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PYTHON FOR HPC

Day 1 Outline

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- Why use python?
- Some features of the python language
- Inner workings and performance
- Multithreading and multiprocessing examples
- A few words on concurrency

Repo: https://github.com/appeltel/python-hpc-seminar

(repo has links, code examples, etc…)

Why Python?

What is Python?

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- "Scripting" Language named after Monty Python
- Created in 1989 by Guido van Rossum, who is now the Benevolent Dictator for Life
- Multi-paradigm, with object-oriented and functional features
- CPython reference implementation (current version 3.6)
- Type "import this" for language philosophy

Easy to Learn, Read, and Use

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```
>>> def fibonacci(n):
...     a, b = 0, 1
...     for _ in range(n):
...         a, b = b, a + b
...     return a
...
>>> fibonacci(7)
13
>>>
```

High Level

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- Built-in generic dynamic array (list) and mapping (dict) types
- Memory managed
- REPL, Notebooks, features for rapid prototyping
- BATTERIES INCLUDED

BATTERIES INCLUDED

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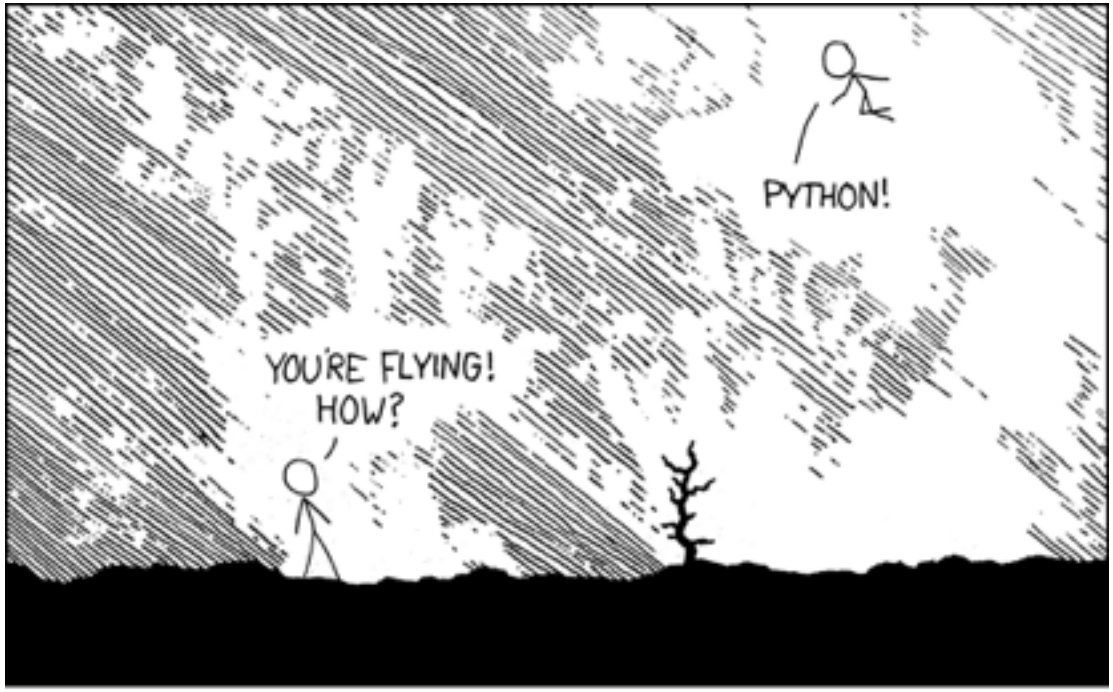

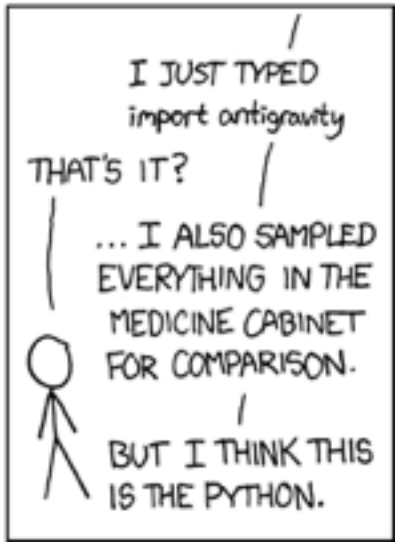

BATTERIES INCLUDED

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- Full-featured standard library
- Extensive third-party packages
- PyPI service for distributing third party packages
- pip - tool for installing and managing packages
- virtualenv - tool for creating sandboxed environments for installing package sets

MORE BATTERIES INCLUDED

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- Pre-packaged distribution of python and many scientific libraries and tools
- Tools for managing environments, installing yet more packages

Great Community

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python SOFTWARE FOUNDATION

django girls

PyOhio

About Python

Some Basics

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- REPL - Read - Eval - Print - Loop
- Some basic things to explore on the REPL:
  - Names, assignment
  - Functions, modules, import system, namespaces
  - Dynamic typing, memory management
  - EAFP style - “We’re all responsible users here”
  - lists and dicts

More on Lists and Dicts

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- Built in list type “list” - (dynamic array)
- Built in mapping type “dict” - (hash table)
- Dynamic typing allows for easy representation of semi-structured data

