

UCB/LBL Training Anaconda

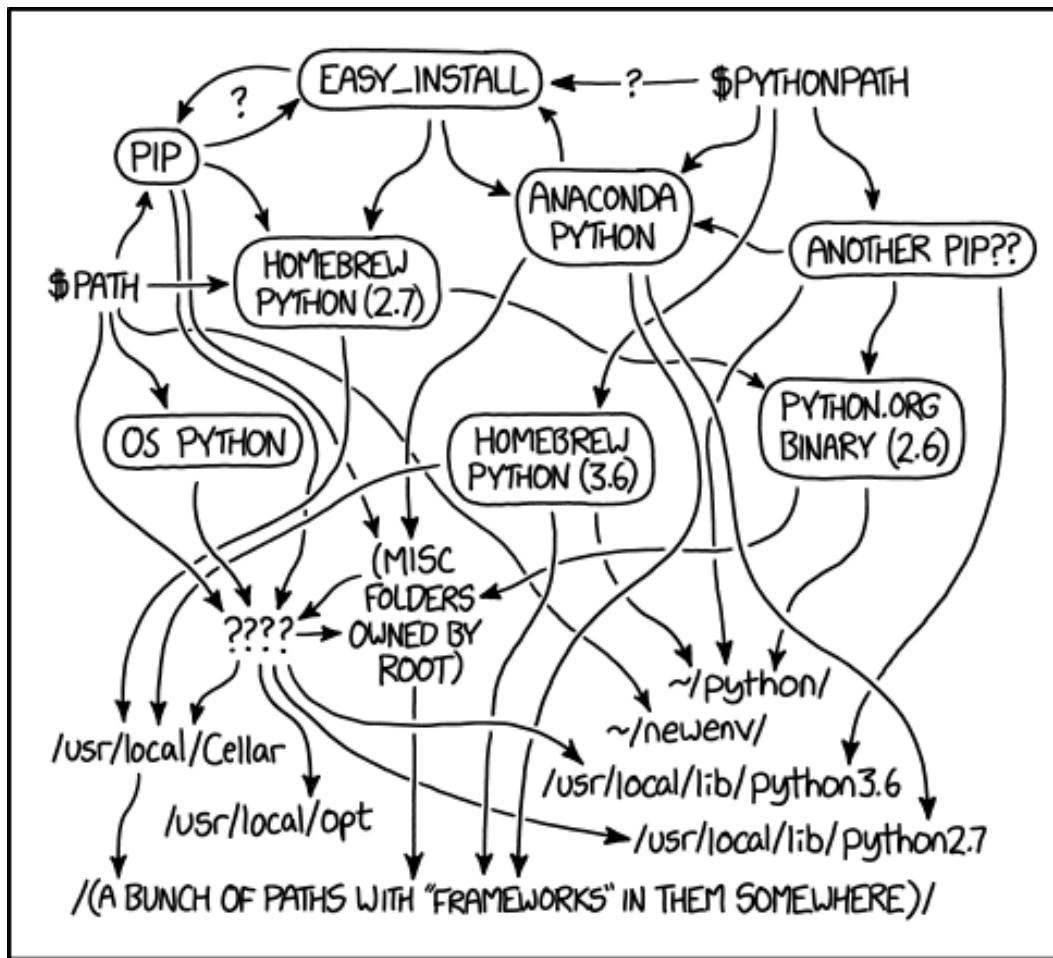
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May 2, 2018*



Why Anaconda

- Users want us to provide a stable, yet flexible Python environment
- From a support point of view, this can be challenging
 - Users will want different Python versions (some still need Python 2!)
 - The number of packages and modules seems almost infinite
 - Some users will require access to old versions of modules. This seems to be common among grad students nearing the end of their thesis projects who don't want subtle changes in results from bioinformatics pipelines.
 - Some Python packages can have dependencies on systems libraries
- Using Anaconda, users can easily manage their own Python installations, with the added bonus that they can maintain consistency from laptop to cluster

How some view the Python ecosystem



MY PYTHON ENVIRONMENT HAS BECOME SO DEGRADED
THAT MY LAPTOP HAS BEEN DECLARED A SUPERFUND SITE.

