Software

RSE CONFERENCE 2018: GETTING MORE PYTHON PERFORMANCE WITH INTEL® OPTIMIZED DISTRIBUTION FOR PYTHON

Plan for the Workshop: What do YOU want to do?

We have a bit under 90 minutes…

I have a bunch of slides, but we can skip through fast.

We have three hands-on examples

- kmeans clustering (`04_kmeans`) shows
  - Intel optimization benefit in a machine learning application
  - Intel® Vtune profiling
- Black-Scholes shows
  - Profiling (timing in Python, using Intel® Vtune)
  - Use of numpy, numba, Cython (general approaches to Python performance optimization)
- SVM shows
  - How to use scikit-learn for handwritten digit recognition
  - Intel performance gains if you compare runs with/without Intel Python

Proposal: short intro, kmeans (until we've had enough), Black-Scholes

MORE PERFORMANCE USING INTEL® DISTRIBUTION FOR PYTHON

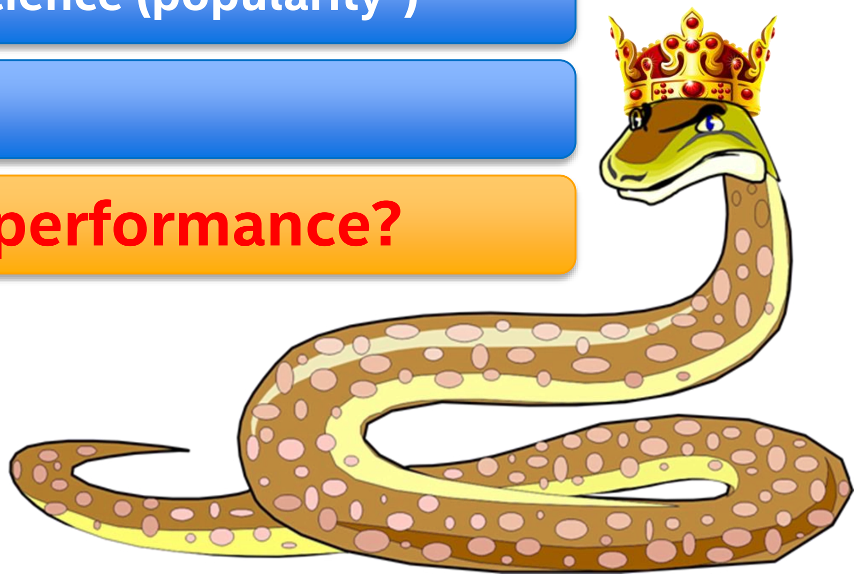
Most Wanted: Python

~7.8 Million out of ~21 Million developers use python (EDC 2016)

#1 language for machine learning/data science (popularity[1])

>100000 python packages on PyPI

But...often slow. Can we get better performance?



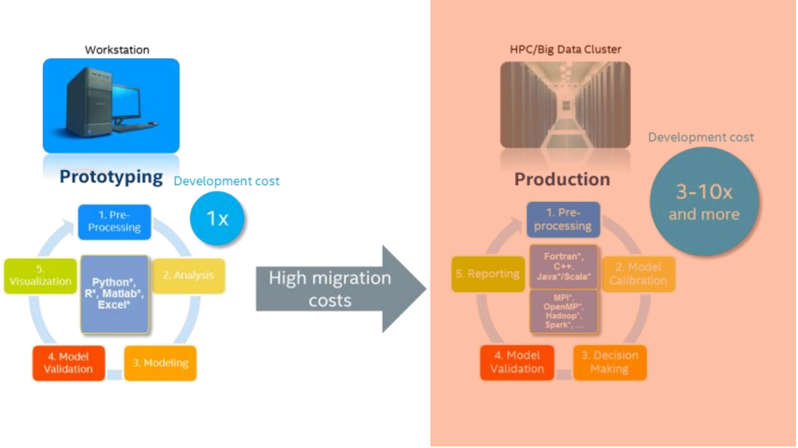
[1] https://www.kdnuggets.com/2017/01/most-popular-language-machine-learning-data-science.html

Faster Python* with Intel® Distribution for Python 2018

High Performance Python Distribution

- Accelerated NumPy, SciPy, scikit-learn well suited for scientific computing, machine learning & data analytics
- Drop-in replacement for existing Python. **No code changes required**
- Highly optimized for latest Intel processors
- **Free for everyone**, or pay to get Priority Support – a direct connection with Intel engineers for technical questions