```
>>> record = {
...     "name": "Eric Appelt",
...     "email": "eric.appelt@gmail.com",
...     "uid": 111694,
...     "dogs": ["Abby", "Rocky"]
... }
>>> record['dogs'][1]
'Rocky'
>>>
```

How Python Works

WARNING: This section covers the current version of the reference implementation of python called CPython. There are other implementations of the python language that do not work this way and are more performant. However, people often refer to the reference implementation when they say "python".

Python Memory Management

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- Each python object has a reference count
- Binding to a name, placement in a list position, increments the reference count
- When the reference count is zero, the object is destroyed and memory freed
- A garbage collector runs periodically to take care of circular references.

Python Objects in Memory

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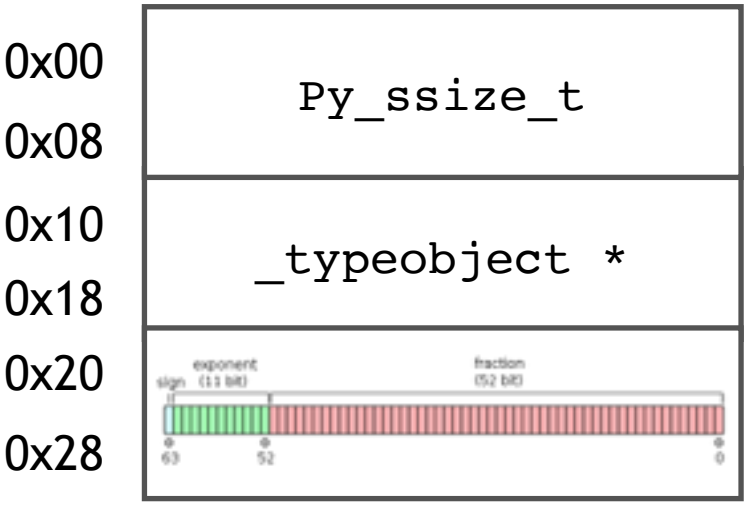
Python dynamic typing and memory management by reference counting incurs memory overhead (64-bit architecture):



Reference count integer (8 byte)

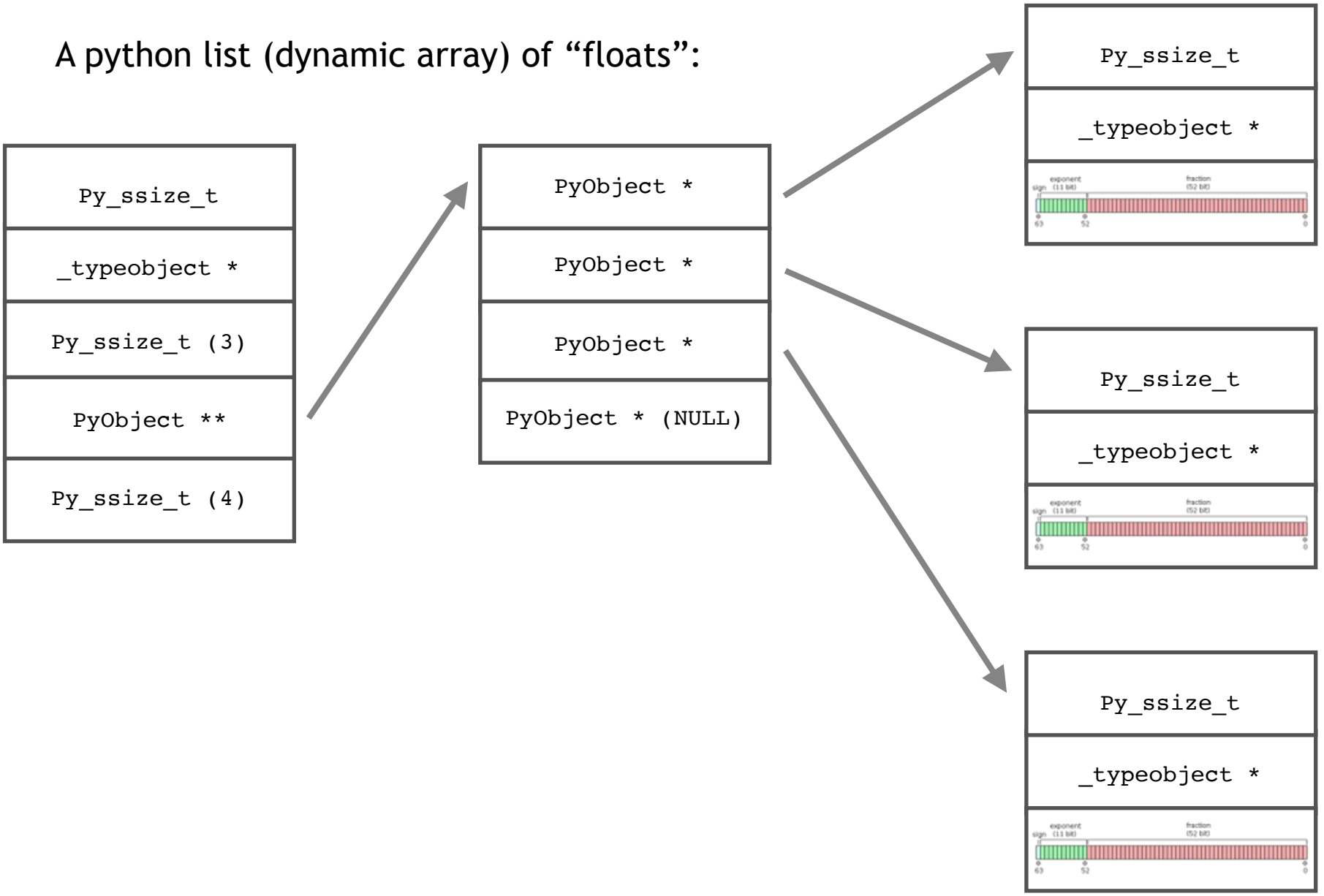
Pointer to type (8 byte)

Double precision floating point data (8 byte)

A python “float” object.

A Python List of Floats

A python list (dynamic array) of “floats”:



SOMETHING BETTER FOR HPC

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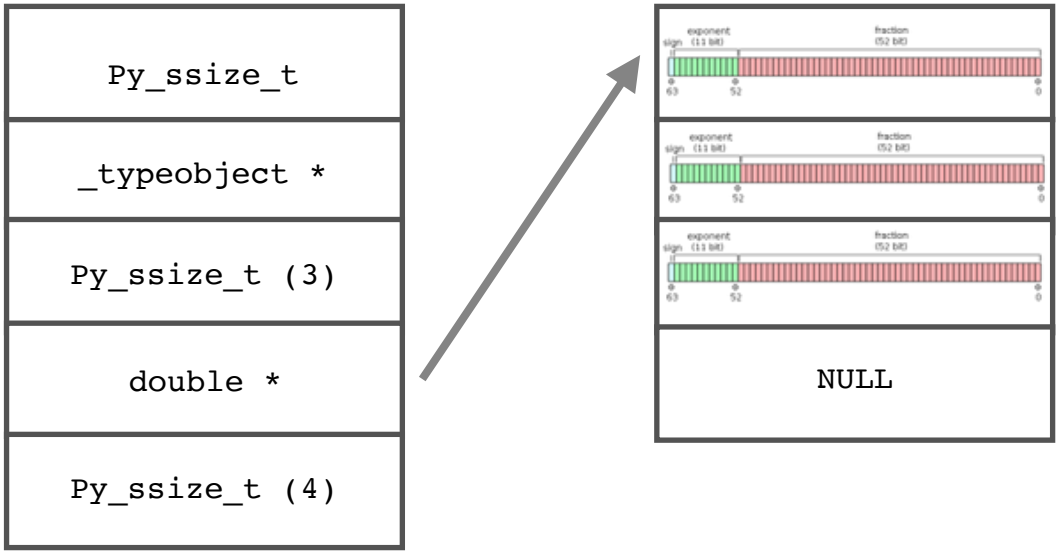
Something like this would be better for performance



8 bytes per double, no dereferencing individual pointers, checking types for each one.

SOMETHING BETTER FOR HPC

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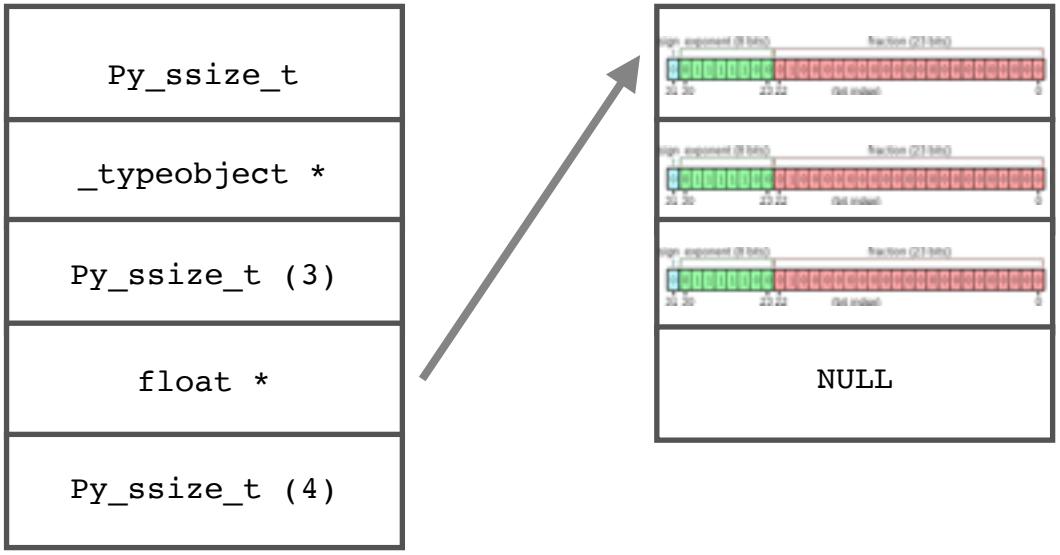
Or even better if you don't need double precision!



4 bytes per float, no dereferencing individual pointers, checking types for each one.

Python Bytecode and Interpretation

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- Python source is compiled into a platform-independent bytecode
- (CPython) A simple virtual stack machine, written in C, executes the bytecode
- (CPython) bytecode is NOT just-in-time compiled to native processor instructions
- Other implementations of python, such as pypy, do improve performance by compiling to native processor instructions.

Example Function

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```
>>> import dis
>>> def foo(x, y):
...     return x * y + 17
...
>>> foo.__code__.co_varnames
('x', 'y')
>>> foo.__code__.co_consts
(None, 17)
>>> [hex(b) for b in foo.__code__.co_code]
['0x7c', '0x0', '0x7c', '0x1', '0x14', '0x0', '0x64', '0x1', '0x17', '0x0', '0x53', '0x0']
>>> dis.dis(foo)
  2           0 LOAD_FAST                0 (x)
              2 LOAD_FAST                1 (y)
              4 BINARY_MULTIPLY
              6 LOAD_CONST               1 (17)
              8 BINARY_ADD
             10 RETURN_VALUE
>>>
```

