Scientific Programming with the SciPy Stack

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https://github.com/scw/scipy-devsummit-2017-talk

High Quality PDF (5MB)

Resources Section

Scientific Computing

Scientific Computing

The application of computational methods to all aspects of the process of scientific investigation – data acquisition, data management, analysis, visualization, and sharing of methods and results.

Extending ArcGIS

- ArcGIS is a *system of record*. Combine data and analysis from many fields and into a common environemnt.
- Why extend? Can't do it all, we support over 1000 GP tools — enabling *integration* with other environments to extend the platform.

Python

Why Python?

- Accessible for new-comers, and the most taught first language in US universites
- Extensive package collection (56k on PyPI), broad user-base
- Strong glue language used to bind together many environments, both open source and commercial
- Open source with liberal license — do what you want

- Brand new to Python? This talk may be challenging
- Resources include materials that for getting started

Python in ArcGIS

- Python API for driving ArcGIS Desktop and Server
- A fully integrated module: `import arcpy`
- Interactive Window, Python Addins, Python Tooboxes
- Extensions:
  - Spatial Analyst: `arcpy.sa`
  - Map Document: `arcpy.mapping`
  - Network Analyst: `arcpy.na`
  - Geostatistics: `arcpy.ga`
  - Fast cursors: `arcpy.da`
- ArcGIS API for Python

Python in ArcGIS

- Python 3.5 in Pro (Desktop vs Pro Python)
  - `arcpy.mp` instead of `arcpy.mapping`
- Continue to add modules: NetCDF4, xlrd, xlwt, PyPDF2, dateutil, pip
- Python raster function, with a repository of examples using SciPy for on the fly visualizations

Python in ArcGIS

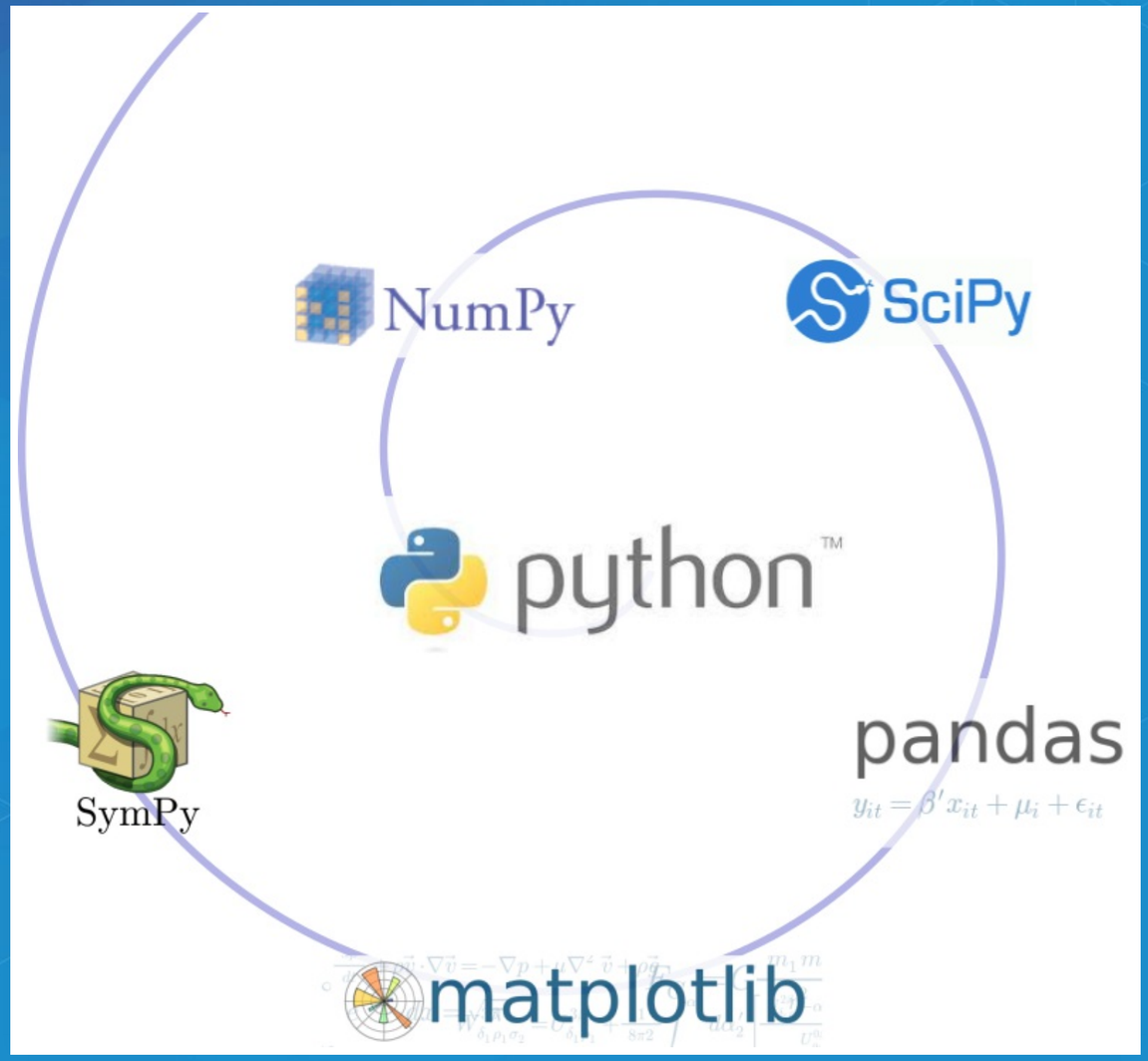
- Here, focus on SciPy stack, what's included out of the box
- Move toward maintainable, reusable code and beyond the "one-off"
- Recurring theme: multi-dimensional data structures
- Also see Brendan Collins talk tomorrow which covers dask

