A nicer numpy

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What is this about?

Two libraries to make working in numpy nicer.

- These are public tools, available for some years
- Installable from Debian and related distros.
- Python2 and Python3 both supported

numpysane (`https://github.com/dkogan/numpysane`)

- Provides some routines to improve core functionality
- These are new functions, so there're no compatibility concerns

gnuplotlib (`https://github.com/dkogan/gnuplotlib`)

- Plotting
- Does a similar thing as `matplotlib` but (I claim) better

What's wrong with numpy?

- Some core functionality is mysterious and unintuitive
- Things work as expected *only* with 2-dimensional arrays, no more and no less

Areas addressed by `numpysane`:

- Nicer array manipulation
- Nicer basic linear algebra routines
- Better broadcasting support

Mostly stolen from the PDL project

Matrix concatenation

Basic example: stick two identical 2D arrays together to extend each row

- The docs say to use `hstack()`

Let's try it:

```
>>> import numpy as np
>>> arr32 = np.arange(3*2).reshape(3,2)
>>> print(arr32)
[[0 1]
 [2 3]
 [4 5]]

>>> print(arr32.shape)
(3, 2)
```

Matrix concatenation

What do we expect `hstack(arr32,arr32)` to do?

```
[[0 1 0 1]
 [2 3 2 3]
 [4 5 4 5]]
```

or

```
[[0 1]
 [2 3]
 [4 5]
 [0 1]
 [2 3]
 [4 5]]
```

?

Matrix concatenation

This was a trick question. Here's what it does:

```
>>> np.hstack(arr32,arr32)
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
TypeError: hstack() takes 1 positional argument ...
    ... but 2 were given
```

Apparently `hstack()` wants an iterable of the arguments, instead of the arguments themselves

Matrix concatenation

Fine. Here's what it does if you feed it what it wants:

```
>>> print(np.hstack((arr32,arr32)))
[[0 1 0 1]
 [2 3 2 3]
 [4 5 4 5]]
```

That makes sense! Looks "horizontal".

Matrix concatenation

What if I don't feed it strictly 2D matrices?

```
>>> arr132 = np.arange(3*2).reshape(1,3,2)
>>> print(arr132)
[[[0 1]
  [2 3]
  [4 5]]]

>>> print(arr132.shape)
(1, 3, 2)
```

Matrix concatenation

Same question as before: what do we expect `hstack((arr132,arr132))` to do?

```
[[[0 1 0 1]
  [2 3 2 3]
  [4 5 4 5]]]
```

or

```
[[[0 1]
  [2 3]
  [4 5]
  [0 1]
  [2 3]
  [4 5]]]
```

or something else?

Matrix concatenation

Here's what it does:

```
>>> print(np.hstack((arr132,arr132)))
[[[0 1]
  [2 3]
  [4 5]
  [0 1]
  [2 3]
  [4 5]]]

>>> np.hstack((arr132,arr132)).shape
(1, 6, 2)
```

Whoa. That is *not* horizontal at all! I would have expected a result with shape `(1,3,4)`

Matrix concatenation

What if I give it 1-dimensional arrays?

```
>>> arr3  = np.arange(3)
>>> arr13 = np.arange(3).reshape(1,3)
>>> print(arr3)
[0 1 2]

>>> arr3.shape
(3,)

>>> print(arr13)
[[0 1 2]]

>>> arr13.shape
(1, 3)
```

Matrix concatenation

```
>>> np.hstack((arr3,arr3)).shape
(6,)

>>> np.hstack((arr13,arr13)).shape
(1, 6)

>>> np.hstack((arr13,arr3)).shape
ValueError: all the input arrays must have ...
    ... same number of dimensions
```

- Do the stacking functions want the dimension counts to match up, or something?

Well, no:

```
>>> np.vstack((arr13,arr3))
[[0 1 2]
 [0 1 2]]
```

Matrix concatenation

So what's wrong?

- numpy is inconsistent about which is the most significant dimension in an array

There's an arbitrary design choice that must be made: if I stack `N` arrays of shape `(A,B,C)` into a new array, do I get

1. an array of shape `(N,A,B,C)` or
2. an array of shape `(A,B,C,N)`?