Example Function Invocation

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CALLED: foo(3, 5)

function code

```
  0 LOAD_FAST                0 (x)
  2 LOAD_FAST                1 (y)
  4 BINARY_MULTIPLY
  6 LOAD_CONST               1 (17)
  8 BINARY_ADD
 10 RETURN_VALUE
```

co_varnames

PyObject * (3)	PyObject * (5)

co_consts

PyObject * (None)	PyObject * (17)

object stack

Example Function Invocation

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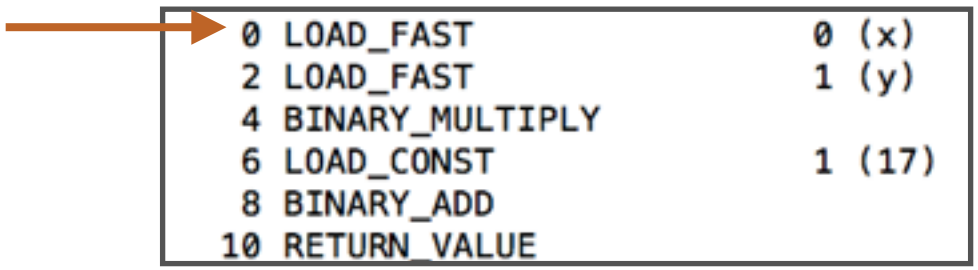
CALLED: foo(3, 5)

function code



co_varnames

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Example Function Invocation

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```

co_varnames

PyObject * (3)	PyObject * (5)

co_consts

PyObject * (None)	PyObject * (17)

PUSH!

object stack

PyObject * (3)

Example Function Invocation

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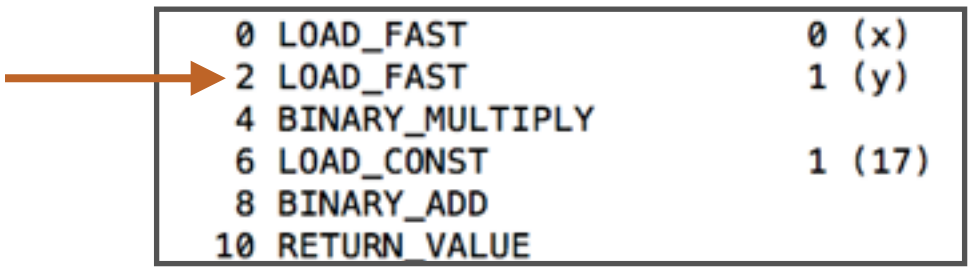
CALLED: foo(3, 5)

function code



co_varnames

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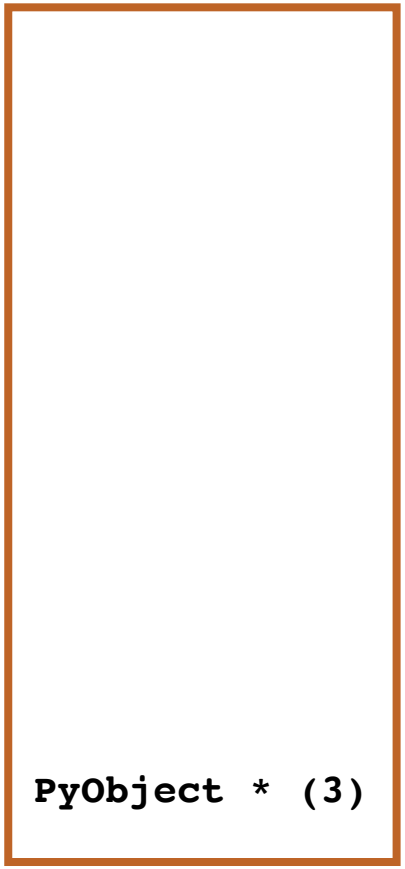
object stack



Example Function Invocation

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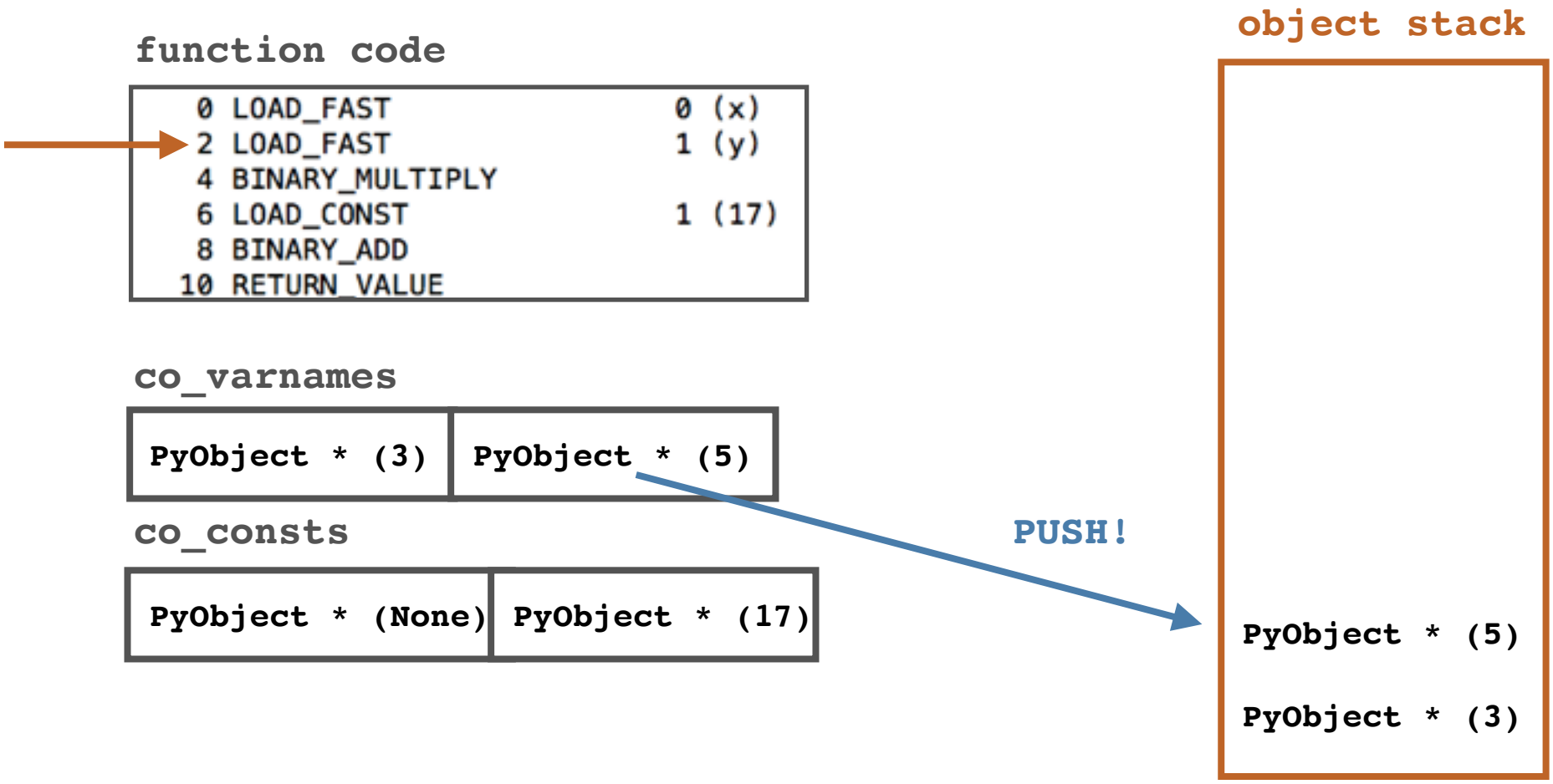