SciPy

Why SciPy?

- Most languages don’t support things useful for science, e.g.:
  - Vector primitives
  - Complex numbers
  - Statistics
- Object oriented programming isn’t always the right paradigm for analysis applications, but is the only way to go in many modern languages
- SciPy brings the pieces that matter for scientific problems to Python.

SciPy Stack


NumPy
SciPy
python
SymPy
pandas
$y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$
matplotlib

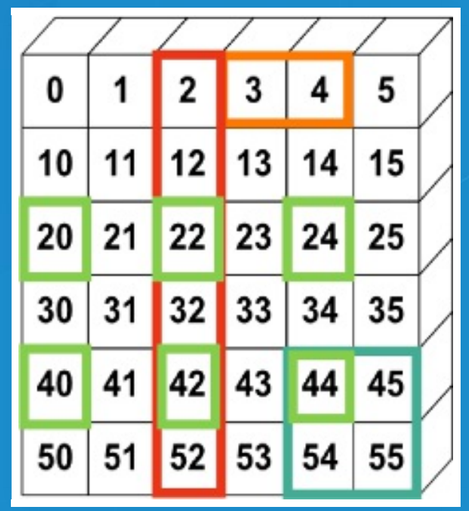
Included SciPy

Package	KLOC	Contributors	Stars
matplotlib	118	441	4909
Nose	7	75	1053
NumPy	236	429	4011
Pandas	183	408	8765
SciPy	387	387	2930
SymPy	243	443	3642
Totals	1174	1885	

Testing with Nose

- Nose — a Python framework for testing
- Tests improve your productivity, and create robust code
- Nose builds on unittest framework, extends it to make testing easy.
- Plugin architecture, includes a number of plugins and can be extended with third-party plugins.

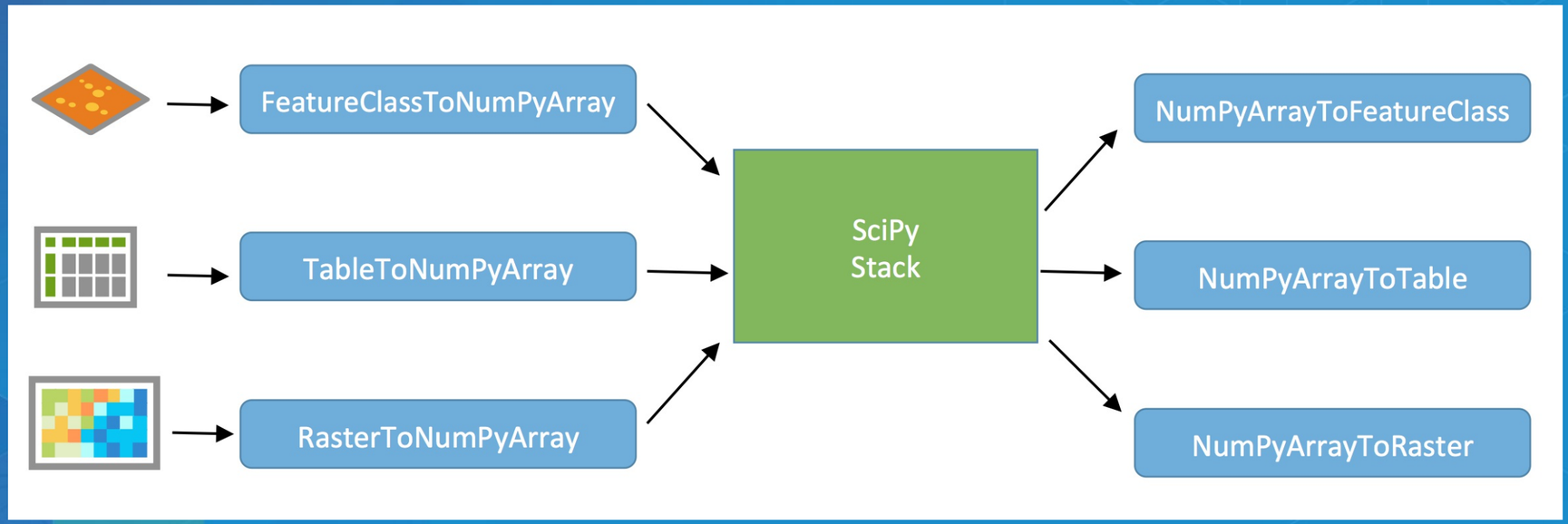
1. An array object of arbitrary homogeneous items
2. Fast mathematical operations over arrays
3. Random Number Generation