Most of numpy makes the *first* choice, but some of it (concatenation functions most notably) makes the second choice

Dimensionality example

Example:

- Let's say I have a 1-dimensional array containing simultaneous temperature measurements at different locations:

```
>>> print(T1)
[ t_where0 t_where1 t_where2 ... ]

>>> print(T1.shape)
(Nlocations,)
```

We have one dimension, so the locations are indexed by `axis = 0` and `axis = -1`. These are the same axis.

Dimensionality example

Now, let's say I measured all the temperatures multiple times throughout the day, and I record the measurements into a joint array T2.
I have a choice:

```
>>> print(T2.shape)
(Ntimes,Nlocations)
```

or

```
>>> print(T2.shape)
(Nlocations,Ntimes)
```

?

Dimensionality example

When I extend `T1` into `T2` I want consistent printing:
The dimensions printed horizontally and vertically should not change
I.e. I want this:

```
>>> print(T2)
[[ t_when0where0 t_when0where1 t_when0where2 ... ]
 [ t_when1where0 t_when1where1 t_when1where2 ... ]
 ...]

>>> print(T2.shape)
(Ntimes, Nlocations)
```

This way each horizontal row describes *one* point in time and *multiple* locations, just like when printing `T1`

Dimensionality example

When I extend `T1` into `T2` I want consistent indexing:
The axis index corresponding to locations should not change

- For `T1`, locations are in `axis = 0` and `axis = -1` (same axis)
- For `T2`, locations are in `axis = 1` and `axis = -1` (same axis)

So counting *from the back* gives me consistency, and I want to always use `axis = -1`
Thus I want

- The *first* concatenation option: stacking `N` arrays of shape `(A,B,C)` produces an array of shape `(N,A,B,C)`
- All axes to be indexed from the end. Always.

Dimensionality example

If we really wanted to index the axes from the front while remaining self-consistent, numpy could do what PDL does:

- the horizontally-printed dimension is the *first* dimension
- `N` arrays of shape `(A,B,C)` produce an array of shape `(A,B,C,N)`

But then a core convention of linear algebra would be violated: a matrix of `N` rows and `M` columns would have shape `(M,N)`. Can't please everybody.

Matrix concatenation: conclusion

So why are `hstack()` and friends weird?

- Because `hstack()` tries to concatenate along `axis = 1`, while it should use `axis = -1`
- This works for 2D arrays (and 1D arrays because of special-case logic in `hstack()`), but not for others

Many other core functions in numpy have this issue, and routines in `numpysane` do this in a consistent and predictable way.

Matrix concatenation with numpysane

There are two functions, both stolen from the PDL project.

- `glue()` concatenates any N arrays along the given axis
- `cat()` concatenates N arrays along a new outer dimension

These both add leading length-1 dimensions to the input as needed: "something" is logically equivalent to "1 of something". This is one of the *broadcasting* rules I'll get to in a bit

Matrix concatenation with numpysane

`nps.glue()` works as expected:

```
>>> import numpysane as nps

>>> nps.glue(arr32, arr32,  axis=-1).shape
(3, 4)

>>> nps.glue(arr32, arr32,  axis=-2).shape
(6, 2)

>>> nps.glue(arr132,arr132, axis=-1).shape
(1, 3, 4)

>>> nps.glue(arr13, arr3,   axis=-1).shape
(1, 6)

>>> nps.glue(arr13, arr3,   axis=-2).shape
(2, 3)
```

Matrix concatenation with numpysane

`nps.cat()` works as expected too. It always adds a new leading dimension

```
>>> nps.cat(arr32,arr32).shape
(2, 3, 2)

>>> nps.cat(arr132,arr32).shape
(2, 1, 3, 2)
```

Matrix multiplication

The funny business extends to other core areas of numpy. For instance multiplying matrices is non-trivial