Get sufficient performance without an extra development cycle



What's Inside Intel® Distribution for Python

High Performance Python* for Scientific Computing, Data Analytics, Machine Learning

HIGHER PERFORMANCE	GREATER PRODUCTIVITY	ECOSYSTEM COMPATIBILITY
Performance Libraries, Parallelism, Multithreading, Language Extensions	**Prebuilt & Accelerated Packages**	**Supports Python 2.7 & 3.6, conda, pip**
Accelerated NumPy/SciPy/scikit-learn with Intel® MKL[1] & Intel® DAAL[2]	Prebuilt & optimized packages for numerical computing, machine/deep learning, HPC, & data analytics	Compatible & powered by Anaconda*, supports conda & pip
Data analytics, machine learning & deep learning with scikit-learn, pyDAAL	Drop in replacement for existing Python - **No code changes required**	Distribution & individual optimized packages also available at conda & Anaconda.org, YUM/APT, Docker image on DockerHub
Scale with Numba* & Cython*	Jupyter* notebooks, Matplotlib included	Optimizations upstreamed to main Python trunk
Includes optimized mpi4py, works with Dask* & PySpark*	Conda build recipes included in packages	Commercial support through Intel® Parallel Studio XE 2017
Optimized for latest Intel® architectures	**Free download & free for all uses including commercial deployment**	

Intel® Architecture Platforms

Operating System: Windows*, Linux*, MacOS[1]*

[1]Intel® Math Kernel Library
[2]Intel® Data Analytics Acceleration Library

[1] Available only in Intel® Parallel Studio Composer Edition.

Installing Intel® Distribution for Python* 2018

Standalone Installer

Download full installer from
https://software.intel.com/en-us/intel-distribution-for-python

ANACONDA CLOUD

anaconda.org
anaconda.org/intel channel

```
> conda config --add channels intel
> conda install intelpython3_full
> conda install intelpython3_core
```

python™ Package Index

pip
Intel-optimized packages

```
> pip install intel-<pkg-name>
```

Docker Hub
docker

Docker Hub

```
> docker pull intelpython/intelpython3_full
```

YUM/APT
repositories

yum/apt

Access for yum/apt:
https://software.intel.com/en-us/articles/installing-intel-free-libs-and-python

What's New? Intel® Distribution for Python*

What's New in 2018 version

- Updated to latest version of Python 3.6
- Optimized scikit-learn for machine learning speedups
- Conda build recipes for custom infrastructure

What's new in 2019 beta?

Faster Machine learning with Scikit-learn functions

- Support Vector Machine (SVM) and K-means prediction, accelerated with Intel® DAAL

Built-in access to XGBoost library for Machine Learning

- Access to Distributed Gradient Boosting algorithms

Ease of access installation

- Now integrated into Intel® Parallel Studio XE installer.

Access Intel-optimized Python packages through

ACCELERATE PYTHON* PERFORMANCE

Software.intel.com/en-us/distribution-for-python

ANACONDA CLOUD

python Package Index

Docker Hub

docker

YUM/APT

repositories

OUT-OF-THE-BOX PERFORMANCE WITH ACCELERATED NUMERICAL PACKAGES

NUMPY & SCIPY OPTIMIZATIONS

- BLAS/LAPACK using MKL
- MKL-based FFT functionality
- Vectorized, threaded universal functions
  - Use of Intel® C Compiler, and Intel® Fortran Compiler
  - Aligned memory allocation
- Threaded memory copying

https://github.com/IntelPython/mkl_random

MKL-BASED RANDOM NUMBER GENERATION

- Added numpy subpackage numpy.random_intel that mirrors numpy.random in the scope
- Exposes all basic random number generators provided in Intel® MKL.

```
In [3]: import numpy as np, numpy.random_intel as irnd, numpy.random as vrnd

In [4]: irnd.seed(1234,brng='SFMT19937')

In [5]: %time x1 = irnd.randn(10**6)
        CPU times: user 4 ms, sys: 4 ms, total: 8 ms
        Wall time: 7.73 ms

In [6]: %time x2 = vrnd.randn(10**6)
        CPU times: user 44 ms, sys: 0 ns, total: 44 ms
        Wall time: 44.8 ms
```

Intel random number generator

Default numpy random number generator

MKL-BASED FFT

https://github.com/IntelPython/mkl_fft

Intel® Math Kernel Library provides:

- Full stride support, no extra copying
- In-place & out-of-place transforms
- Native support for ND-transforms
- Support for double and single precision

```
In [1]: import scipy.fftpack, numpy as np

In [2]: size = (23, 45, 34)
        x = np.random.randn(*size) + 1j*np.random.randn(*size)
        x = x.T

In [3]: y = scipy.fftpack.fftn(x,overwrite_x=True)

In [4]: y is x

Out[4]: True
```

OPTIMIZED UNIVERSAL FUNCTION LOOPS

Compiler-generated vectorized instructions

with automatic run-time dispatching for different architectures

Vectorized transcendental functions

using Intel® Compiler's SVML

Threaded evaluation

using Intel® MKL's Vector Math Library.

But Wait…There’s More!

Moving beyond optimized Python*, how efficient is your Python/C/C++ application code?

Are there any hard to find sources of performance loss?

Performance analysis gives the answer!

INTRODUCTION TO INTEL® VTUNE™ FOR PYTHON

Tune Python* + Native Code for Better Performance

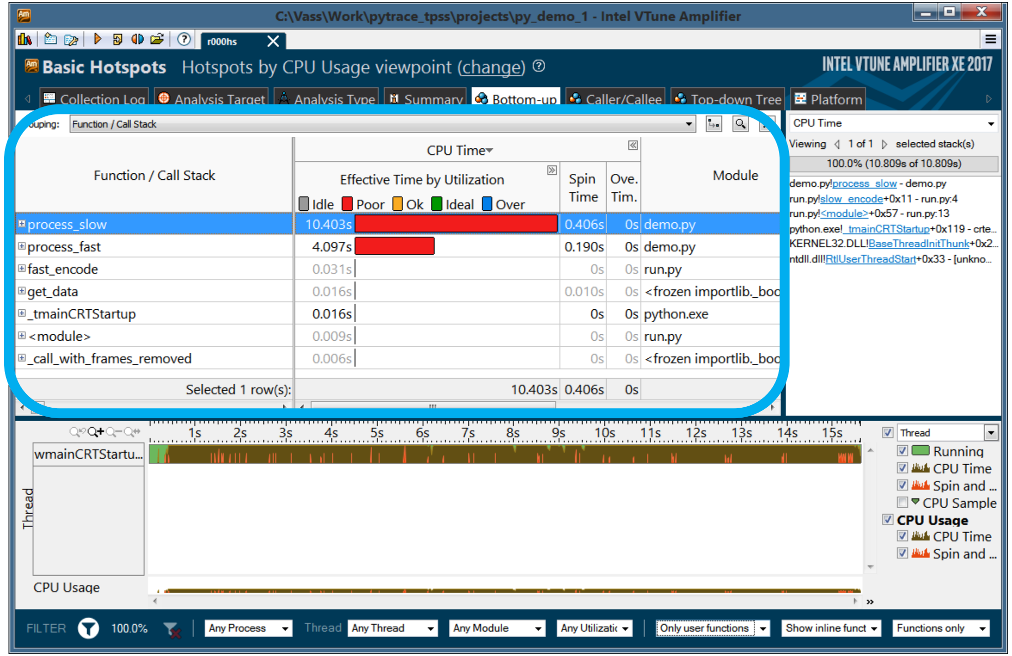
Analyze Performance with Intel® VTune™ Amplifier (available in Intel® Parallel Studio XE)

Challenge

- Single tool that profiles Python + native mixed code applications
- Detection of inefficient runtime execution