ArcGIS + NumPy

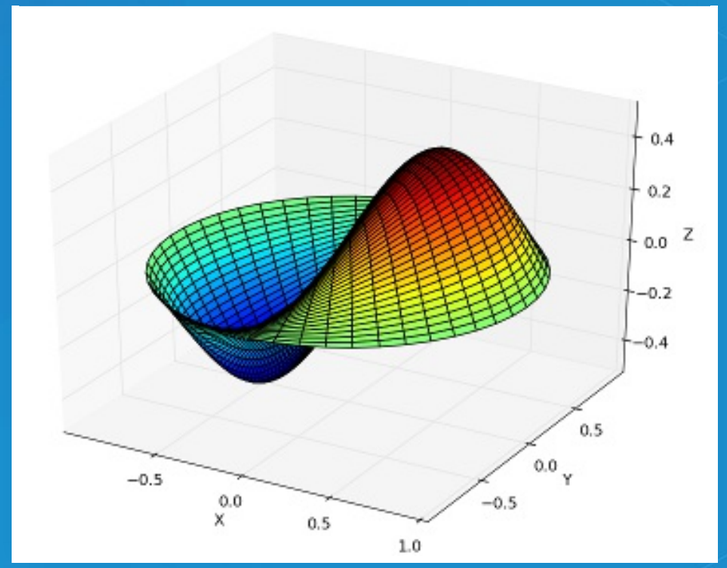
- ArcGIS and NumPy can interoperate on raster, table, and feature data.
- See Working with NumPy in ArcGIS
- In-memory data model. Example script to process by blocks if working with larger data.