<https://xkcd.com/1987/>

Anaconda installation

Installing Anaconda on the cluster is easy and doesn't require root access or any special knowledge. Nonetheless, there are a few things that you can do to make it easier for your users.

- Direct users to the installation page
<https://conda.io/docs/user-guide/install/index.html>
- Encourage users to download directly to cluster rather than installing on laptop and copying to cluster (right click download button to copy link location)
`wget https://repo.anaconda.com/archive/Anaconda3-5.1.0-Linux-x86_64.sh`
- Let users know that the download page will likely direct them to the download for the architecture where their browser is running (see next slide)

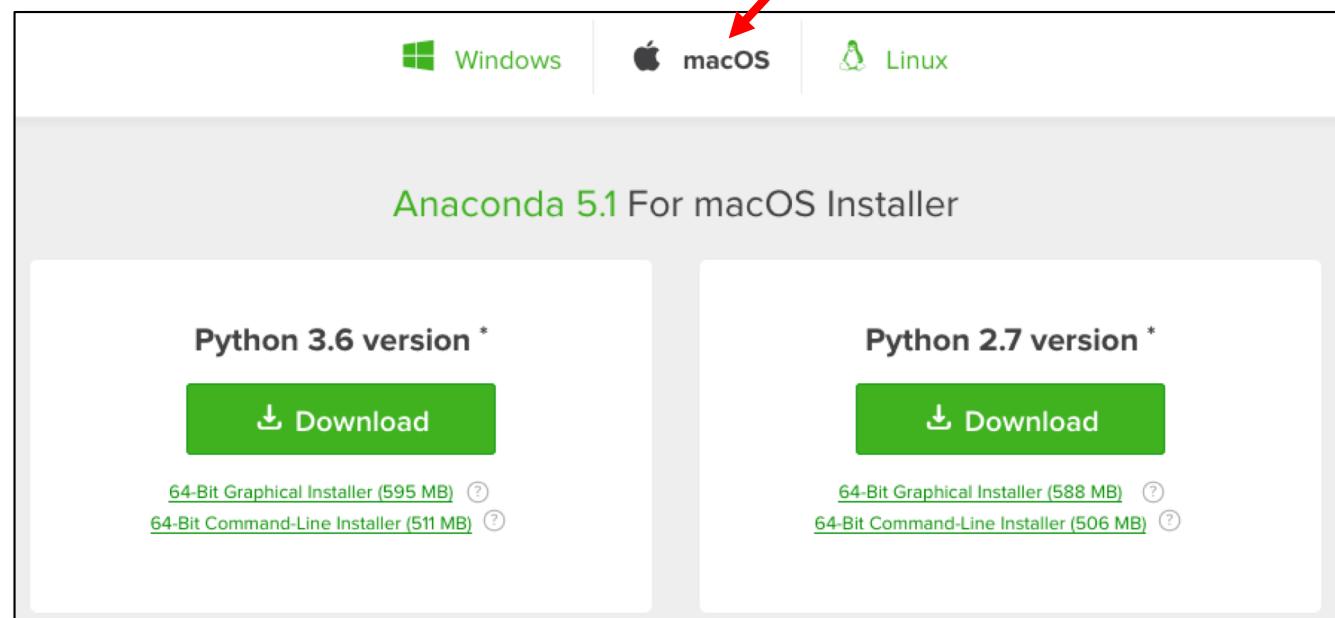
Anaconda install gotcha

Installing on Linux

1. Download the installer:

- Miniconda installer for Linux.
- **Anaconda installer for Linux.**

Using the browser on my Mac and following link to Linux install took me to the macOS download instead of Linux download. Click the penguin to remedy.



