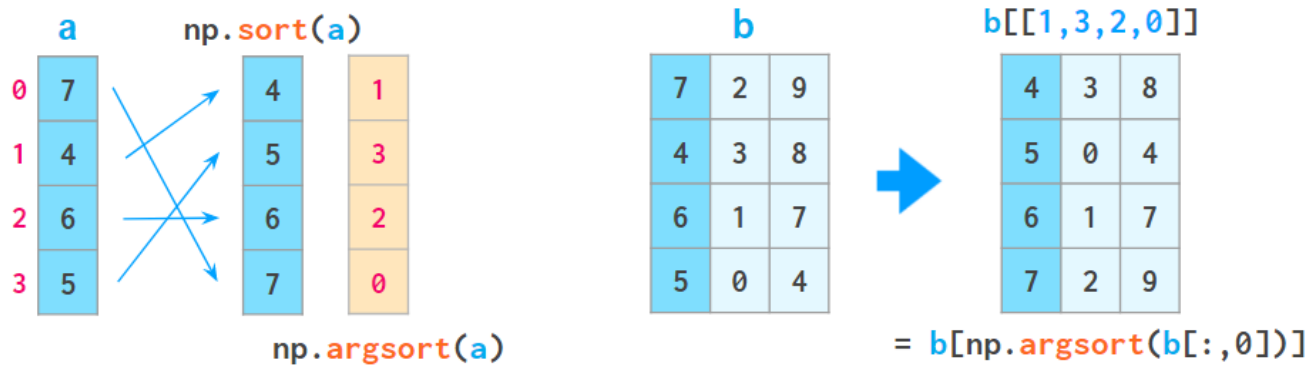
As helpful as the `axis` argument is for the functions listed above, it is as unhelpful for the 2D sorting:

python lists	numpy arrays	
`a.sort()`	`a.sort()`	sorts in-place
`sorted(a)`	`np.sort(a)`	returns new sorted array
`a.sort(key=f)`	–	key function
`a.sort(reversed=False)`	-	ascending/descending
–	`a.sort(axis=-1)`	which axis to sort along



It is just not what you would usually want from sorting a matrix or a spreadsheet: `axis` is in no way a replacement for the `key` argument. But luckily, NumPy has several helper functions which allow sorting by a column — or by several columns, if required:

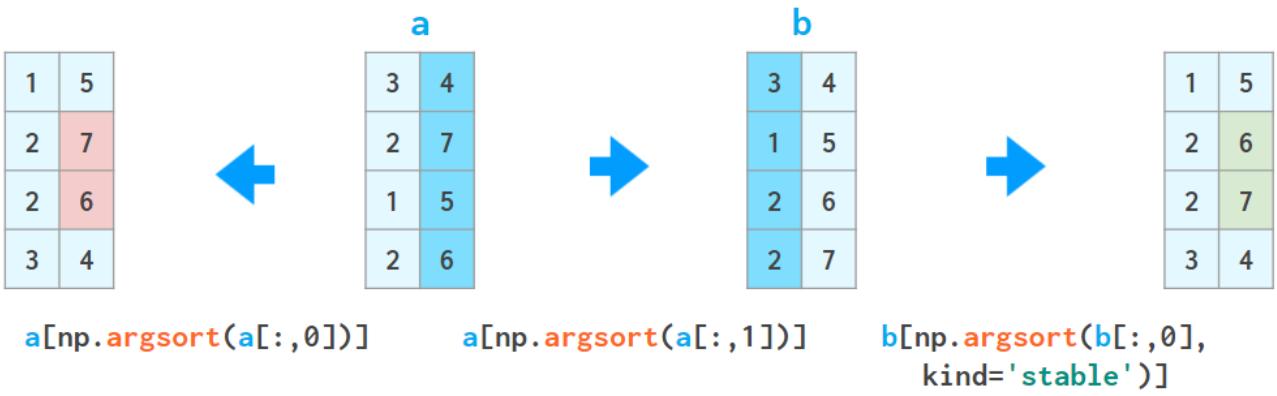
1. `a[a[:,0].argsort()]` sorts the array by the first column:



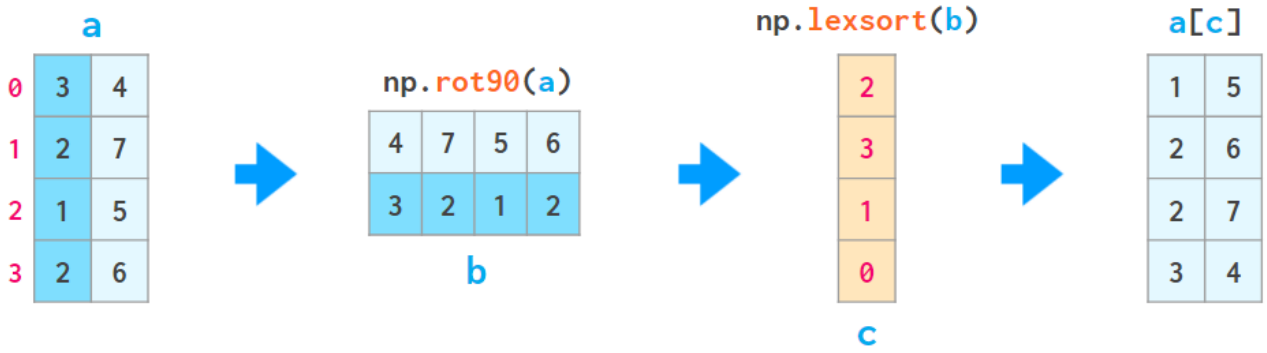
Here `argsort` returns an array of indices of the original array after sorting.

This trick can be repeated, but care must be taken so that the next sort does not mess

```
a = a[a[:,1].argsort(kind='stable')]
a = a[a[:,0].argsort(kind='stable')]
```

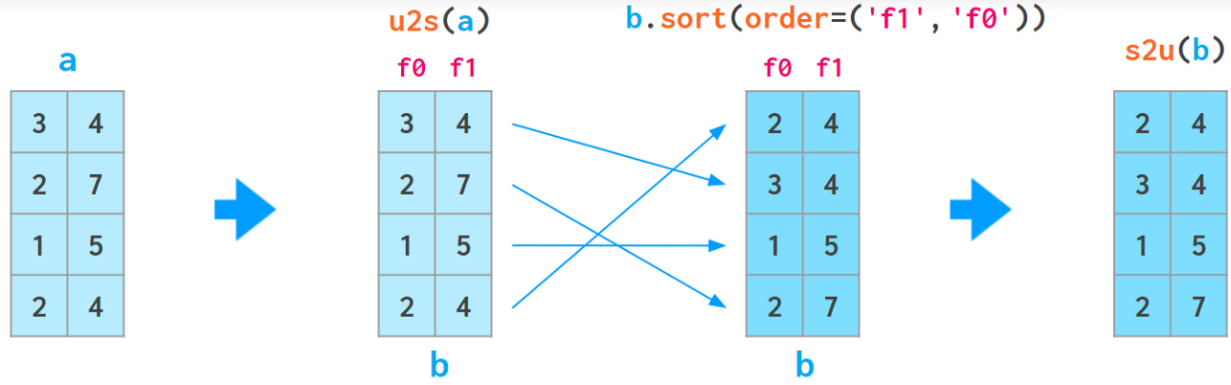


2. There's a helper function `lexsort` which sorts in the way described above by all available columns, but it always performs row-wise, and the order of rows to be sorted is inverted (i.e., from bottom to top) so its usage is a bit contrived, e.g.
– `a[np.lexsort(np.rot90(a))]` sorts by all columns in left-to-right order.