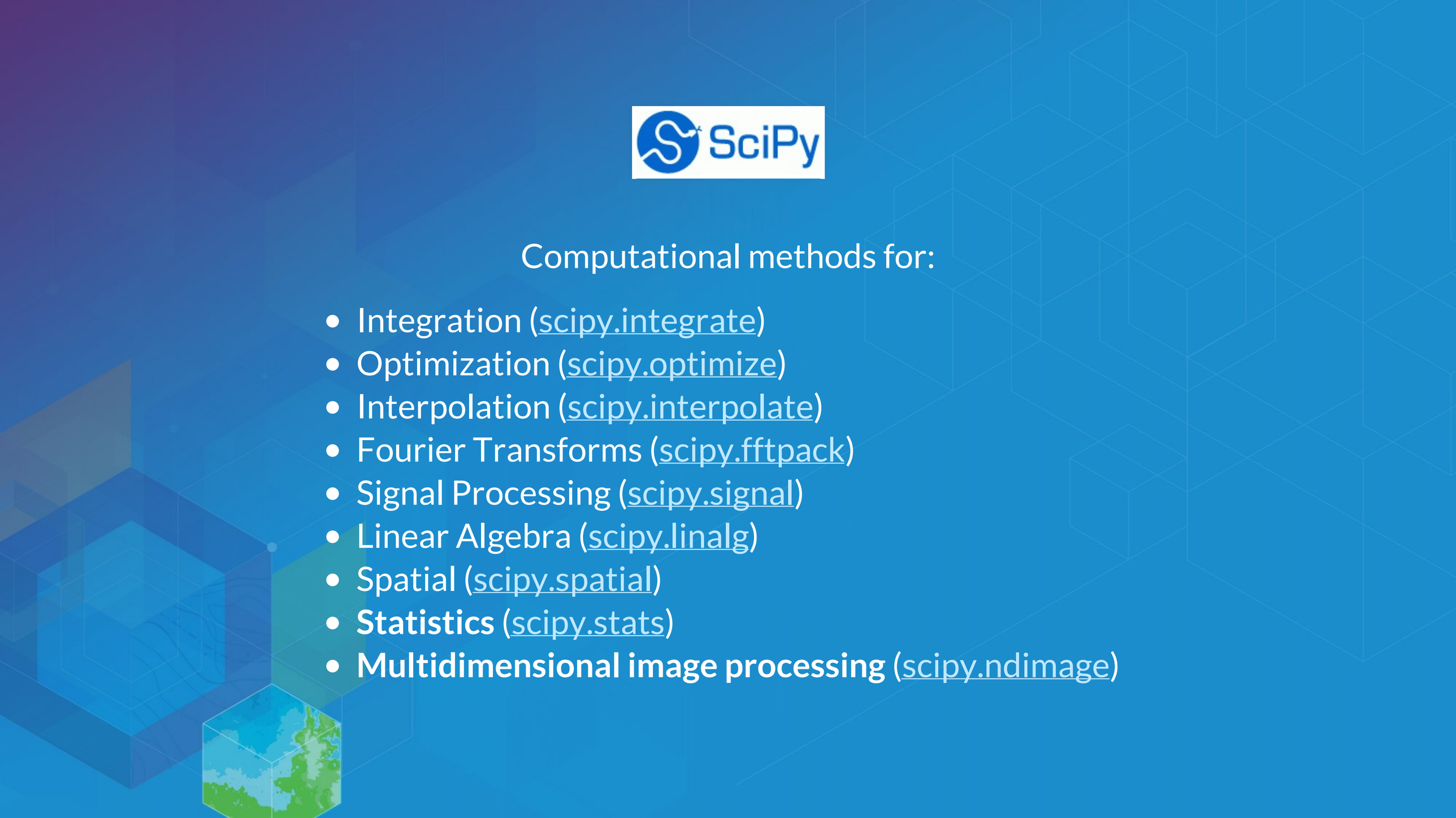
ArcGIS + NumPy



matplotlib

- Plotting library and API for NumPy data
- Matplotlib Gallery





Computational methods for:

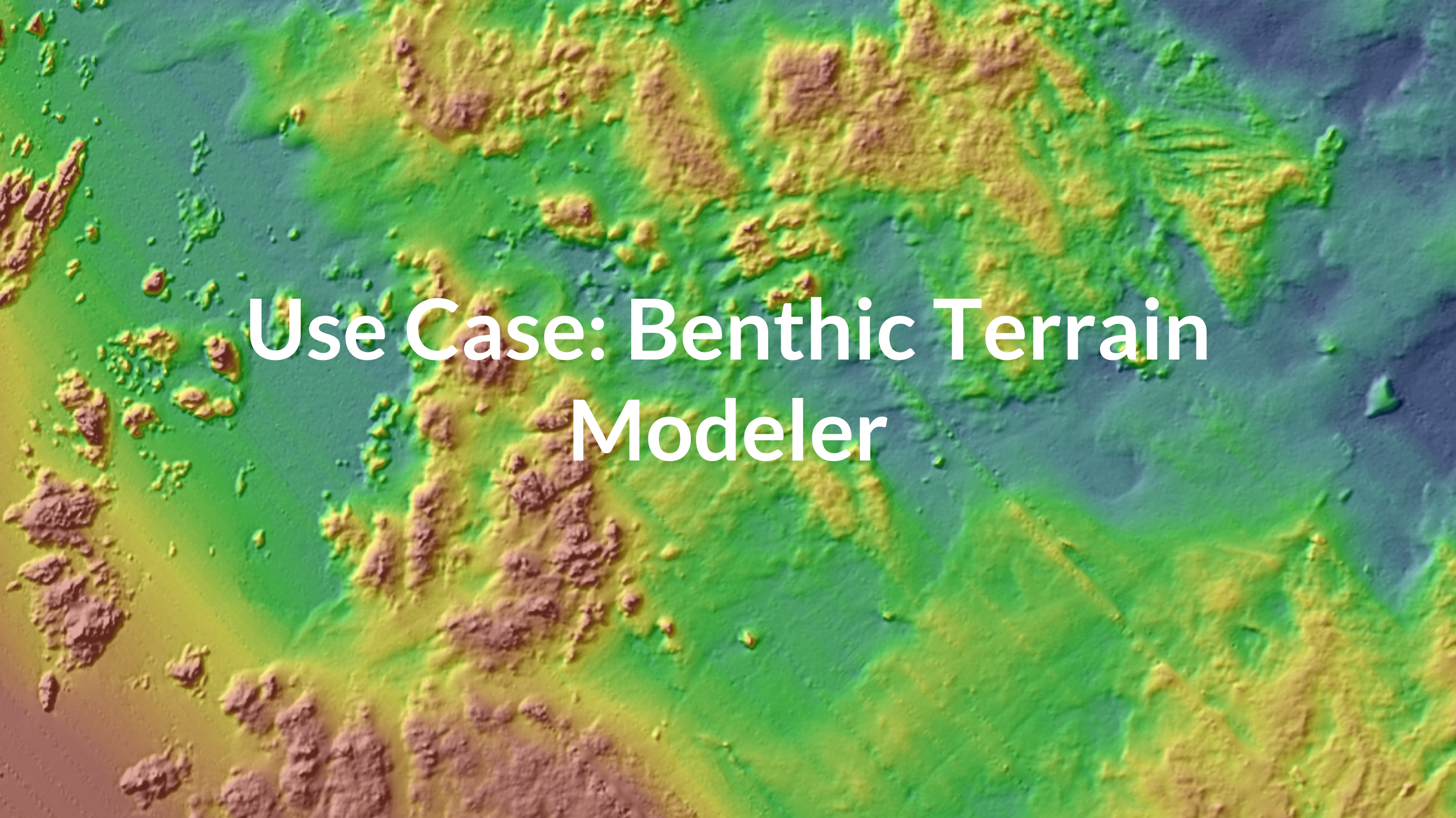
- Integration (scipy.integrate)
- Optimization (scipy.optimize)
- Interpolation (scipy.interpolate)
- Fourier Transforms (scipy.fftpack)
- Signal Processing (scipy.signal)
- Linear Algebra (scipy.linalg)
- Spatial (scipy.spatial)
- **Statistics** (scipy.stats)
- **Multidimensional image processing** (scipy.ndimage)