Example Function Invocation

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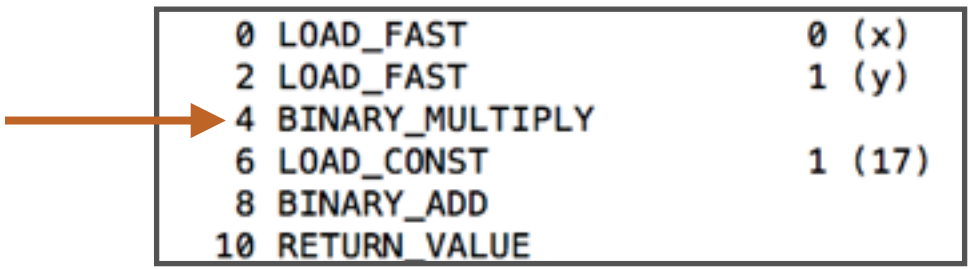
CALLED: foo(3, 5)

function code



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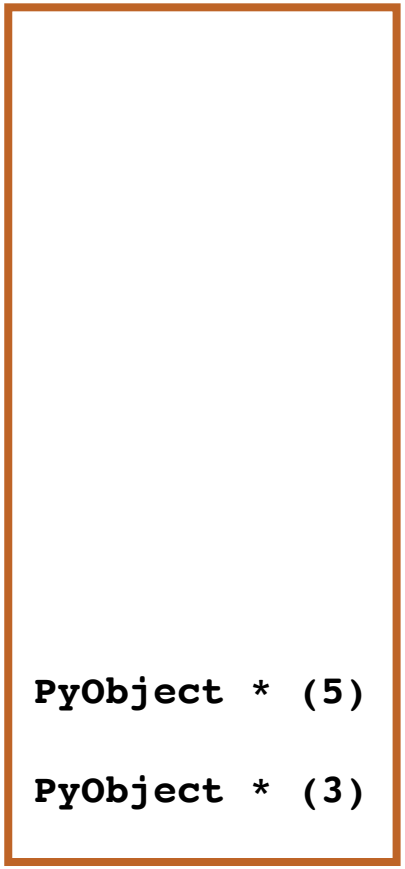
object stack



Example Function Invocation

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CALLED: foo(3, 5)

function code

```
  0 LOAD_FAST                0 (x)
  2 LOAD_FAST                1 (y)
  4 BINARY_MULTIPLY
  6 LOAD_CONST               1 (17)
  8 BINARY_ADD
 10 RETURN_VALUE
```

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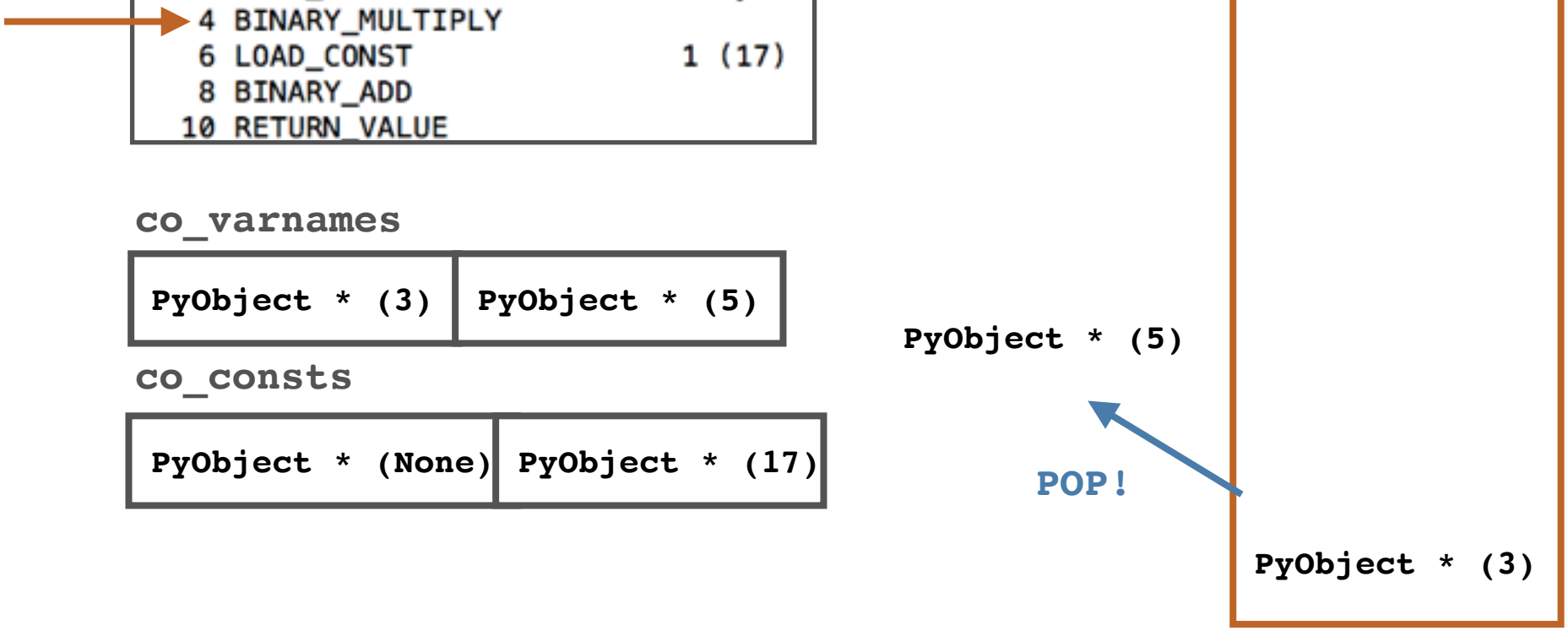

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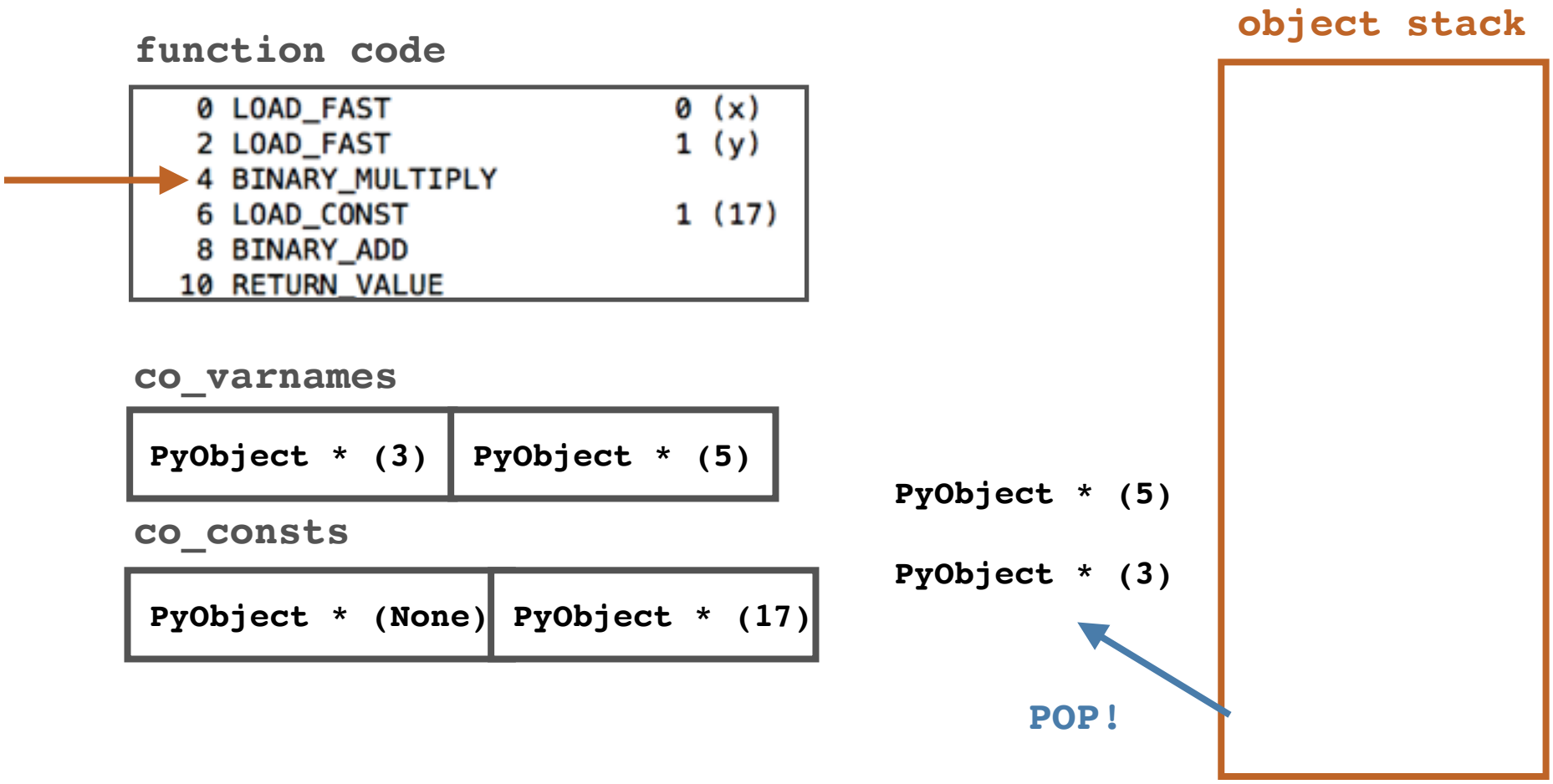