– `a[np.lexsort(np.rot90(a[:,[2,5]]))]` sorts by column 2 first and then (where the values in column 2 are equal) by column 5. An alternative form is `a[np.lexsort(np.flipud(a.T[[2,5]]))]`

Here `flipud` flips the matrix in the up-down direction (to be precise, in the `axis=0` direction, same as `a[::-1,...]`, where three dots mean "all other dimensions"— so it's all of a sudden `flipud`, not `fliplr`, that flips the 1D arrays) and `rot90` rotates the matrix in the positive direction (i.e., counter-clockwise) by 90 degrees. Both flips and rot90 return views



Both conversions are actually views, so they are fast and don't require any extra memory. But the functions `u2s` and `s2u` need to be imported first with the horrific `from numpy.lib.recfunctions import unstructured_to_structured as u2s, structured_to_unstructured as s2u`

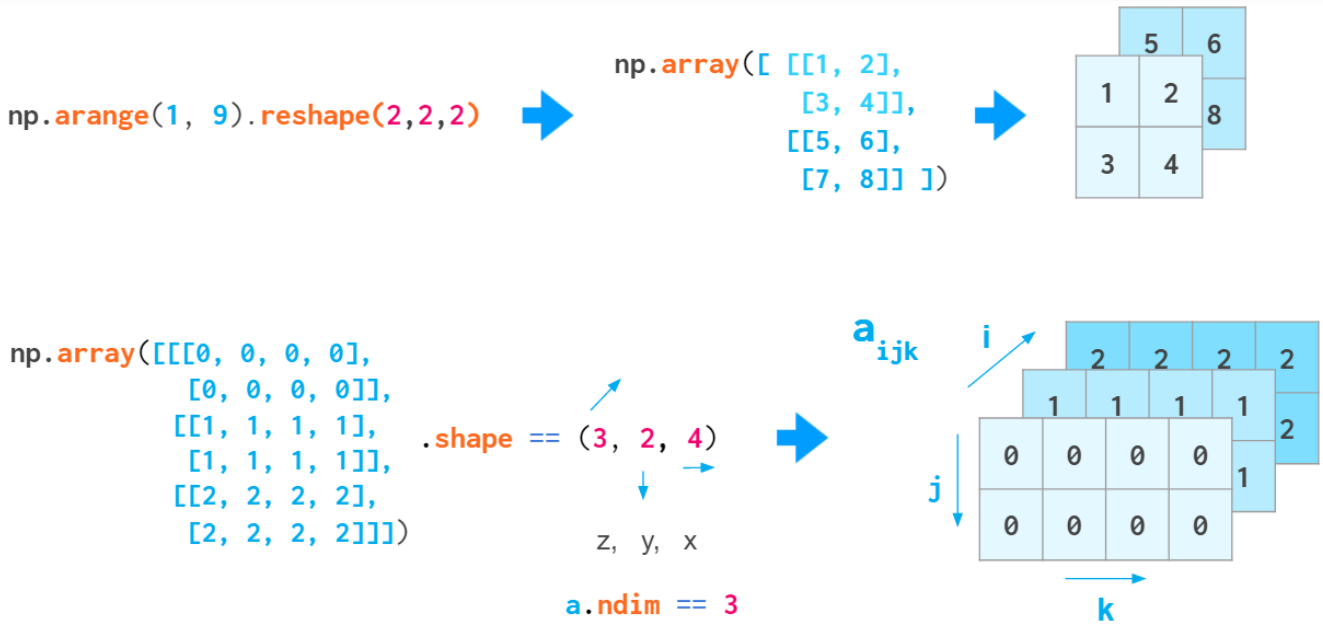
4. It might be a better option to do it in Pandas since this particular operation is more readable and less error-prone there:

– `pd.DataFrame(a).sort_values(by=[2,5]).to_numpy()` sorts by column 2, then by column 5.

– `pd.DataFrame(a).sort_values().to_numpy()` sorts by all columns in the left-to-right order.