Anaconda installation

Download to cluster (Comet) is fast and takes about 10 seconds

```
$ wget https://repo.anaconda.com/archive/Anaconda3-5.1.0-Linux-x86_64.sh  
--2018-04-30 10:41:45--  https://repo.anaconda.com/archive/Anaconda3-5.1.0-  
Linux-x86_64.sh  
Resolving repo.anaconda.com... 104.17.108.77, 104.17.109.77, 104.17.111.77,  
...  
Connecting to repo.anaconda.com|104.17.108.77|:443... connected.  
HTTP request sent, awaiting response... 200 OK  
Length: 577996269 (551M) [application/x-sh]  
Saving to: "Anaconda3-5.1.0-Linux-x86_64.sh"  
  
100%[=====>] 577,996,269 58.0M/s   in 9.4s
```

Anaconda installation

Full anaconda installation in home directory takes just under six minutes and requires 3.4 GB of disk space

```
$ time bash Anaconda3-5.1.0-Linux-x86_64.sh
Welcome to Anaconda3 5.1.0
...
Thank you for installing Anaconda3!
real 5m50.775s
user 1m39.212s
sys 0m42.248s

$ du -hs anaconda3/
3.4G anaconda3/
```

Anaconda installation

The Anaconda installer can automatically modify the .bashrc to point to the newly installed Python location. Beware of possible conflicts due to existing PYTHONPATH.

WARNING:

You currently have a PYTHONPATH environment variable set. This may cause unexpected behavior when running the Python interpreter in Anaconda3. For best results, please verify that your PYTHONPATH only points to directories of packages that are compatible with the Python interpreter in Anaconda3: /home/etrain109/anaconda3

Do you wish the installer to prepend the Anaconda3 install location to PATH in your /home/etrain109/.bashrc ? [yes/no]

[no] >>> yes

*Appending source /home/etrain109/anaconda3/bin/activate to
/home/etrain109/.bashrc*

A backup will be made to: /home/etrain109/.bashrc-anaconda3.bak

```
$ which python3  
~/anaconda3/bin/python3
```

Installing packages

Although Anaconda comes with a large number of standard packages, users may still need to install additional packages. This can be done using conda

```
$ python3
Python 3.6.4 |Anaconda, Inc.| (default, Jan 16 2018, 18:10:19)
[GCC 7.2.0] on linux
>>> from Bio import SeqIO
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ModuleNotFoundError: No module named 'Bio'

$ conda install BioPython

$ python3
Python 3.6.4 |Anaconda, Inc.| (default, Jan 16 2018, 18:10:19)
[GCC 7.2.0] on linux
>>> from Bio import SeqIO
>>>
```

Installing packages

But beware that sometimes special installations may be needed

<https://stackoverflow.com/questions/33433274/anaconda-graphviz-cant-import-after-installation>

```
$ python3
$ conda install graphviz
Solving environment: done
    graphviz:          2.40.1-h25d223c_0
Downloading and Extracting Packages
graphviz

$ python3
>>> import graphviz
Traceback (most recent call last):
ModuleNotFoundError: No module named 'graphviz'

$ pip install graphviz
Installing collected packages: graphviz
Successfully installed graphviz-0.8.3

$ python3
>>> import graphviz
>>> graphviz.__version__
'0.8.3'
```

Miniconda vs. Anaconda

- Miniconda includes only conda (open source package manager and environment management system) and its dependencies. Anaconda includes conda plus about 720 widely used packages.
- Installing Miniconda is quick (~ one minute) and requires little space (348 MB)
- Which one is right for you? It depends. According to
<https://stackoverflow.com/questions/45421163/anaconda-vs-miniconda>

Choose Anaconda if you:

- Are new to conda or Python
- Like the convenience of having Python and over 150 scientific packages automatically installed at once
- Have the time and disk space (a few minutes and 3 GB), and/or
- Don't want to install each of the packages you want to use individually.

Choose Miniconda if you:

- Do not mind installing each of the packages you want to use individually.
- Do not have time or disk space to install over 150 packages at once, and/or
- Just want fast access to Python and the conda commands, and wish to sort out the other programs later.

I use Miniconda myself. Anaconda is bloated. Many of the packages are never used and could still be easily installed if and when needed.