Example Function Invocation

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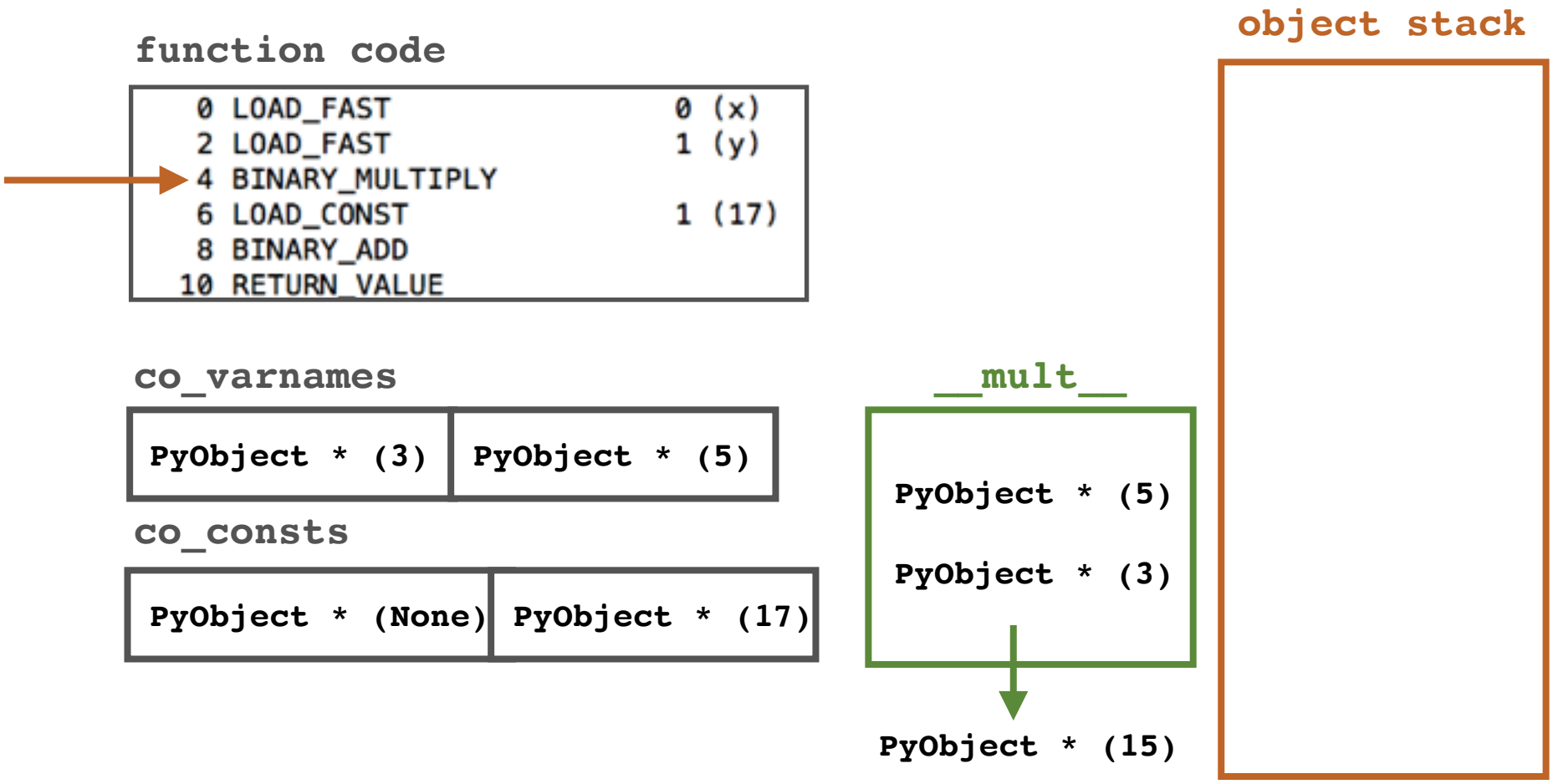
CALLED: foo(3, 5)



Example Function Invocation

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co_varnames

PyObject * (3)	PyObject * (5)

co_consts

PyObject * (None)	PyObject * (17)

object stack

PyObject * (15)

PyObject * (15)

PUSH!

Example Function Invocation

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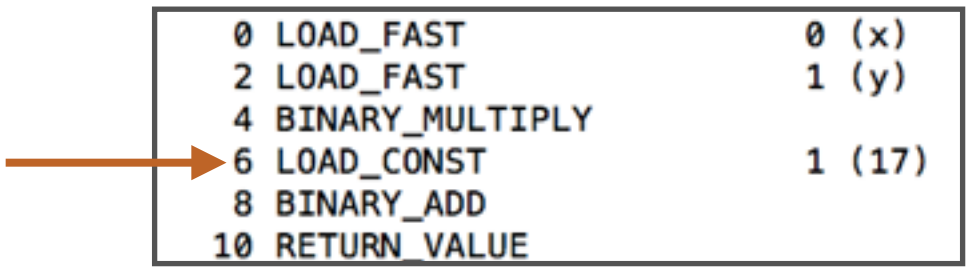
CALLED: foo(3, 5)

function code



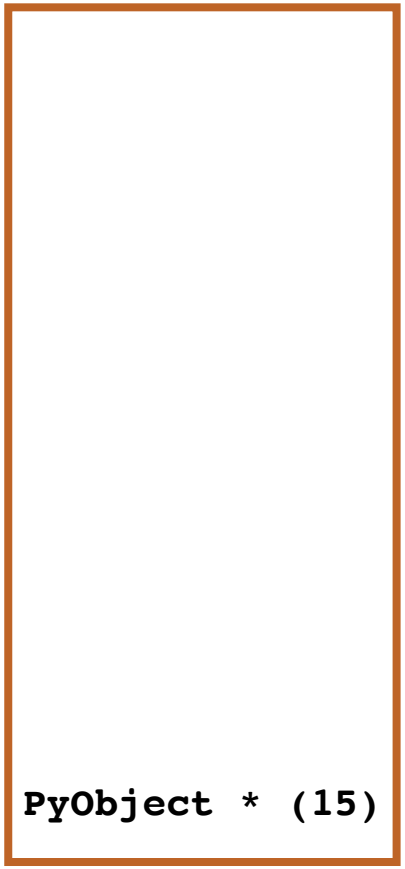
co_varnames

PyObject * (3)	PyObject * (5)

co_consts

PyObject * (None)	PyObject * (17)

object stack



Example Function Invocation

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CALLED: foo(3, 5)

function code

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```

co_varnames

PyObject * (3)	PyObject * (5)

co_consts

PyObject * (None)	PyObject * (17)