3. 3D and Above

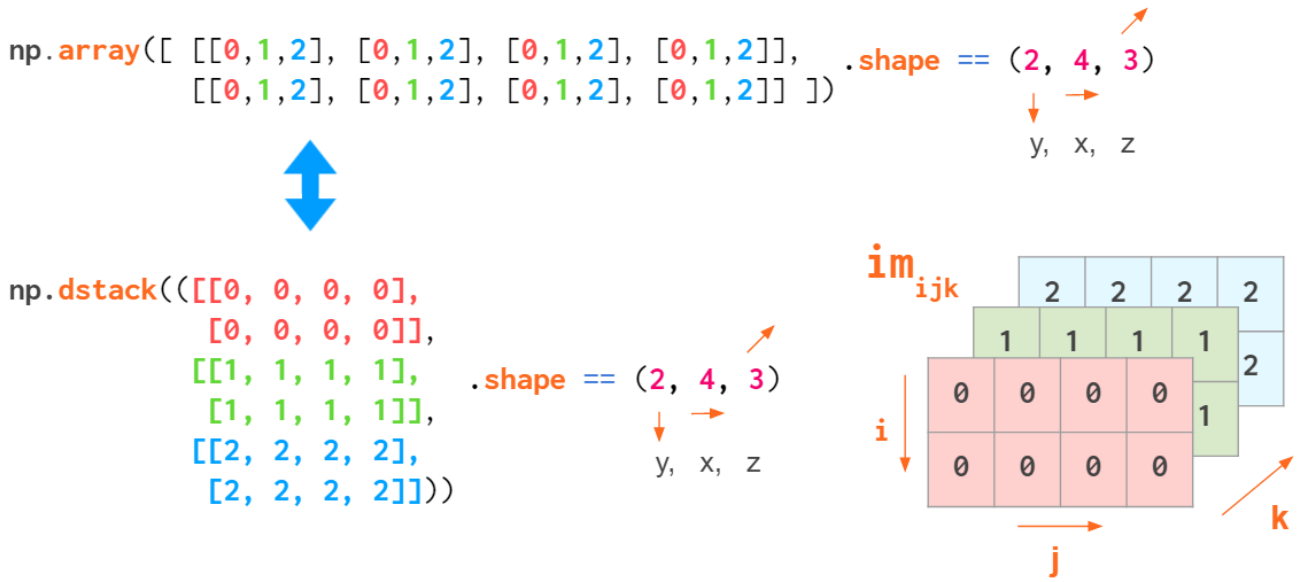
When you create a 3D array by reshaping a 1D vector or converting a nested Python list, the meaning of the indices is (z,y,x). The first index is the number of the plane, then the coordinates go in that plane:



Generic 3D arrays

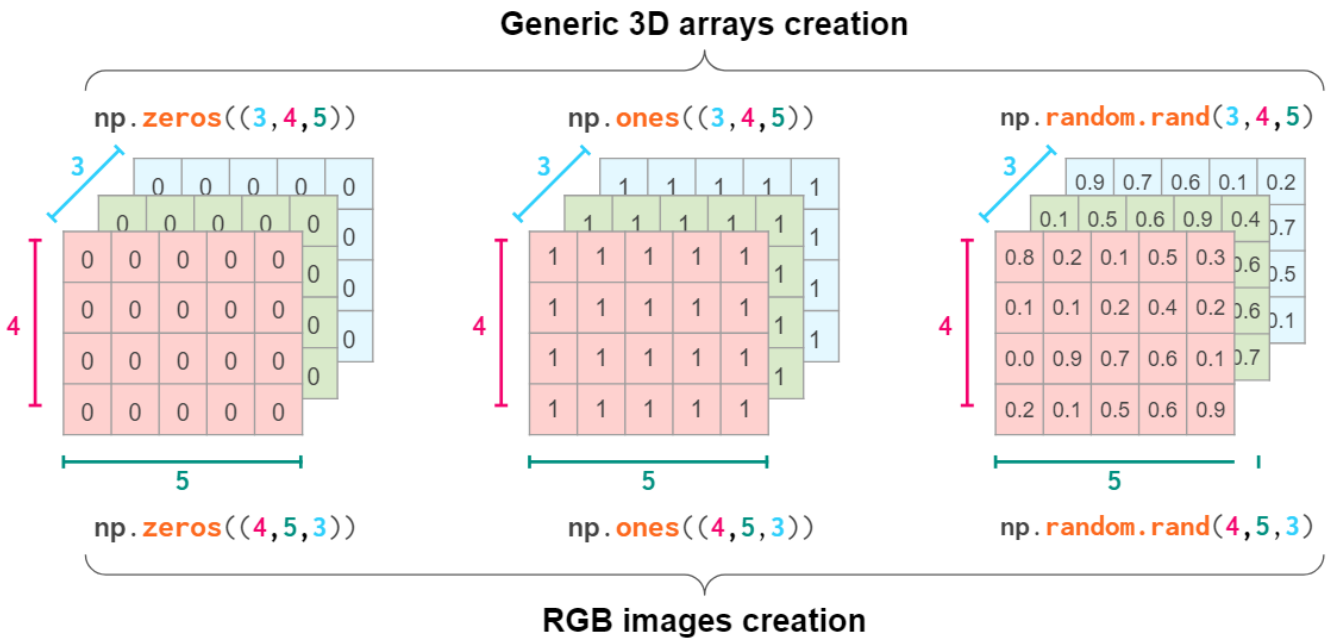
This index order is convenient, for example, for keeping a bunch of gray-scale images: `a[i]` is a shortcut for referencing the i-th image.