Listing installed packages

Installed packages and their versions can be listed using “conda list”. Of course, you can still get this information from the Python prompt using the appropriate dunder (e.g. numpy.__version__)

```
$ conda list
# packages in environment at /home/etrain109/anaconda3:
#
#           Name                Version          Build  Channel
_ipyw_jlab_nb_ext_conf      0.1.0            py36he11e457_0
alabaster                   0.7.10           py36h306e16b_0
anaconda                    5.1.0            py36_2
anaconda-client              1.6.9            py36_0
anaconda-navigator          1.7.0            py36_0
...
yaml                        0.1.7            had09818_2
zeromq                      4.2.2            hbedb6e5_2
zict                         0.1.3            py36h3a3bf81_0
zlib                         1.2.11           ha838bed_2
```

A few words about MKL

To get the best performance for numerically intensive applications, we recommend using the Intel MKL library of threaded and vectorized math routines. Anaconda 2.5 (February 2016) and later come with MKL-powered versions of NumPy, SciPy and Scikit-learn.

<https://docs.anaconda.com/mkl-optimizations/>

It is possible to opt out of using MKL

<https://docs.anaconda.com/mkl-optimizations/#uninstalling-mkl>

Not sure why anyone would want to do that when running on a modern cluster or supercomputer other than for benchmarking purposes when testing new math libraries.

A few words about MKL

Can confirm that NumPy, SciPy and scikit-learn were built using MKL with the `show_config()` method

```
>>> import numpy as np
>>> np.show_config()
mkl_info:
    libraries = ['mkl_rt', 'pthread']
    library_dirs = ['/home/etrain109/anaconda3/lib']
    define_macros = [('SCIPY_MKL_H', None), ('HAVE_CBLAS', None)]
    include_dirs = ['/home/etrain109/anaconda3/include']
blas_mkl_info:
    libraries = ['mkl_rt', 'pthread']
    library_dirs = ['/home/etrain109/anaconda3/lib']
    define_macros = [('SCIPY_MKL_H', None), ('HAVE_CBLAS', None)]
    include_dirs = ['/home/etrain109/anaconda3/include']
blas_opt_info:
    libraries = ['mkl_rt', 'pthread']
    library_dirs = ['/home/etrain109/anaconda3/lib']
...
...
```

A few words about MKL

```
>>> a = np.random.rand(20000,20000)
>>> ainv = np.linalg.inv(a)
```

```
top - 16:48:24 up 43 days,  2:23,  1 user,  load average: 5.11, 3.85, 3.16
Tasks: 1351 total,  26 running, 1325 sleeping,   0 stopped,   0 zombie
Cpu(s): 95.5%us,  2.8%sy,  0.0%ni,  1.5%id,  0.0%wa,  0.0%hi,  0.2%si,  0.0%st
Mem: 131777004k total, 16082468k used, 115694536k free,    21496k buffers
Swap:      0k total,       0k used,       0k free,  143224k cached

          PID USER      PR  NI    VIRT    RES   SHR S %CPU %MEM     TIME+ COMMAND
23082 etrain10  20   0 17.5g  12g  16m R 100.5 10.0   0:49.38 python3
23089 etrain10  20   0 17.5g  12g  16m R 100.5 10.0   0:50.25 python3
23091 etrain10  20   0 17.5g  12g  16m R 100.5 10.0   0:47.83 python3
23096 etrain10  20   0 17.5g  12g  16m R 100.5 10.0   0:48.01 python3
23097 etrain10  20   0 17.5g  12g  16m R 100.5 10.0   0:47.69 python3
23102 etrain10  20   0 17.5g  12g  16m R 100.5 10.0   0:47.15 python3
23104 etrain10  20   0 17.5g  12g  16m R 100.5 10.0   0:49.19 python3
22809 etrain10  20   0 17.5g  12g  16m R 100.1 10.0   1:01.06 python3
23084 etrain10  20   0 17.5g  12g  16m R 100.1 10.0   0:49.32 python3
23086 etrain10  20   0 17.5g  12g  16m R 100.1 10.0   0:50.35 python3
23087 etrain10  20   0 17.5g  12g  16m R 100.1 10.0   0:50.22 python3
23088 etrain10  20   0 17.5g  12g  16m R 100.1 10.0   0:50.14 python3
23090 etrain10  20   0 17.5g  12g  16m R 100.1 10.0   0:48.63 python3
23093 etrain10  20   0 17.5g  12g  16m R 100.1 10.0   0:47.59 python3
23098 etrain10  20   0 17.5g  12g  16m R 100.1 10.0   0:46.22 python3
23100 etrain10  20   0 17.5g  12g  16m R 100.1 10.0   0:47.04 python3
23103 etrain10  20   0 17.5g  12g  16m R 100.1 10.0   0:47.41 python3
23083 etrain10  20   0 17.5g  12g  16m R 99.8 10.0   0:49.35 python3
23092 etrain10  20   0 17.5g  12g  16m R 99.8 10.0   0:46.16 python3
23085 etrain10  20   0 17.5g  12g  16m R 92.6 10.0   0:48.50 python3
23101 etrain10  20   0 17.5g  12g  16m R 80.0 10.0   0:46.93 python3
23094 etrain10  20   0 17.5g  12g  16m R 79.7 10.0   0:45.18 python3
23095 etrain10  20   0 17.5g  12g  16m R 75.1 10.0   0:44.29 python3
23099 etrain10  20   0 17.5g  12g  16m R 74.4 10.0   0:44.57 python3
22318 etrain10  20   0 113m 5216 1464 S  0.0  0.0   0:00.08 bash
```