- Up until numpy 1.10.0 `np.dot()` was the function for that, and it is surprising in all sorts of ways (which should be expected since a "dot product" is not the same thing as "matrix multiplication")
- In 1.10.0 we got `np.matmul`, which is *much* better, but even then it has strange corners. Trying to compute an outer product:

```
>>> a = np.arange(5).reshape(5,1)
>>> b = np.arange(3)

>>> np.matmul(a,b)
ValueError: matmul: Input operand 1 has a mismatch in
   its core dimension 0, with gufunc signature
   (n?,k),(k,m?)->(n?,m?) (size 3 is different from 1)
```

Matrix multiplication with numpysane

numpysane provides its own `matmult()` routine that does what one expects:

```
>>> nps.matmult(a,b).shape

(5, 3)
```

There're many more functions in numpysane in this area. Everything's documented, and I'd like to move on to. . .

Broadcasting

What is broadcasting?

- *Broadcasting* is a generic way to vectorize functions
- A broadcasting-aware function has a *prototype*: it knows the dimensionality of its inputs and of its outputs
- When calling a broadcasting-aware function, any extra dimensions in the input are automatically used for vectorization

Broadcasting: an example

This is best described with an example: a broadcasting-aware inner product. An inner product (also known as a dot product) is a function that

- takes in two identically-sized 1-dimensional arrays
- outputs a scalar

`inner( [ 1 2 3 4], [1 2 3 4] )` $\rightarrow$ 30

Broadcasting: an example

If one calls a broadcasting-aware inner product (such as `nps.inner()`) with two arrays of shape (2,3,4) as input, it would

- compute 6 inner products of length-4 each
- report the output in an array of shape (2,3)

Because `nps.inner()` knows the dimensionality of its inputs and of its outputs, it can figure out how to parse the input arrays

Broadcasting: an example

```
>>> a234 = np.arange(2*3*4).reshape(2,3,4)

>>> print(a234)
[[[ 0  1  2  3]
  [ 4  5  6  7]
  [ 8  9 10 11]]

 [[12 13 14 15]
  [16 17 18 19]
  [20 21 22 23]]]

>>> print(nps.inner(a234,a234))
[[  14  126  366]
 [ 734 1230 1854]]
```

The values in the output are `inner([0,1,2,3], [0,1,2,3])` and `inner([4,5,6,7],[4,5,6,7])` and so on.

Broadcasting rules

In short:

- Line up the shapes of the inputs to their *trailing* dimensions
- Match the trailing dimensions with the expected shapes of the inputs
- Any leading dimensions left over are used for vectorization
- The extra leading dimensions must be compatible across all the inputs. This means that each leading dimension must either
  - equal 1
  - be missing (thus assumed to equal 1)
  - equal to some positive integer >1, consistent across all arguments
- The leading dimensions of the inputs determine the shape of the output

Broadcasting: more involved example

Let's say we have a function with

- input prototype `( (3,), ('n',3), ('n',), ('m',) )`
- output prototype `('n','m')`

Given inputs of shape

```
(1,5,    3)
(2,1,  8,3)
(        8)
(  5,    9)
```

the broadcasting logic will set `n = 8` and `m = 9`.
The call will then return an output array of shape `(2,5,8,9)`

OK, so what about broadcasting?

In stock numpy, broadcasting is documented, but

- it is sparse and incomplete
- little end-user awareness that it exists

`numpysane` provides routines to add broadcasting awareness

- to any python function (via a decorator)
- to any C function (via generated C code that produces an extension module)

Broadcasting: an example

Let's write a broadcasting-aware inner product.

```
import numpysane as nps
@nps.broadcast_define( (('n',), ('n',)), () )
def inner(a,b):
    # We could use numpy for this: return a.dot(b)
    sum = 0.
    for i in range(len(a)): sum += a[i]*b[i]
    return sum
```

Broadcasting: an example

- We had a function `inner(a,b)` that computes *one* inner product. It knows nothing about vectorization
- And it assumes that `a` and `b` are 1-dimensional arrays of the same length
- Then we applised the `nps.broadcast_define()` decorator to add broadcasting awareness
- The decorator is told about the number of input and outputs and all of their expected dimensions
- The internal `nps.broadcast_define()` machinery ensures that the dimensions of the given inputs and outputs match. If not, it raises an exception
- If we call `inner()` with higher-dimensional input, we'll get multiple inner products computed, and an array of output returned