SciPy: Geometric Mean

- Calculating a geometric mean of an *entire raster* using SciPy (source)

$$\left(\prod_{i=1}^{n} a_i\right)^{1/n} = \sqrt[n]{a_1 \cdot a_2 \cdots a_n}$$

```
import scipy.stats
rast_in = 'data/input_raster.tif'
rast_as_numpy_array = arcpy.RasterToNumPyArray(rast_in)
raster_geometric_mean = scipy.stats.stats.gmean(
    rast_as_numpy_array, axis=None)
```



Use Case: Benthic Terrain Modeler

Benthic Terrain Modeler

- A Python Add-in and Python toolbox for geomorphology
- Open source, can borrow code for your own projects: https://github.com/EsriOceans/btm
- Active community of users, primarily marine scientists, but also useful for other applications

Lightweight SciPy Integration

- Using scipy.ndimage to perform basic multiscale analysis
- Using scipy.stats to compute circular statistics

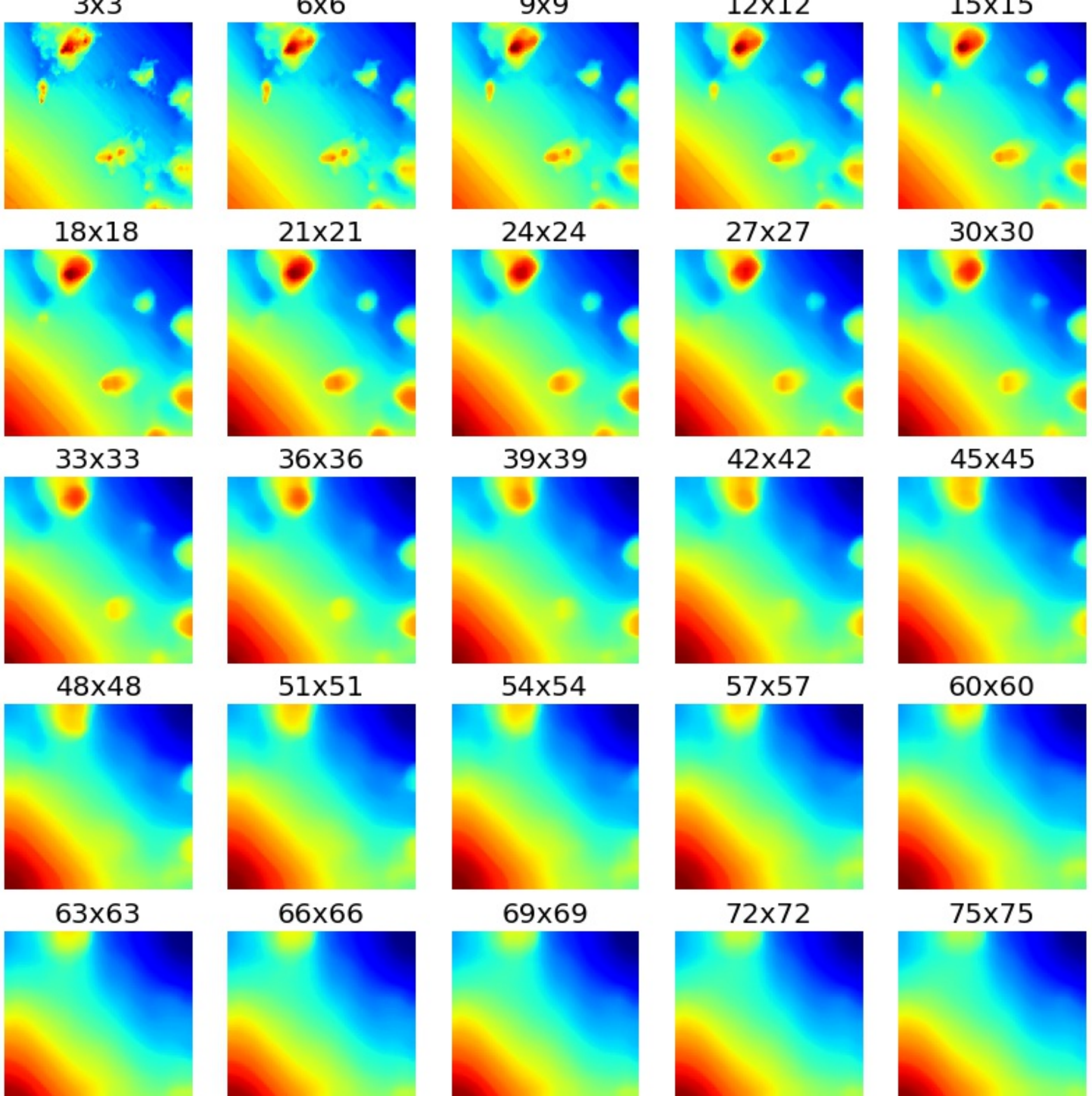
Lightweight SciPy Integration

Example source

```
import arcpy
import scipy.ndimage as nd
from matplotlib import pyplot as plt

ras = "data/input_raster.tif"
r = arcpy.RasterToNumPyArray(ras, "", 200, 200, 0)

fig = plt.figure(figsize=(10, 10))
```

Lightweight SciPy Integration

```
for i in xrange(25):
    size = (i+1) * 3
    print "running {}".format(size)
    med = nd.median_filter(r, size)

    a = fig.add_subplot(5, 5,i+1)
    plt.imshow(med, interpolation='nearest')
    a.set_title('{}x{}'.format(size, size))