PUSH!

object stack

PyObject * (17)

PyObject * (15)

Example Function Invocation

ACCRE
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CALLED: foo(3, 5)

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```

co_varnames

PyObject * (3)	PyObject * (5)

co_consts

PyObject * (None)	PyObject * (17)

object stack

PyObject * (17)

PyObject * (15)

Example Function Invocation

ACCRE
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CALLED: foo(3, 5)

function code

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 10 RETURN_VALUE
```

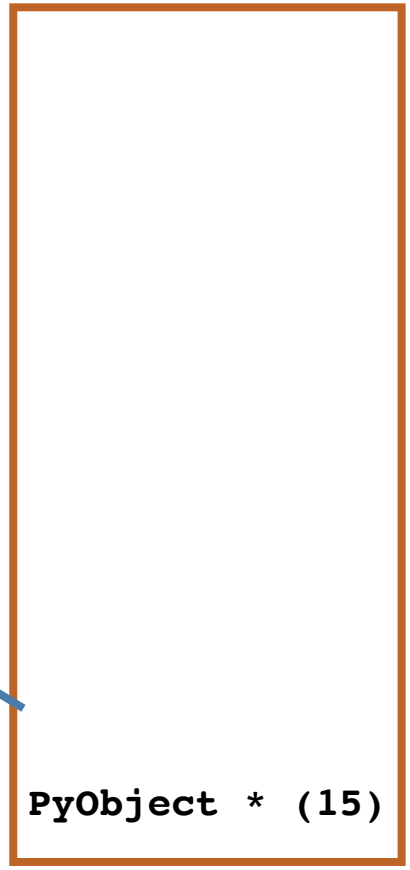
co_varnames

PyObject * (3)	PyObject * (5)

co_consts

PyObject * (None)	PyObject * (17)

object stack



Example Function Invocation

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CALLED: foo(3, 5)

function code

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  0 LOAD_FAST                0 (x)
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 10 RETURN_VALUE
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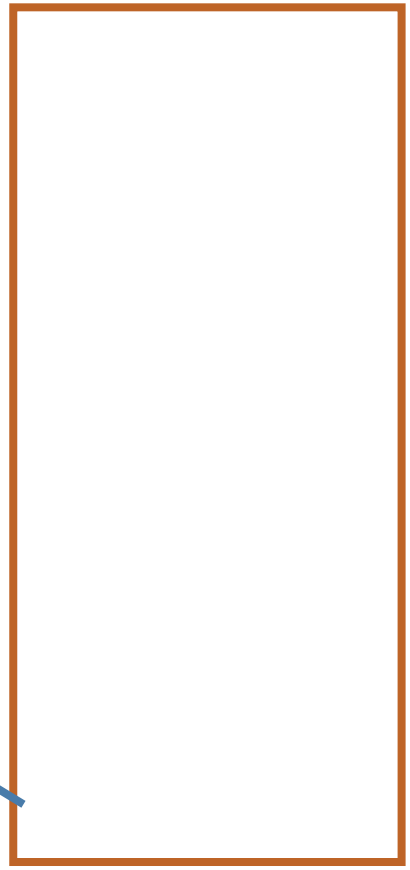
co_varnames

PyObject * (3)	PyObject * (5)

co_consts

PyObject * (None)	PyObject * (17)

object stack



Example Function Invocation

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CALLED: foo(3, 5)

function code

```
  0 LOAD_FAST                0 (x)
  2 LOAD_FAST                1 (y)
  4 BINARY_MULTIPLY
  6 LOAD_CONST               1 (17)
  8 BINARY_ADD
 10 RETURN_VALUE
```

co_varnames

PyObject * (3)	PyObject * (5)

co_consts

PyObject * (None)	PyObject * (17)

__add__

PyObject * (17)

PyObject * (15)

PyObject * (32)

object stack

Example Function Invocation

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CALLED: foo(3, 5)

function code

```
  0 LOAD_FAST                0 (x)
  2 LOAD_FAST                1 (y)
  4 BINARY_MULTIPLY
  6 LOAD_CONST               1 (17)
  8 BINARY_ADD
 10 RETURN_VALUE
```

co_varnames

PyObject * (3)	PyObject * (5)

co_consts

PyObject * (None)	PyObject * (17)

object stack

PyObject * (32)

PyObject * (32)

PUSH!

Example Function Invocation

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CALLED: foo(3, 5)

function code

```
  0 LOAD_FAST                0 (x)
  2 LOAD_FAST                1 (y)
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  6 LOAD_CONST               1 (17)
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 10 RETURN_VALUE
```

co_varnames

PyObject * (3)	PyObject * (5)

co_consts

PyObject * (None)	PyObject * (17)

object stack

PyObject * (32)

Example Function Invocation

ACCRE
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CALLED: foo(3, 5)

function code

```
  0 LOAD_FAST                0 (x)
  2 LOAD_FAST                1 (y)
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  6 LOAD_CONST               1 (17)
  8 BINARY_ADD
 10 RETURN_VALUE
```

co_varnames

PyObject * (3)	PyObject * (5)

co_consts

PyObject * (None)	PyObject * (17)

PyObject * (32)

POP!

object stack

PyObject * (32)

Example Function Invocation

ACCRE
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CALLED: foo(3, 5)

function code

```
  0 LOAD_FAST                0 (x)
  2 LOAD_FAST                1 (y)
  4 BINARY_MULTIPLY
  6 LOAD_CONST               1 (17)
  8 BINARY_ADD
 10 RETURN_VALUE
```

co_varnames

PyObject * (3)	PyObject * (5)

co_consts

PyObject * (None)	PyObject * (17)

(return to caller)

PyObject * (32)

object stack

Parallelism in Python

Matrix Inversion Example

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- Take some LU-decompositon and inversion example code written in pure python
- Run it serially over a set of random matrices
- Try improving performance by multithreading
- Try improving performance by multiprocessing

Example code in the repo if you (or I) fall behind!

About Concurrency

Concurrency vs Parallelism

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- Parallelism: Do multiple things at the same time
- Concurrency: Deal with multiple things going on at the same time
- Cooking example

Python supports multiple paradigms for achieving concurrent programming including os-level threads and also native coroutines

Python Coroutine Example

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```
import asyncio

import aiohttp

BASE_URL = 'https://ericappelt.com/animals/'


async def speak(animal, session):

    async with session.get('{}/{}'.format(BASE_URL, animal)) as response:
        response.raise_for_status()
        sound = await response.text()

    return 'The {} says "{}".'.format(animal, sound)
```

Day Two

Day 2 Outline

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- Packaging, pip, and anaconda
- Numpy
- Revisiting matrix inversions with numpy
- A quick tour of scientific packages
- Jupyter notebooks and literate programming
- Making pretty and interactive plots

Repo: https://github.com/appeltel/python-hpc-seminar

(repo has links, code examples, etc…)

External Libraries

Pip and Virtualenv

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- pip: download and additional python libraries
- pypi/warehouse: central repository for community libraries
- virtualenv: tool for managing lightweight python “environments” of installed libraries
- system python: Python installed as part of your operating system - you don’t want to mess with this

Pip and Virtualenv

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Quick Demo (… or read below if something goes wrong …)

```
eric@laptop:tmp$ python -m virtualenv venv
Using base prefix '/Users/eric/.pyenv/versions/3.6.2'
New python executable in /Users/eric/tmp/venv/bin/python
Installing setuptools, pip, wheel...done.
eric@laptop:tmp$ source venv/bin/activate
(venv) eric@laptop:tmp$ pip install numpy
Collecting numpy
  Downloading numpy-1.14.2-cp36-cp36m-macosx_10_6_intel.macosx_10_9_intel.ma
ntel.macosx_10_10_x86_64.whl (4.7MB)
    100% |████████████████████████████████| 4.7MB 193kB/s
Installing collected packages: numpy
Successfully installed numpy-1.14.2
(venv) eric@laptop:tmp$ python -c "import numpy as np; print(np.arange(5))"
[0 1 2 3 4]
(venv) eric@laptop:tmp$ deactivate
eric@laptop:tmp$ rm -r venv
eric@laptop:tmp$
```

ANACONDA

- Pre-packaged distribution of python and many scientific libraries and tools
- Tools for managing environments, installing yet more packages
- Available on ACCRE cluster via LMOD

Intro to Numpy

NUMPY

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NumPy is the fundamental package for scientific computing with Python. It contains among other things:

- a powerful N-dimensional array object
- sophisticated (broadcasting) functions
- tools for integrating C/C++ and Fortran code
- useful linear algebra, Fourier transform, and random number capabilities

Besides its obvious scientific uses, NumPy can also be used as an efficient multi-dimensional container of generic data. Arbitrary data-types can be defined. This allows NumPy to seamlessly and speedily integrate with a wide variety of databases.