Working with environments

Environments give you the flexibility to use different versions of Python and/or Python packages without altering your default environment (i.e. the one created when installing Anaconda or Miniconda). Before creating new environments, you may need to update conda to the latest version

```
$ conda update -n base conda
Solving environment: done

## Package Plan ##

environment location: /home/etrain109/anaconda3

added / updated specs:
- conda

The following packages will be downloaded:
package              |      build
-----              | -----
conda-4.5.1          |      py36_0    1.0 MB
```

Creating environments

Environments are created using the conda create command. A few examples are shown below for creating environments based on different Python versions and/or packages

```
# Environment with different Python version (3.4)
$ conda create -n py34 python=3.4

# Environment with older zlib version
$ conda create -n ozl zlib=1.2.8

# Environment with older Python and zlib versions
$ conda create -n py35ozl python=3.5 zlib=1.2.8
```

Creating environments

The new environment builds on the base environment that was created during the Anaconda installation and can be found under anaconda3/env. It encompasses the minimal set of changes that are necessary to deal with dependencies

```
$ ls anaconda3/envs/oz1/lib/
libz.a libz.so  libz.so.1  libz.so.1.2.8  pkgconfig

$ ls anaconda3/lib
cairo  libharfbuzz-gobject.so      libpng.so libQt5XmlPatterns.so
cmake  libharfbuzz-gobject.so.0    libpython3.6m.a
libQt5XmlPatterns.so.5
[-- 903 lines not shown --]
libharfbuzz-gobject.a  libpng.a      libQt5XmlPatterns.la
xsltConf.sh
libharfbuzz-gobject.la  libpng.la    libQt5XmlPatterns.prl
```

Listing and removing environments

Environments are listed and removed with the conda info and remove commands. In the example below, we list the environments before and after removing the "ozl" environment.

```
$ conda info --envs
base          * /home/etrain109/anaconda3
ozl
py35ozl
py34

$ conda remove -n ozl --all

$ conda info --envs
base          * /home/etrain109/anaconda3
py35ozl
py34
```

Activating/deactivating environments

Use source activate and source deactivate to change environments. Note that the prompt changes to reflect the new environment and that repeated calls to activate create a stack of environments.

```
$ python3 -V
Python 3.6.4 :: Anaconda, Inc.
$ source activate py34

(py34) $ python3 -V
Python 3.4.5 :: Continuum Analytics, Inc.
(py34) $ source activate p35_oldzlib

(p35_oldzlib) $ python3 -V
Python 3.5.5 :: Anaconda, Inc.

(p35_oldzlib) $ source deactivate
(py34) $ source deactivate
$
```