Solution

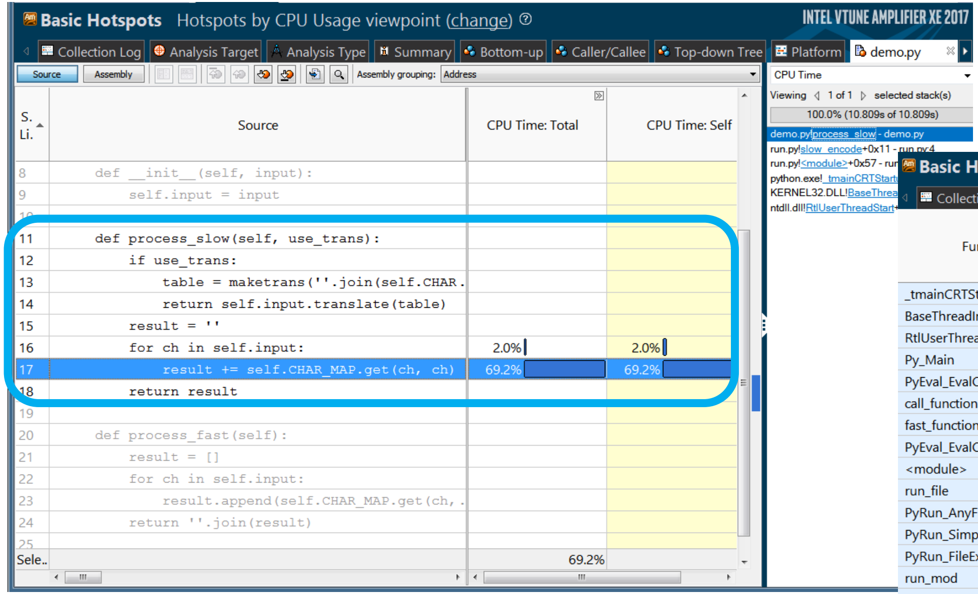
- Auto-detect mixed Python/C/C++ code & extensions
- Accurately identify performance hotspots at line-level
- Low overhead, attach/detach to running application
- Focus your tuning efforts for most impact on performance



Auto detection & performance analysis of Python & native functions

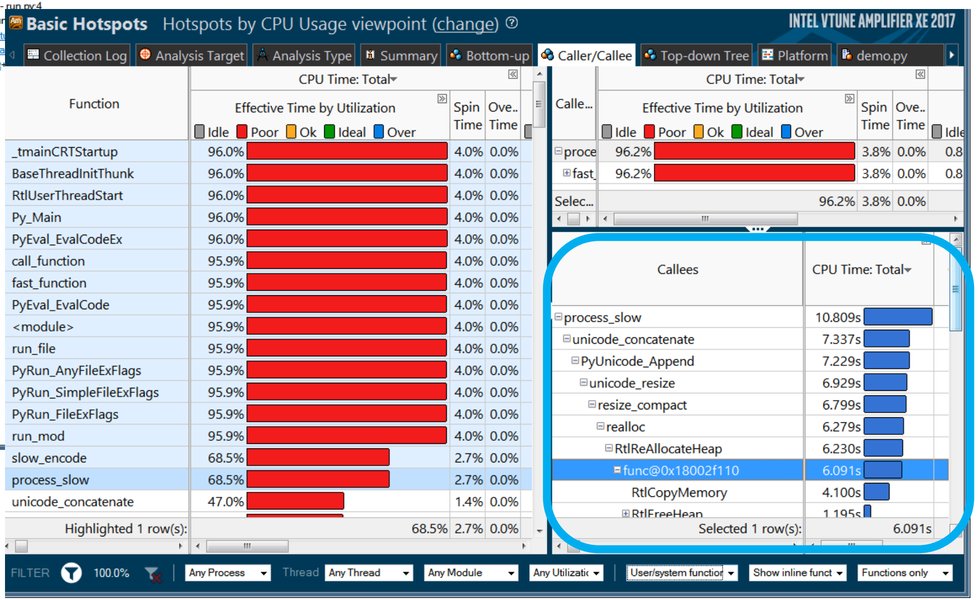
Available in Intel® VTune™ Amplifier & Intel® Parallel Studio XE

Diagnose Problem code quickly & accurately



Identifies exact line of code that is a bottleneck

Details Python* calling into native functions



A two-pronged approach to Higher Python* Performance

Step 1: Use Intel® Distribution for Python

- Leverage optimized native libraries for performance
- Drop-in replacement for your current Python - **no code changes required**
- Optimized for multi-core and latest Intel processor

Step 2: Use **Intel® VTune™ Amplifier** for profiling

- Get detailed summary of entire application execution profile
- Auto-detects & profiles Python/C/C++ mixed code & extensions with low overhead
- Accurately detect hotspots - line level analysis helps you to make smart optimization decisions fast!
- Available in Intel® Parallel Studio XE Professional & Cluster Edition

More Resources

Intel® Distribution for Python

- Product page – overview, features, FAQs…
- Training materials – movies, tech briefs, documentation, evaluation guides…
- Support – forums, secure support…

Intel® VTune Amplifier

- Product page – overview, features, FAQs…
- Training materials – movies, tech briefs, documentation, evaluation guides…
- Reviews
- Support – forums, secure support…

USING CONDA

Conda

Package manager

- install/remove packages
- handles dependences
- also non-python packages (such as native libs)