Broadcasting: an example

So we can give it two arrays, and get inner products of each corresponding row:

```
>>> a234 = np.arange(2*3*4).reshape(2,3,4)

>>> print(inner(a234,a234).shape)
(2,3)
```

Or we can compute the inner product of some arbitrary vector and each row of one array:

```
>>> a234 = np.arange(2*3*4).reshape(2,3,4)
>>> a4   = np.arange(4)

>>> print(inner(a234,a4).shape)
(2,3)
```

Broadcasting: summary

- This is a very powerful technique. The `nps.broadcast_define()` decorator is written in Python and wraps Python code. With lots of iterations this is *slow*.
- A much faster analogue exists in C: `nps.numpysane_pywrap()`. The iteration code and the code for the inner function are all in C, so this is fast. Please see the documentation for more detail.
- A stock numpy broadcasting-in-C API exists: `https://docs.scipy.org/doc/numpy-1.13.0/reference/c-api.generalized-ufuncs.html`
  I found this after implementing my own, and have not tried it.

Plotting: gnuplotlib

Let's switch gears, and talk about plotting.

- As with the numpy core, there's a dominant choice here: matplotlib
- I'm not aware of any *major* issues: if it's not pissing you off right now, there probably isn't a lot of reason to switch to my library

However, matplotlib ...

- is python-specific
- is slow
- has a weird API
- is missing useful interactivity

Plotting: gnuplotlib

`gnuplotlib`: a plotting library for numpy

- Uses `gnuplot` as the plotting backend, so
  - The plots look and feel like `gnuplot` plots have for decades
  - It's fast
  - Lots of features and backends available
- Has a reasonable API (I claim)
- A direct port of `PDL::Graphics::Gnuplot`

Plotting: gnuplotlib design choices

One `plot()` function does everything

- Can still build up the plot components programmatically: using python

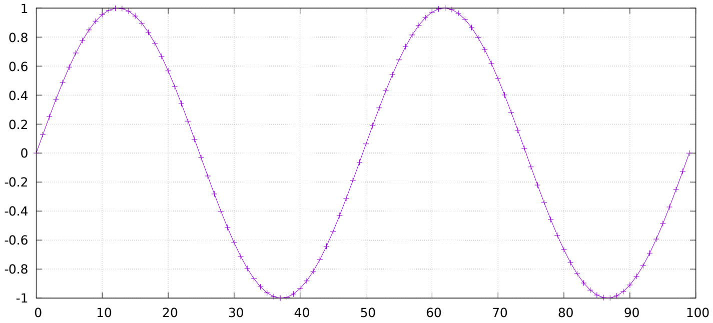
`gnuplotlib` is a thin shim

- strings are passed to `gnuplot` verbatim (like in `feedgnuplot`)
- so we get a powerful library and a friendly learning curve

Plotting: gnuplotlib: a *very* brief tutorial

To plot something, just call plot:

```
import numpy      as np
import numpysane  as nps
import gnuplotlib as gp
th = np.linspace(-2.*np.pi, 2.*np.pi, 100)
gp.plot(np.sin(th))
```



Plotting: gnuplotlib: a *very* brief tutorial

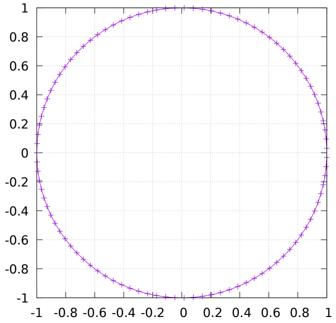
```
import numpy      as np
import numpysane  as nps
import gnuplotlib as gp
th = np.linspace(-2.*np.pi, 2.*np.pi, 100)
gp.plot(np.sin(th))
```

- We're plotting in 2D, so default is `tuplesize=2` arrays
- We gave it just 1 array, so integers 0,1,2,... were used for the x

Plotting: gnuplotlib: a *very* brief tutorial

- We can pass in 2 arrays to make an x-y plot:

```
th = np.linspace(-np.pi, np.pi, 100)
gp.plot(np.cos(th), np.sin(th), square = True)
```