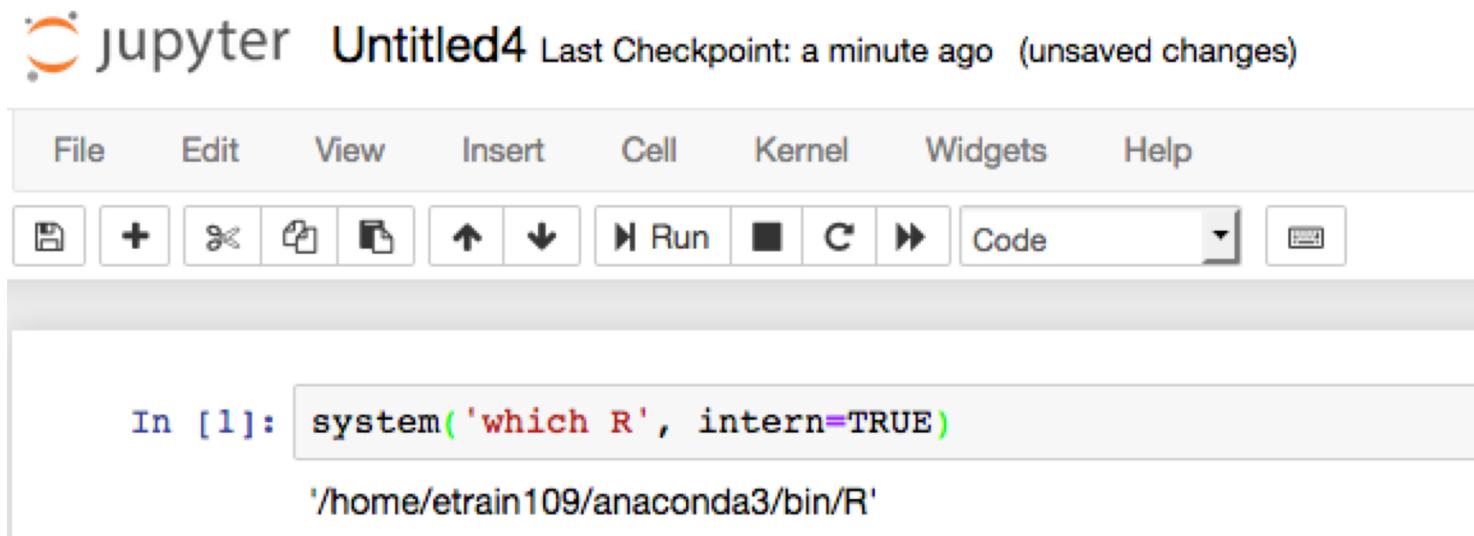
Managing R with conda

Although Anaconda and Jupyter are usually associated with the Python community, keep in mind that conda is language agnostic.

```
$ which R  
/opt/R/bin/R  
  
$ conda install -c r r-irkernel  
Solving environment: done  
## Package Plan ##  
environment location: /home/etrain109/anaconda3  
  
$ which R  
/home/etrain109/anaconda3/bin/R
```

Managing R with conda

R notebooks executed in Jupyter will use the R version found in Anaconda and packages will be installed in anaconda3/lib/R/library. Personally, I find this more convenient than dealing with a mix of system wide and local installations.