    plt.axis('off')
    plt.subplots_adjust(hspace = 0.1)
    prev = med
```


3x3
6x6
9x9
12x12
15x15
18x18
21x21
24x24
27x27
30x30
33x33
36x36
39x39
42x42
45x45
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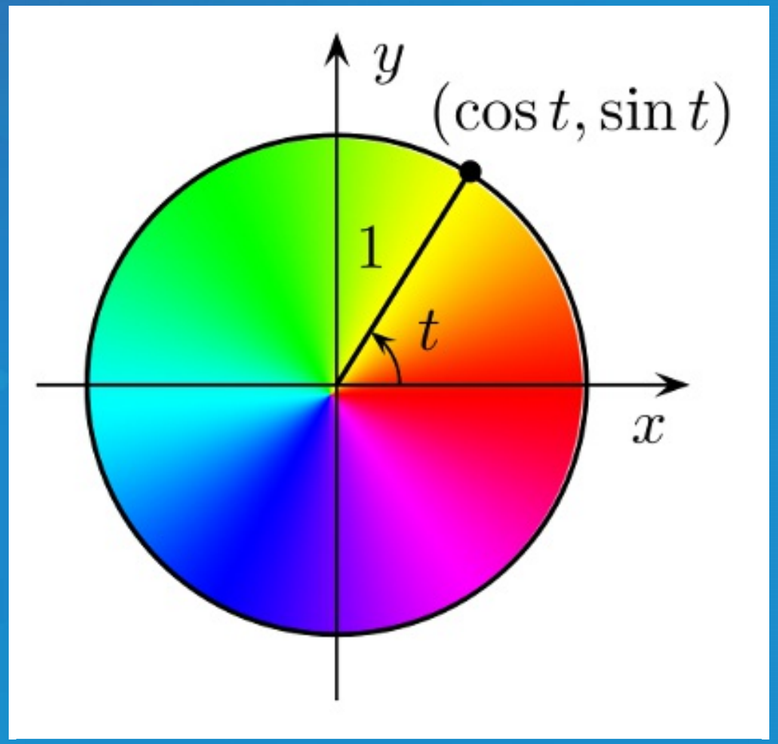
60x60
63x63
66x66
69x69
72x72
75x75

SciPy Statistics



- Break down aspect into sin() and cos() variables
- Aspect is a circular variable — without this 0 and 360 are opposites instead of being the same value

SciPy Statistics

Summary statistics from SciPy include circular statistics (source).

```
import scipy.stats.morestats

ras = "data/aspect_raster.tif"
r = arcpy.RasterToNumPyArray(ras)

morestats.circmean(r)
morestats.circstd(r)
morestats.circvar(r)
```

Demo: SciPy

Multidimensional Data

NetCDF4

- Fast, HDF5 and NetCDF4 read+write support, OPeNDAP
- Heirarchical data structures
- Widely used in meterology, oceanography, climate communities
- Easier: Multidimensional Toolbox, but can be useful

(Source)

```
import netCDF4
nc = netCDF4.Dataset('test.nc', 'r', format='NETCDF4')
print nc.file_format
# outputs: NETCDF4
nc.close()
```

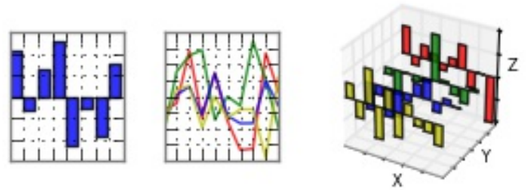
Multidimensional Improvements

- Multidimensional formats: HDF, GRIB, NetCDF
- Access via OPeNDAP, vector renderer, Raster Function Chaining
- An example which combines mutli-D with time
- Multi-D supported as WMS, and in Mosaic datasets (10.2.1+)