Plotting: gnuplotlib: a *very* brief tutorial

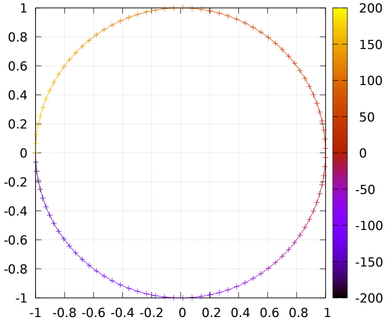
```
th = np.linspace(-np.pi, np.pi, 100)
gp.plot(np.cos(th), np.sin(th), square = True)
```

- We passed in *two* arrays
- We also passed in `square = True`. This is a *plot option* to autoscale the x and y axes evenly. Otherwise the circle will looks like an ellipse

Plotting: gnuplotlib: a *very* brief tutorial

- It's possible to have more values per point. For instance:

```
th = np.linspace(-np.pi, np.pi, 100)
gp.plot(np.cos(th), np.sin(th),
        # The angle (in degrees) is shown as the color
        th * 180./np.pi,
        tuplesize = 3,
        _with     = 'linespoints palette',
        square    = True)
```



Plotting: gnuplotlib: a *very* brief tutorial

```
th = np.linspace(-np.pi, np.pi, 100)
gp.plot(np.cos(th), np.sin(th),
        # The angle (in degrees) is shown as the color
        th * 180./np.pi,
        tuplesize = 3,
        _with     = 'linespoints palette',
        square    = True)
```

- The style `linespoints palette` is given to gnuplot directly. `gnuplotlib` doesn't know what that means
- `tuplesize=3` tells `gnuplotlib` that there are 3 values per point. Because of `palette`, these will be interpreted as x,y,color
- The `gnuplot` documentation talks in detail about what kind of input each style expects

Plotting: gnuplotlib: a *very* brief tutorial

An explicit invocation of `plot()` looks like this:

```
plot( curve, curve, ..., plot_options )
```

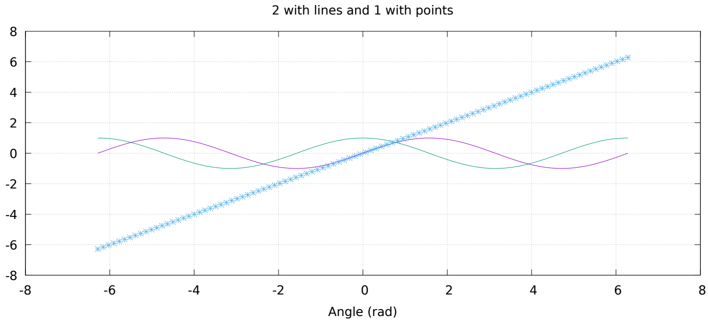
where each `curve` is a `tuple`:

```
curve = (array, array, ..., curve_options)
```

- *plot options* apply to the whole plot, and are given as keyword args to `plot()`
- *curve options* apply to each separate curve (dataset); given in a `dict()` in the end of each `curve` tuple. Or defaults given in the `plot()` kwargs
- If we have one dataset, we can inline the tuples, like we did above

Plotting: gnuplotlib: a *very* brief tutorial

```
th = np.linspace(-2.*np.pi, 2.*np.pi, 100)
gp.plot( ( th, np.sin(th), ),
         ( th, np.cos(th), ),
         ( th, th, dict(_with = 'points ps 1') ),
         _with = 'lines',
         xlabel = "Angle (rad)",
         title  = "2 with lines and 1 with points")
```