Environments

- isolate different sets of packages/versions
- creates hard-links when possible
- similar to virtualenv

Conda basics

Getting started

- conda --help
- conda list
- conda search numpy
- conda search numpy -c intel -c conda-forge

Environments

- conda env list
- conda create -n sandbox -c intel python=3.6
- source activate sandbox
- conda list

- Package management
  - conda install numpy
  - conda remove numpy

Jupyter Notebooks

NOTEBOOKS

- Interactive (via web browser)
- Python, markup, and shell (and other)
- Python kernel running
- Cells get executed individually
- State is carried over between cell execution
- Output appears back in the notebook
- Can also be used to run julia codes (ask me about Julia later if you're interested!)

Preparing hands-on sessions

```
% To enable Vtune profiling (password: workshops)
sudo bash
echo 0 > /proc/sys/kernel/yama/ptrace_scope
exit
cd ~/Cownie
source conda.sh
conda deactivate
% To use pre-installed code (easier...)
conda activate intel_env
% Or, to update packages if you have internet access
conda create -n <your_env_name> -c intel python=3.6 \
notebook numpy mpi4py matplotlib numexpr numba cython
conda activate <your_env_name>
source /opt/intel/vtune_amplifier/amplxe-vars.sh
which amplxe-cl && which amplxe-gui && which icc
cd material
which python
jupyter notebook
```

Hands-on files

Initial versions of the codes are at the top level in files with obvious names

- These may be incomplete, and require that you fill in some code

Suggested solutions are in … the `solutions` sub-directory

Hands-On: Kmeans

Cluster Analysis

Problems

A news provider wants to group the news with similar headlines in the same section

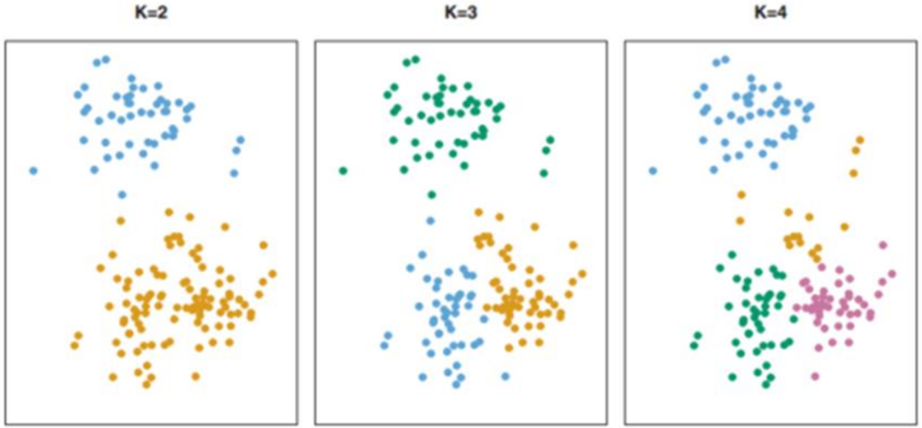
Humans with similar genetic pattern are grouped together to identify correlation with a specific disease

Solution: K-Means

Pick ***k*** centroids

Repeat until converge:

- Assign data points to the closest centroid
- Re-calculate centroids as the mean of all points in the current cluster
- Re-assign data points to the closest centroid



Source: Gareth James, Daniela Witten, Trevor Hastie, Robert Tibshirani. (2014). *An Introduction to Statistical Learning*. Springer

Hands-On Example: Kmeans (1)

Use kmeans clustering to choose an optimal small number of colours to compress an image

Use `04_kmeans.ipynb` and walk through the code.

- To see original performance, disable Intel optimizations by finding this and executing it before running the code.

```
from sklearn.daal4sklearn import dispatcher
# TODO: Disable Intel-optimizations (DAAL) and repeat fit and predict and get timings
# call disable() on dispatcher before calling KMeans
dispatcher.disable()
```

- Don't worry about the deprecated function used for reading the image.

Hands-On Example: Kmeans (2)

- You could profile this version, or just change this to enable(), as below, run that cell and then run the fit again.

```
from sklearn.daal4sklearn import dispatcher
# TODO: Disable Intel-optimizations (DAAL) and repeat fit and predict and
get timings
# call disable() on dispatcher before calling KMeans
dispatcher.enable()
```

Kmeans conclusions

With no code changes at all Intel® Distribution for Python can give >100x speedup on this machine-learning code (precise gain will depend on the machine you are running on, of course, you'd get more on a many core server…)

We started to use Intel® Vtune Amplifier

- Saw that it can show us parallelism
- Saw that it can show us Python code up the call tree from the expensive operations

HANDS-ON PYTHON PERFORMANCE TOOLS
PERFORMANCE TOOLS APPLIED TO BLACK SCHOLES

Hands-On Example : Black-Scholes What is Black-Scholes?