Quickstart:

https://docs.scipy.org/doc/numpy-dev/user/quickstart.html

Exploring Numpy

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- Some experimentation on the REPL
- Revisiting the matrix inversion code
- Look at multithreading performance

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Tour of Libraries

SciPy

- The SciPy library provides user friendly numerical integration and optimization functions
- Built on NumPy
- SciPy.org is the organization maintaining numpy, scipy, and a set of related tools
- These tools are often referred to as the SciPy stack

Matplotlib

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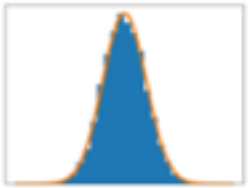
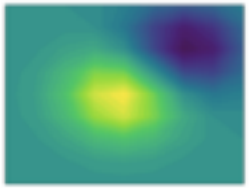
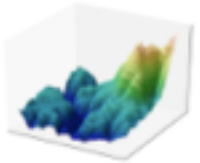
matplotlib

Matplotlib is a Python 2D plotting library which produces publication quality figures in a variety of hardcopy formats and interactive environments across platforms. Matplotlib can be used in Python scripts, the Python and IPython shells, the Jupyter notebook, web application servers, and four graphical user interface toolkits.

Pandas

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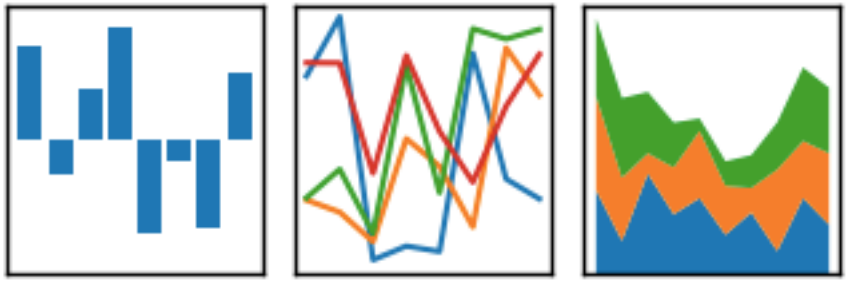
pandas

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



pandas is a Python package providing fast, flexible, and expressive data structures designed to make working with "relational" or "labeled" data both easy and intuitive. It aims to be the fundamental high-level building block for doing practical, **real world** data analysis in Python. Additionally, it has the broader goal of becoming **the most powerful and flexible open source data analysis / manipulation tool available in any language**. It is already well on its way toward this goal.

pandas is well suited for many different kinds of data:

- Tabular data with heterogeneously-typed columns, as in an SQL table or Excel spreadsheet
- Ordered and unordered (not necessarily fixed-frequency) time series data.
- Arbitrary matrix data (homogeneously typed or heterogeneous) with row and column labels
- Any other form of observational / statistical data sets. The data actually need not be labeled at all to be placed into a pandas data structure

Scikit-learn

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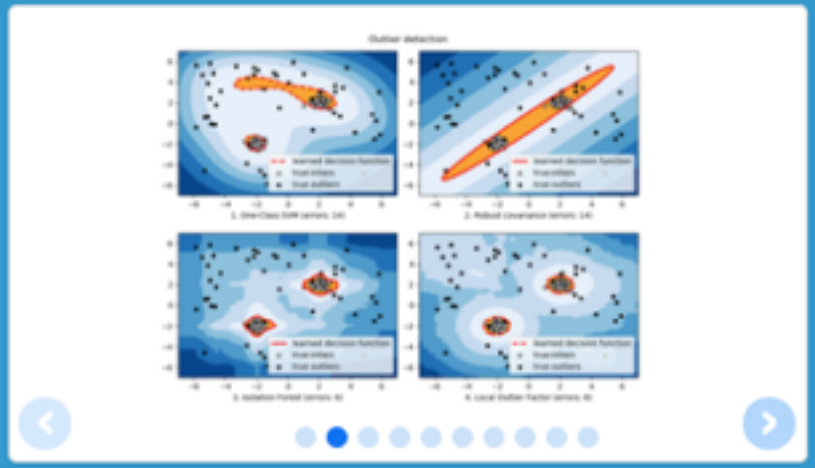

scikit-learn

Machine Learning in Python

- Simple and efficient tools for data mining and data analysis
- Accessible to everybody, and reusable in various contexts
- Built on NumPy, SciPy, and matplotlib
- Open source, commercially usable - BSD license

SCIKIT-LEARN: FREE CAPSTONE PROJECT IDEA

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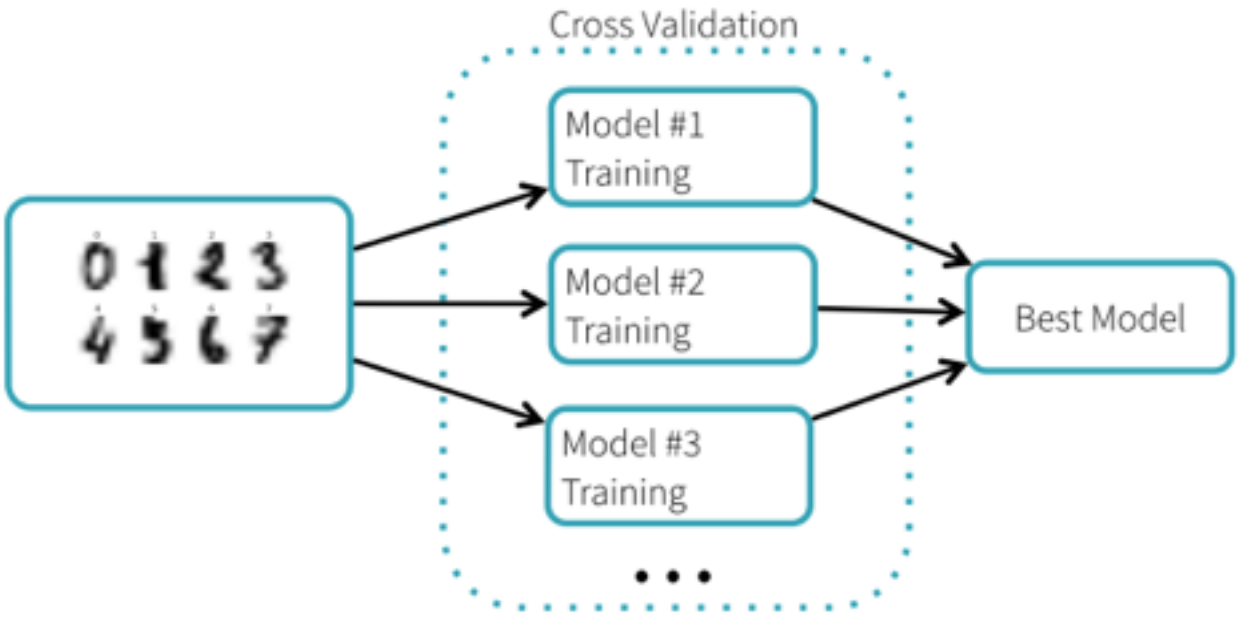
Training a random forest classifier to recognize handwritten digits:



Good candidate for parallelization and distribution over multiple cluster nodes, see:

https://databricks.com/blog/2016/02/08/auto-scaling-scikit-learn-with-apache-spark.html