Plotting: gnuplotlib: a *very* brief tutorial

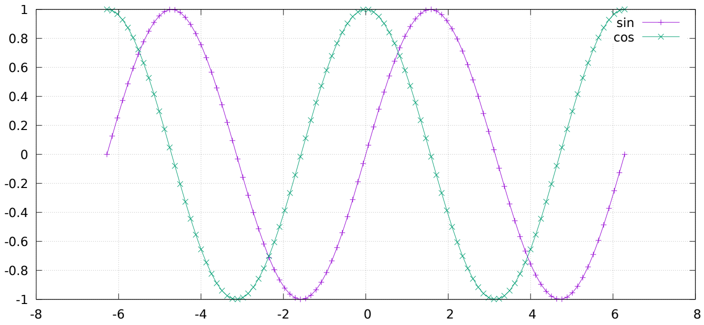
```
th = np.linspace(-2.*np.pi, 2.*np.pi, 100)
gp.plot( ( th, np.sin(th), ),
         ( th, np.cos(th), ),
         ( th, th, dict(_with = 'points ps 1') ),
         _with = 'lines',
         xlabel = "Angle (rad)",
         title  = "2 with lines and 1 with points")
```

- We passed in 3 tuples, one for each dataset
- We passed in the `xlabel` plot option to label the x axis
- We passed in the `title` plot option to title the plot
- We passed in the default `with` curve option: `lines`
- 2/3 datasets don't set their own `with`, so they use `lines`
- 1/3 plots with `points ps 1` instead. `gnuplotlib` doesn't know what that is, but `gnuplot` knows that `ps` is a synonym for `pointsize`

Plotting: gnuplotlib: a *very* brief tutorial

- Broadcasting is fully supported:

```
th = np.linspace(-2.*np.pi, 2.*np.pi, 100)
gp.plot( th,
         nps.cat(np.sin(th),
                 np.cos(th)),
         legend = np.array( ("sin", "cos"), ) )
```



Plotting: gnuplotlib: a *very* brief tutorial

```
th = np.linspace(-2.*np.pi, 2.*np.pi, 100)
gp.plot( th,
         nps.cat(np.sin(th),
                 np.cos(th)),
         legend = np.array( ("sin", "cos"), ) )
```

- I plotted two datasets, but didn't use tuples
- Using default `tuplesize=2`, and gave it two arrays:
  - First array has the expected shape of `(100,)`
  - Second array has the shape `(2,100)`
- This thus broadcasts: I get two plots: `sin(th)` vs `th` and `cos(th)` vs `th`
- curve options broadcast too: I have it two different `legend` options, and `gnuplotlib` knows to use each one for the two datasets

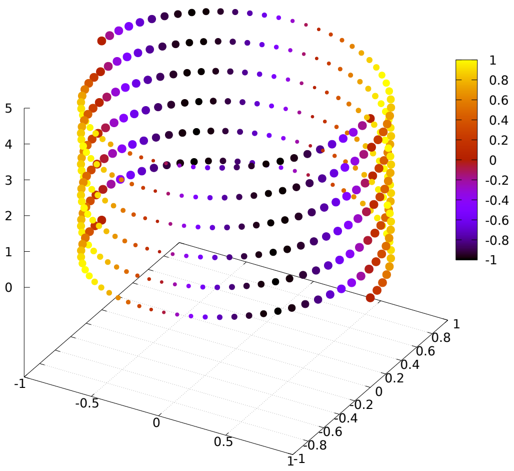
Plotting: gnuplotlib: a *very* brief tutorial

- What does this do?

```
th    = np.linspace(0, 6*np.pi, 200)
z     = np.linspace(0, 5,       200)
size  = 0.5 + np.abs(np.cos(th))
color = np.sin(2*th)

gp.plot3d( np.cos(th) * nps.transpose(np.array((1,-1))),
           np.sin(th) * nps.transpose(np.array((1,-1))),
           z,
           size,
           color,
           tuplesize = 5,
           _with = 'points ps variable pt 7 palette',
           squarexy = True)
```

Plotting: gnuplotlib: a *very* brief tutorial



Plotting: gnuplotlib

That's it for the overview. Lots of examples in the guide:

- `https://github.com/dkogan/gnuplotlib/blob/master/guide/guide.org`

The API docs are on the main page:

- `https://github.com/dkogan/gnuplotlib`

Thanks for listening!

The documentation and sources and links to this talk:

- `https://github.com/dkogan/numpysane`
- `https://github.com/dkogan/gnuplotlib`

Or you can

```
apt install python3-numpysane python3-gnuplotlib
```