But this index order is not universal. When working with RGB images, the (y,x,z) order is usually used: First are two pixel coordinates, and the last one is the color coordinate (RGB in Matplotlib, BGR in OpenCV):

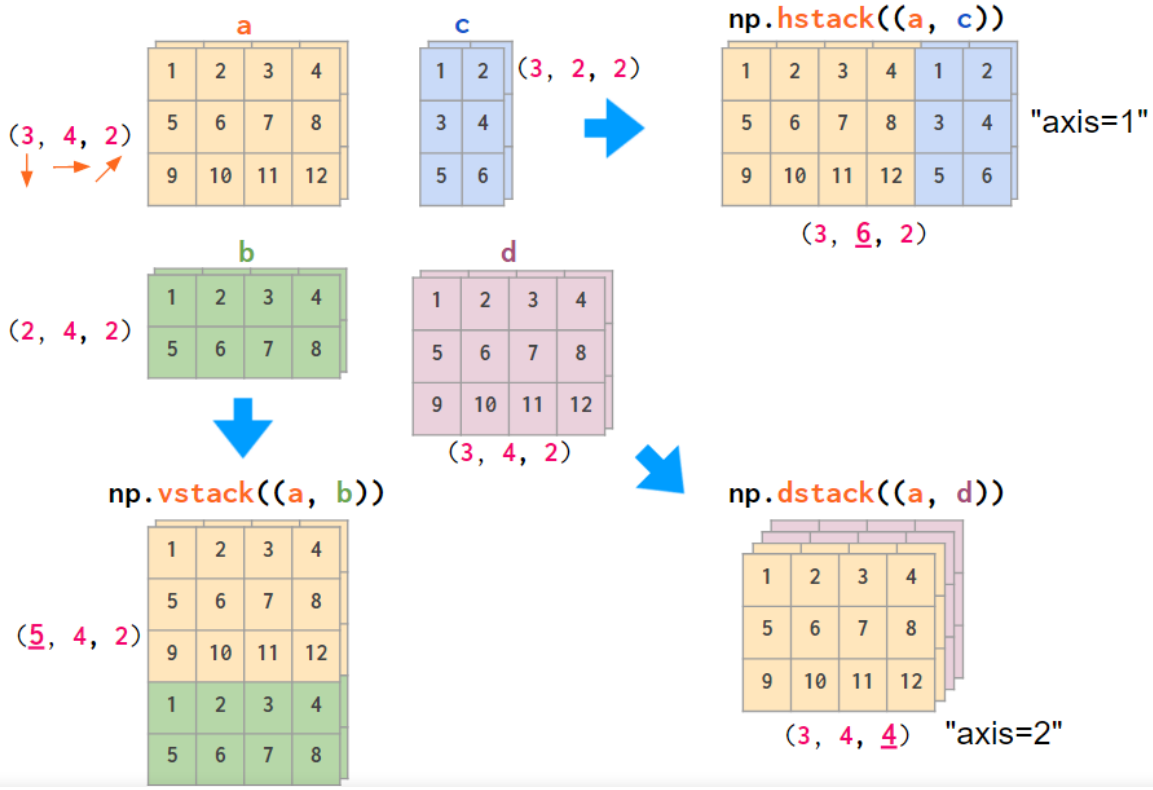


RGB images

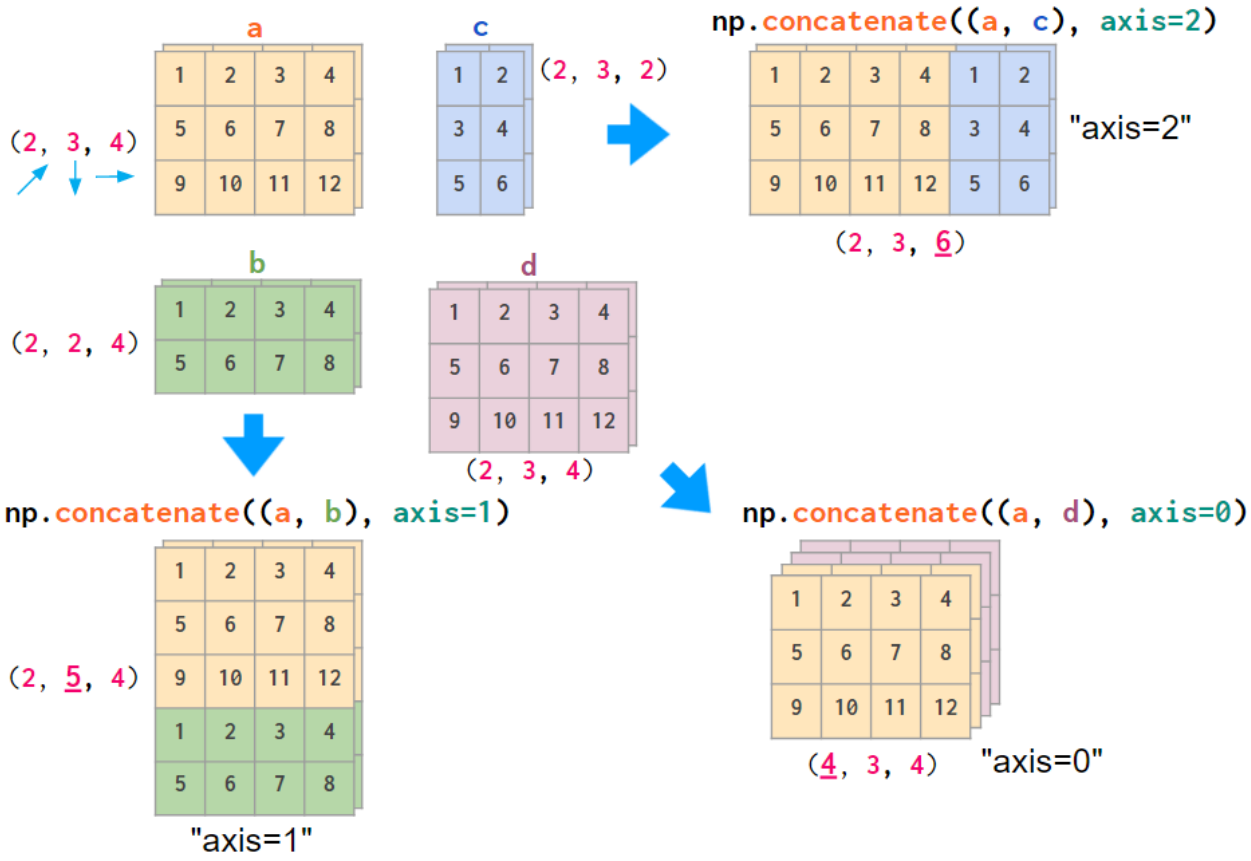
So the actual command to create a certain geometrical shape depends on the conventions of the domain you're working on:



Obviously, NumPy functions like `hstack`, `vstack`, or `dstack` are not aware of those conventions. The index order hardcoded in them is (y,x,z), the RGB images order:

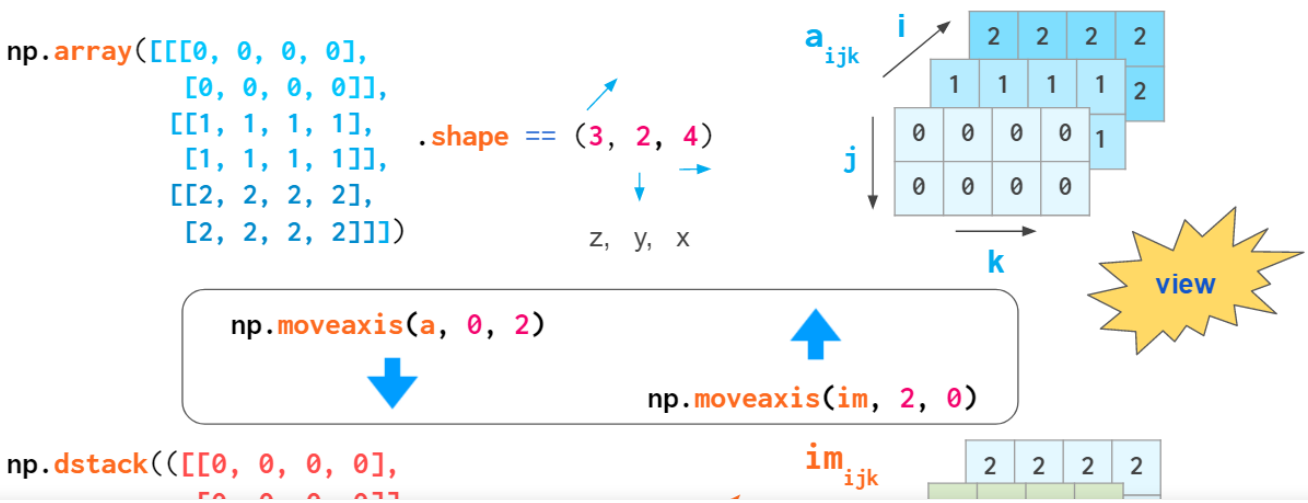


If your data is laid out differently, it is more convenient to stack images using the `concatenate` command, feeding it the explicit index number in an `axis` argument:



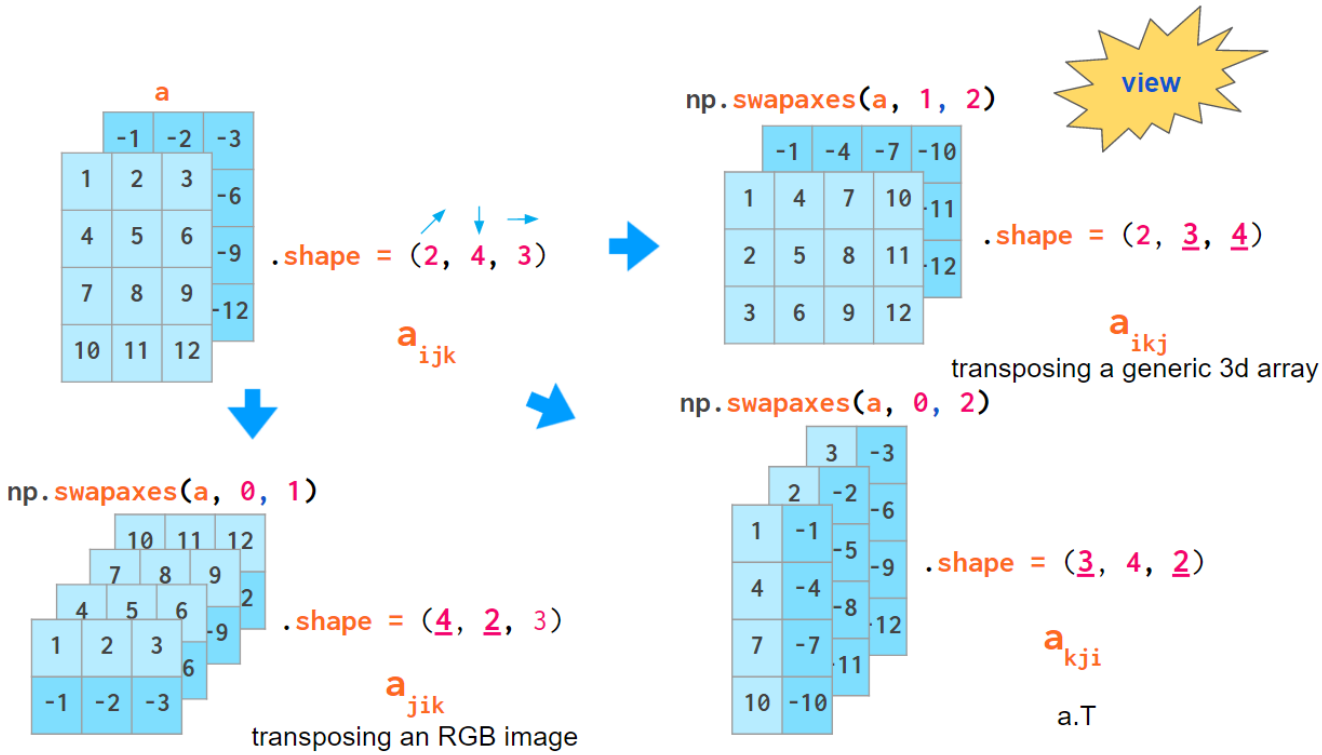
Stacking generic 3D arrays

If thinking in terms of axes numbers is not convenient to you, you can convert the array to the form that is hardcoded into `hstack` and co:



This conversion is cheap: No actual copying takes place; it just mixes the order of indices on the fly.

Another operation that mixes the order of indices is array transposition. Examining it might make you feel more familiar with 3D arrays. Depending on the order of axes you've decided on, the actual command to transpose all planes of your array will be different: For generic arrays, it is swapping indices 1 and 2, for RGB images it is 0 and 1:



Interesting though that the default `axes` argument for `transpose` (as well as the only `a.T` operation mode) reverses the index order, which coincides with neither of the index order conventions described above.

Broadcasting works with higher dimensions as well, see my note "Broadcasting in NumPy" for details.

And finally, here's a function that can save you a lot of Python loops when dealing with the multidimensional arrays and can make your code cleaner — `einsum` (Einstein summation):

Matrix multiplication

$$c_{ik} = \sum_j a_{ij} b_{jk}$$

```
c = np.einsum('ij,jk->ik', a, b)
```

Tensor multiplication

$$c_{ijlm} = \sum_k a_{ijk} b_{klm}$$

```
c = np.einsum('ijk,klm->ijlm', a, b)
```

It sums the arrays along the repeated indices. In this particular example `np.tensordot(a, b, axis=1)` would suffice in both cases, but in the more complex cases `einsum` might work faster and is generally easier to both write and read — once you understand the logic behind it.

If you want to test your NumPy skills, there's a tricky crowd-sourced set of 100 NumPy exercises[10] on GitHub.

Let me know (on reddit, hackernews, or twitter) if I have missed your favorite NumPy feature, and I'll try to fit it in!

References

1. Scott Sievert, NumPy GPU acceleration
2. Jay Alammar, A Visual Intro to NumPy and Data Representation
3. Big-O Cheat Sheet site
4. Python Time Complexity wiki page
5. NumPy Issue #14989, Reverse param in ordering functions
6. NumPy Issue #2269, First nonzero element
7. Numba library homepage

10. 100 NumPy exercises on GitHub

License