The screenshot shows a Jupyter Notebook interface. At the top, there's a toolbar with various icons for file operations, cell selection, and help. Below the toolbar, the title bar reads "jupyter Untitled4 Last Checkpoint: a minute ago (unsaved changes)". The main area is a code cell containing the following R code:

```
In [1]: system('which R', intern=TRUE)
```

The output of the code is displayed below the cell:

```
/home/etrain109/anaconda3/bin/R'
```

Exercises (page 1)

- Install Anaconda Python 3.6 version (<https://conda.io/docs/user-guide/install/index.html>). Use wget to download directly to Comet
- Source .bashrc and confirm paths to python3 and conda (~/anaconda3/bin)
- Edit .bashrc to unset PYTHONPATH (unset PYTHONPATH)
- List info for all Python packages (conda list) and for a few specific packages (conda list pkg)
- Install Miniconda, but don't update your .bashrc (answer 'no' to prepend path question)
- Get an interactive node

```
srun --pty --nodes=1 --ntasks-per-node=24 -p compute --reservation=UCB2018Res -t 01:00:00 --wait 0 /bin/bash
```
- Launch Python3, import numpy as np, and use show_config() to confirm MKL build
- Open a second terminal window, ssh to your interactive node (e.g. ssh comet-12-31), launch top and show threads (Shift-H)
- Execute following at Python prompt and monitor CPU usage in second window

```
a = np.random.rand(20000,20000)
ainv = np.linalg.inv(a)
```

Exercises (page 2)

- Update your conda version – I had to do this to create new environments
`conda update -n base conda`
- Create a new environment using an older version of Python 3
- Create another new environment using an older version of zlib (1.2.8 works)
- List your environments (`conda info --envs`) and explore the the anaconda3/envs directory
- Activate these new environments (`source activate myenv`) and confirm the Python version and zlib version either from the Python prompt or using the `conda list` command
- Deactivate the new environments (`source deactivate`)
- Remove at least one of the new environments
`conda remove -n myenv --all`
- Check out conda documentation
`conda -h`
`conda info -h`

Exercises (page 3)

If you plan to tinker with R notebooks ...

- Get the R version and location before installing R kernel
- Install R kernel
- Get the R version and location after installing R kernel
- Install ggplot2: `install.packages("ggplot2")`

Intermission

Using Jupyter Notebooks

Notebooks provide an excellent way to integrate code, documentation and output into a single file. As one of my colleagues described it, notebooks are essentially executable documentation. Although the Notebook was originally developed for Python (IPython), the concept has been expanded to other languages (we'll also see some examples in R).

Even if you're comfortable developing code the old fashioned way (edit, save, run, repeat), the Jupyter notebook can make you more productive and allows you to execute blocks of code (cells) rather than the entire application. Graphics, results and readable comments can be interspersed between executable statements.

Using Jupyter Notebooks

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OK, Notebooks aren't completely new. They've been a staple of Mathematica for a long time but the Jupyter notebooks take things a step further by allowing the application to other languages and breaking the stand-alone model of Mathematica.

Using Jupyter Notebooks

The Atlantic

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Genomic analysis of elongated skulls suggests extensive female-biased immigration to early Medieval Bavaria

Krishna R. Veeramah^a, Andreas Rott^{b,1}, Melanie Groß^{c,1}, Lucy van Dorp^d, Silvia López^e, Karola Kirsanow^f, Christian Sell^g, Jens Blöcher^e, Daniel Wegmann^{b,9}, Vivian Link^{b,9}, Zuzana Hofmanová^{b,9}, Joris Peters^{b,9}, Bernd Trautmann^b, Anja Gairhosⁱ, Jochen Haberstroh^j, Bernd Päffgen^k, Garrett Hellenthal^b, Brigitte Haas-Gebhardⁱ, Michaela Harbeck^{b,2,3}, and Joachim Burger^{c,2,3}

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Edited by Eske Willerslev, University of Copenhagen, Copenhagen, Denmark, and approved January 30, 2018 (received for review November 21, 2017)

Modern European genetic structure demonstrates strong correlations with geography, while genetic analysis of prehistoric populations can reveal the demographic history of their ancestors. However, population-level genome data can shed light on the demographic processes occurring during the intervening periods have been absent. Therefore, we generated genomic data from 41 individuals dating mostly to the late 5th/early 6th century AD from present-day Bavaria in southern Germany, including 11 whole genomes (mean depth 5.56x). In addition we developed a capture array to sequence neutral regions spanning a total of 5 Mb and 486 functional polymorphic sites to high depth (mean 72x).

to form in the 5th century AD, and that it emanated from a combination of a centralized local population of the border province (Fig. 1B). This finding is consistent with the known fact that some other contemporary groups, an interesting archaeological feature in Bavaria from this period is the presence of skeletons with artificially deformed or elongated skulls (Fig. 1A).