SCIKIT-LEARN: FREE CAPSTONE PROJECT IDEA

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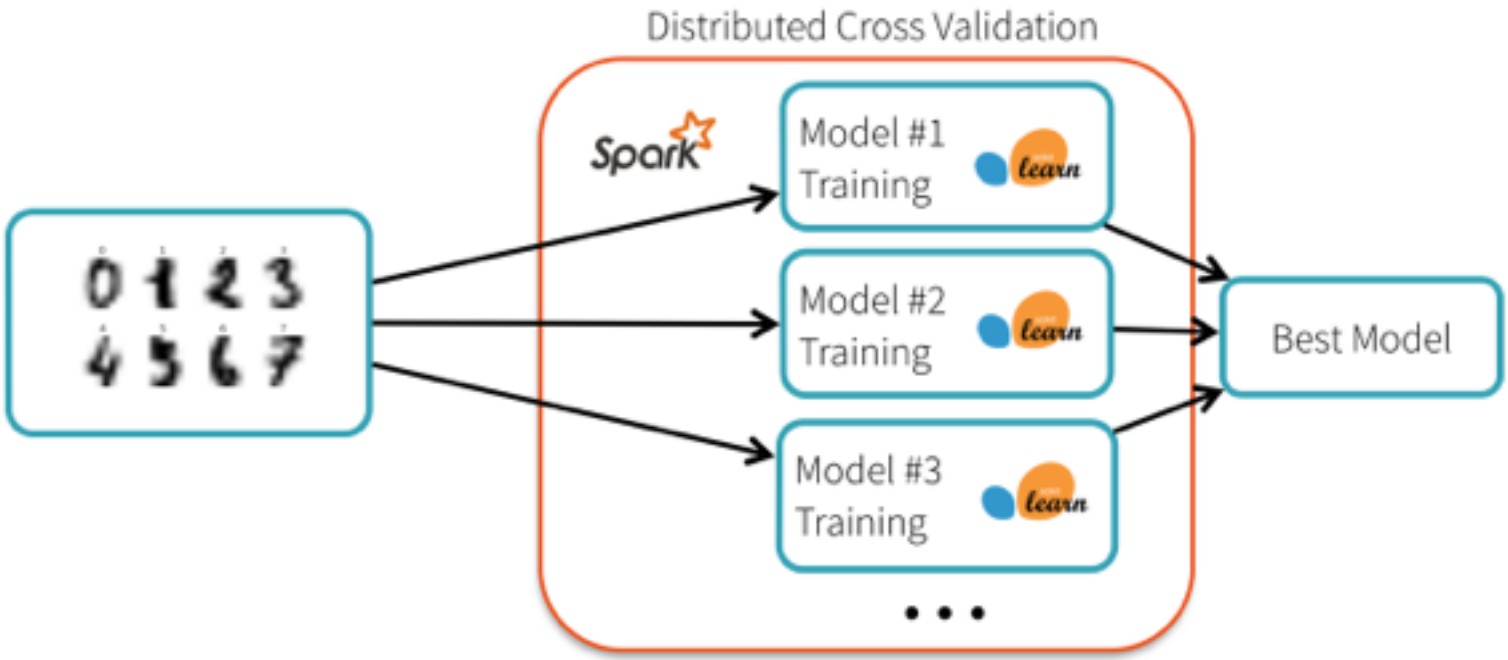
Easy to do on a spark cluster:



- Can it also be done within a slurm job that sets up a joblib cluster for the training?
- Can we use our big data cluster for this?
- How is ACCRE performance?

TENSORFLOW

- Numerical computation with data flow graphs
- Edges represent mathematical operations
- Vertices represent tensors (arrays, matrices)
- Common API for deployment to CPU/GPU
- Deep Learning applications

Fun demo of deep learning: playground.tensorflow.org

TENSORFLOW - IMAGE RECOGNITION

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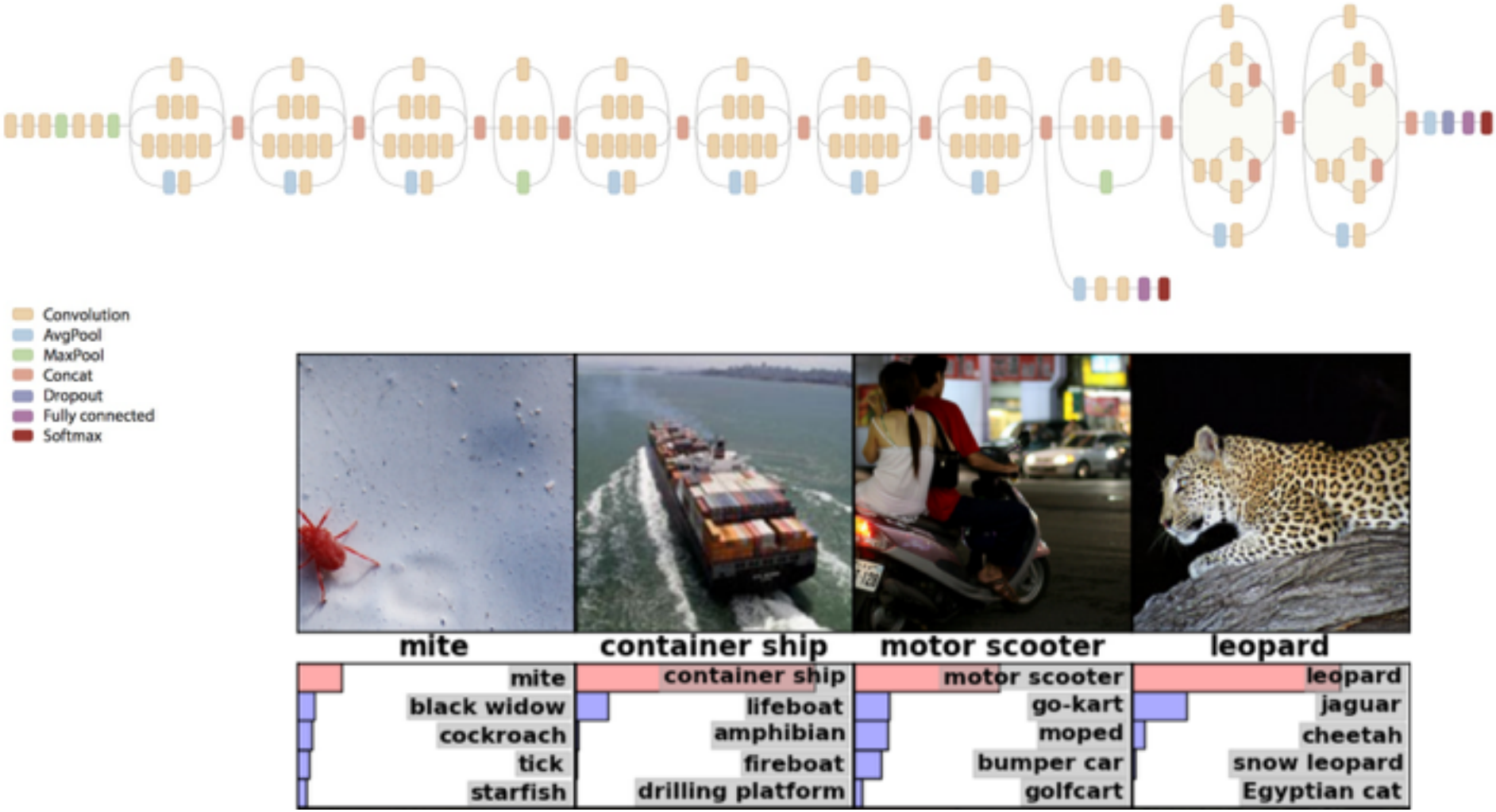
Inception-v3 model:



Jupyter Notebooks

JUPYTER NOTEBOOKS

- Interactive web application
- Embed live code, narrative, and visualizations into notebook files
- Can be run from the ACCRE cluster
- Not just python!

Jupyter Notebooks

- Do some demos
- You can run these directly out of the repo:
- https://github.com/appeltel/python-hpc-seminar