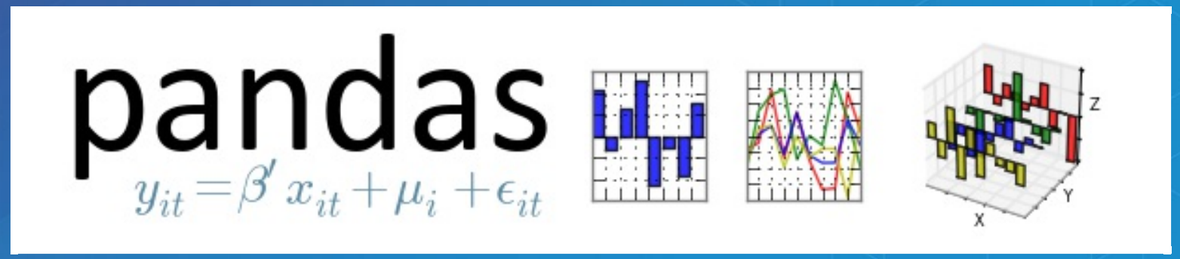
Pandas

pandas

$$y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$$



- **Pan**el **Da**ta — like R "data frames"
- Bring a robust data *analysis* workflow to Python
- Data frames are fundamental — treat tabular (and multi-dimensional) data as a labeled, indexed series of observations.



(Source)

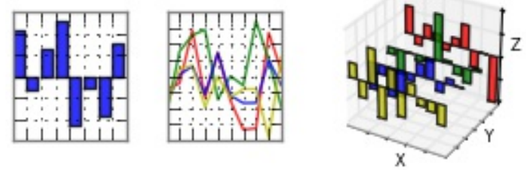
```
import pandas

data = pandas.read_csv('data/season-ratings.csv')
data.columns
```

```
Index([u'season', u'households', u'rank', u'tv_households', \
       u'net_indep', u'primetime_pct'], dtype='object')
```

pandas

$$y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$$




```
majority_simpsons = data[data.primetime_pct > 50]
```

	season	households	tv_households	net_indep	primetime_pct
0	1	13.4m[41]	92.1	51.6	80.751174
1	2	12.2m[n2]	92.1	50.4	78.504673
2	3	12.0m[n3]	92.1	48.4	76.582278
3	4	12.1m[48]	93.1	46.2	72.755906
4	5	10.5m[n4]	93.1	46.5	72.093023
5	6	9.0m[50]	95.4	46.1	71.032357
6	7	8.0m[51]	95.9	46.6	70.713202
7	8	8.6m[52]	97.0	44.2	67.584098
8	9	9.1m[53]	98.0	42.3	64.383562
9	10	7.9m[54]	99.4	39.9	60.916031
10	11	8.2m[55]	100.8	38.1	57.466063
11	12	14.7m[56]	102.2	36.8	53.958944
12	13	12.4m[57]	105.5	35.0	51.094891

Demo: Pandas

SymPy

- A Computer Algebra System (CAS), solve math equations (source)

```
from sympy import *
x = symbol('x')
eq = Eq(x**3 + 2*x**2 + 4*x + 8, 0)
```

$$x^3 + 2x^2 + 4x + 8 = 0$$

```
solve(eq, x)
```

$$[-2, \quad -2i, \quad 2i]$$

Demo: SymPy

Where and How Fast?

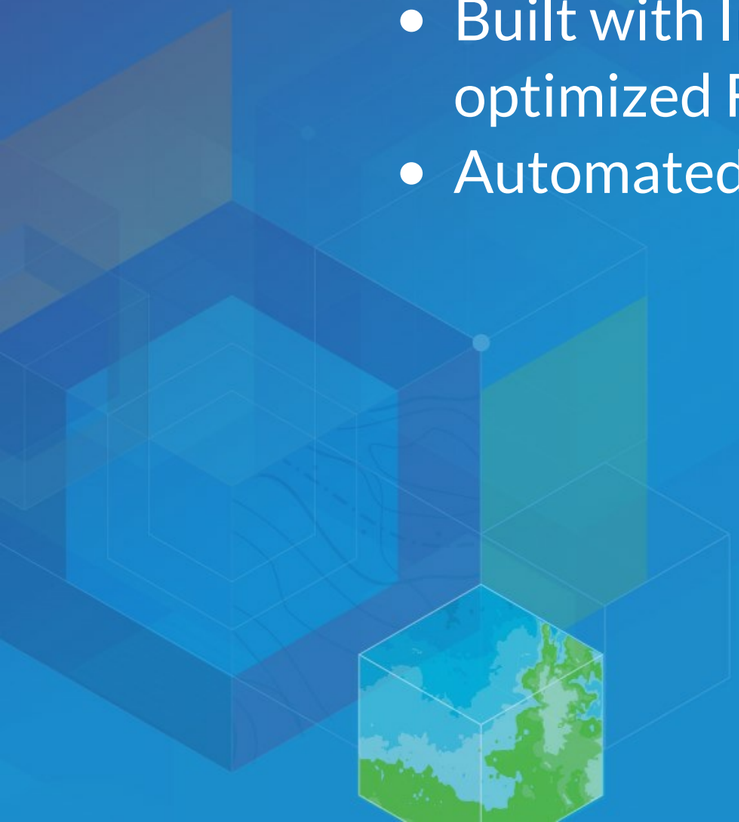
Where Can I Run This?