Artificial cranial deformation (ACD), which is only possible during early childhood, is a deliberate and permanent shaping of the head performed with great effort. In some societies reshaping the human skull has been seen as an ideal of beauty, while it

PNAS / Richard Goerg / Getty / The Atlantic

The Scientific Paper Is Obsolete

Here's what's next.

<https://www.theatlantic.com/science/archive/2018/04/the-scientific-paper-is-obsolete/556676/>

Using Jupyter Notebooks

- **Grab an interactive node**

```
srun --pty --nodes=1 --ntasks-per-node=24 -p compute --reservation=UCB2018Res -t  
01:00:00 --wait 0 /bin/bash
```

- **Load singularity image**

```
module load singularity  
singularity shell /share/apps/gpu/singularity/sdsc_ubuntu_tf1.1_keras_R.img
```

- **Clone repos**

```
git clone https://github.com/sinkovit/PythonSeries  
git clone https://github.com/sinkovit/RSeries
```

Using Jupyter Notebooks

- **Launch notebook**

```
jupyter notebook --no-browser --ip="*" &
```

This will give you an address which has localhost in it and a token. Something like:

```
http://localhost:8888/?token=389587c9d1b69f8f595e7d8bfdd83c9961ed26b8b3f1bb3e
```

You can replace localhost with comet-02-17.sdsc.edu (or what ever host you get) and then paste it into your browser. That should get you into the running notebook. From there everything should be working as a regular notebook. Note: This token is your auth so don't email/send it around (I already stopped the above link).

Using environments with Jupyter

We showed earlier how to create new Python environments that use different versions of Python and/or packages. When working from the command line, it was easy to change environment

```
$ source activate myenv  
(myenv) $
```

When working with Jupyter, a few more steps are needed

- (1) conda install nb_conda_kernels
- (2) Then from each environment
 conda install ipykernel

The first step adds the functionality to the Jupyter notebooks to list the kernels, while the second step adds the environment to the list of kernels

Using environments with Jupyter

We can select a non-default kernel for our new notebooks

The screenshot shows the Jupyter Notebook interface. On the left, there is a file browser with a sidebar showing 0 items. The main area lists several items: 'anaconda3', 'miniconda3', 'PythonSeries', 'RSeries', 'Anaconda3-5.1.0-Linux-x86_64.sh', and 'Miniconda3-latest-Linux-x86_64.sh'. On the right, a large dropdown menu is open under the 'New' button. It contains a list of kernels: 'Python 2', 'Python [conda env:anaconda3]', 'Python [conda env:ozl]', 'Python [conda env:py34]', 'Python [conda root]', 'Python [default]', 'R', and 'R [conda env:anaconda3]'. Below this, under 'Other:', are options for 'Text File', 'Folder', and 'Terminal'.

Using environments with Jupyter

We can also change the kernel for an open notebook

jupyter Python basics Last Checkpoint: 4 hours ago (unsaved changes) Logout

File Edit View Insert Cell Kernel Widgets Help Trusted Python [conda root]

Interrupt Restart Restart & Clear Output Restart & Run All Reconnect Shutdown Change kernel Conda Packages Visit anaconda.org

In []: import sys
sys.version

Python basics

In this brief tutorial, we'll ex...
comments, logical values, t...

If you're new to Python, do...
functions and modules for...

Basic math

Floating point math operations work the way you would expect. For convenience, an exponentiation operator (\star) is provided.

math. strings. lists. dictionaries. tuples, sets, branching, loops, functions and modules for...
Python code.
with a rich syntax, lots of built in functions and operation precedence. As a

Python 2
Python [conda env:anaconda3]
Python [conda env:ozl]
Python [conda env:py34]
Python [conda root]
Python [default]
R
R [conda env:anaconda3]