- Now:
  - ArcGIS Pro (64-bit) Standalone Python Install for Pro
  - 10.4: ArcMap, Server, both 32- and 64- bit environments
    - Both now ship with Scipy Stack (sans IPython)
  - MKL enabled NumPy and SciPy everywhere
    - Older releases: NumPy: ArcGIS 9.2+, matplotlib: ArcGIS 10.1+, SciPy: 10.4+, Pandas: 10.4+
  - Conda for managing full Python environments, consuming and producing packages
  - With the ArcGIS API for Python! Can run anywhere Python runs.

How Does It perform?

- Built with Intel's Math Kernel Library (MKL) and compilers—highly optimized Fortran and C under the hood.
- Automated parallelization for executed code

MKL Performance Chart



from future import *

Opening Doors

- Machine learning (scikit-learn, scikit-image, ...)
- Deep learning (theano, ...)
- Bayesian statistics (PyMC)
  - Markov Chain Monte Carlo (MCMC)
- Frequentist statistics (statsmodels)
- With Conda, not just Python! tensorflow, many others

Resources

Other Sessions

- Exploring Continuum Analytics' Open Source Offerings — tomorrow 10:30 in Mesquite G-H
- Getting Data Science with R and ArcGIS — stick around, in this room in 30 min! 2016 video
- Integrating Open-source Statistical Packages with ArcGIS earlier today, 2016 video
- Harnessing the Power of Python in ArcGIS Using the Conda Distribution yesterday, 2016 video

New to Python

- Courses:
  - Programming for Everybody
  - Codecademy: Python Track
- Books:
  - Learn Python the Hard Way
  - How to Think Like a Computer Scientist

GIS Focused

- Python Scripting for ArcGIS
- ArcPy and ArcGIS - Geospatial Analysis with Python
- Python Developers GeoNet Community
- GIS Stackexchange

Scientific

Courses:

- Python Scientific Lecture Notes
- High Performance Scientific Computing
- Coding the Matrix: Linear Algebra through Computer Science Applications
- The Data Scientist’s Toolbox

Scientific

Books:

- Free:
  - Probabilistic Programming & Bayesian Methods for Hackers
    - very compelling book on Bayesian methods in Python, uses SciPy + PyMC.
  - Kalman and Bayesian Filters in Python

Scientific

- Paid:
  - Coding the Matrix
    - How to use linear algebra and Python to solve amazing problems.
  - Python for Data Analysis: Data Wrangling with Pandas, NumPy, and IPython
    - The cannonical book on Pandas and analysis.

Packages

Only require SciPy Stack:

- Scikit-learn:
  - Lecture material
  - Includes SVMs, can use those for image processing among other things...
- FilterPy, Kalman filtering and optimal estimation:
  - FilterPy on GitHub
- An extensive list of machine learning packages

Code

- ArcPy + SciPy on Github
- raster-functions
  - An open source collection of function chains to show how to do complex things using NumPy + scipy on the fly for visualization purposes
- statistics library with a handful of descriptive statistics included in Python 3.4.
- *TIP*: Want a codebase that runs in Python 2 and 3? Check out future, which helps maintain a single codebase that supports both. Includes the futurize script to initially a project written for one version.

Scientific ArcGIS Extensions

- PySAL ArcGIS Toolbox
- Movement Ecology Tools for ArcGIS (ArcMET)
- Marine Geospatial Ecology Tools (MGET)
  - Combines Python, R, and MATLAB to solve a wide variety of problems
- SDMToolbox
  - species distribution & maximum entropy models
- Benthic Terrain Modeler
- Geospatial Modeling Environment
- CircuitScape

Conferences

- PyCon
  - The largest gathering of Pythonistas in the world
- SciPy
  - A meeting of Scientific Python users from all walks
- GeoPython
  - The Python event for Python and Geo enthusiasts
- PyVideo
  - Talks from Python conferences around the world available freely online.
  - PyVideo GIS talks

Closing

Thanks

- Geoprocessing Team
- The many amazing contributors to the projects demonstrated here.
  - Get involved! All are on GitHub and happily accept contributions.

Rate This Session

iOS, Android: Feedback from within the app

Windows Phone, or no smartphone? Cuneiform tablets accepted.


esri
THE
SCIENCE
OF
WHERE