A Financial Services Industry benchmark (sorry ☺)

It is used for option pricing

Luckily we don't need to understand the details of the theory

From our point of view

- It is a relatively small piece of scientific Python
- It uses transcendental functions (`log, exp, erf, sqrt`)
- It's small enough to play with but big enough to show some general principals

Black Scholes – Naïve

Naïve

Plain obvious python

Kernel works on vectors and scalars

Output 2 vectors

Use timeit, cprofile and line profiler

Using parallelism implicitly

Similar syntax
- Vector based (no loop)
- List -> np.array
- Import from numpy

Numpy

Mathematical building blocks

Universal functions (ufuncs) operate on vectors

Under the hood accelerates computation (e.g. with Intel® MKL)

NumExpr

Hands-On Numpy

Black Scholes option pricing: `01_numpy_blackscholes.ipynb`

Numpy

Naïve '[]' are lists, not arrays

Numpy provides fast array implementation

- contiguous memory
- written in C

Numpy also provides optimized operations on arrays

- vector/array/scalar operations allow calling vectorized libraries
- Umath dispatches to right vector/array/scalar implementation

- Intel-optimized Numpy is accelerated with Intel® Math Kernel Library
- Also accelerates FFT, RNG, Umath, …

Using parallelism under the hood

Numpy

NumExpr

Evaluates strings of numeric expressions

Internally translates to numpy ufuncs

Hands-On numexpr

Black Scholes option pricing: 02_numexpr_blackscholes.ipynb

Compiling Python

Numba

Just-In-Time (LLVM-based, produces parallel code)

Decorators annotate functions

JIT API

Cython

Hands-On numba

Black Scholes option pricing: 03_numba_blackscholes.ipynb

Compiling Python - Numba

Decorators

Defining instantiations

GIL, nopython

API and target

Hands-On: Support Vector Machine classifier

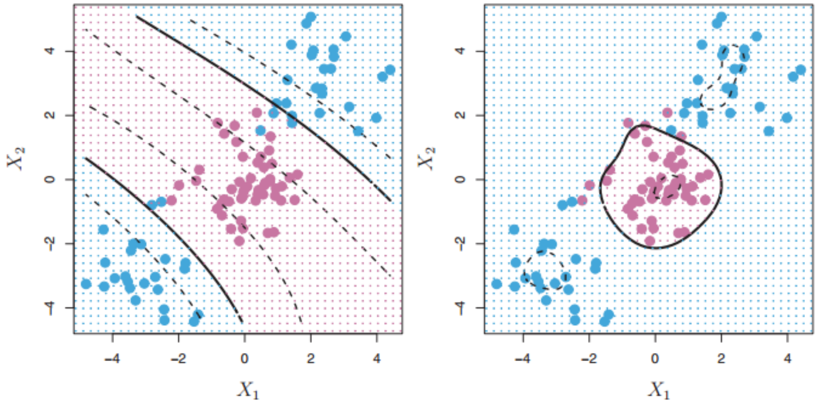
Classification

Problems

- An emailing service provider wants to build a spam filter for the customers
- A postal service wants to implement handwritten address interpretation

Solution: Support Vector Machine (SVM)

- Works well for non-linear decision boundary
- Two kernel functions are provided:
  - Linear kernel
  - Gaussian kernel (RBF)
- Multi-class classifier
  - One-vs-One



Source: Gareth James, Daniela Witten, Trevor Hastie, Robert Tibshirani. (2014). *An Introduction to Statistical Learning.* Springer

Hands-On: SVM

`05_svm.ipynb`

Performs digit recognition for handwritten numerals

Conclusions and learning points are similar to Kmeans

Key Points from the Workshop

Intel® Distribution for Python

- Is **FREE** for everyone and any use (commercial included)
  - If you want guaranteed support you can pay
- Can be installed via `conda`, `pip`, … so it should be easy to add to your environment
- Can hugely improve the performance of *some* unmodified Python code (especially popular areas like ML/DL)
  - Uses threads
  - Uses optimised, vectorized, parallelized, maths libraries

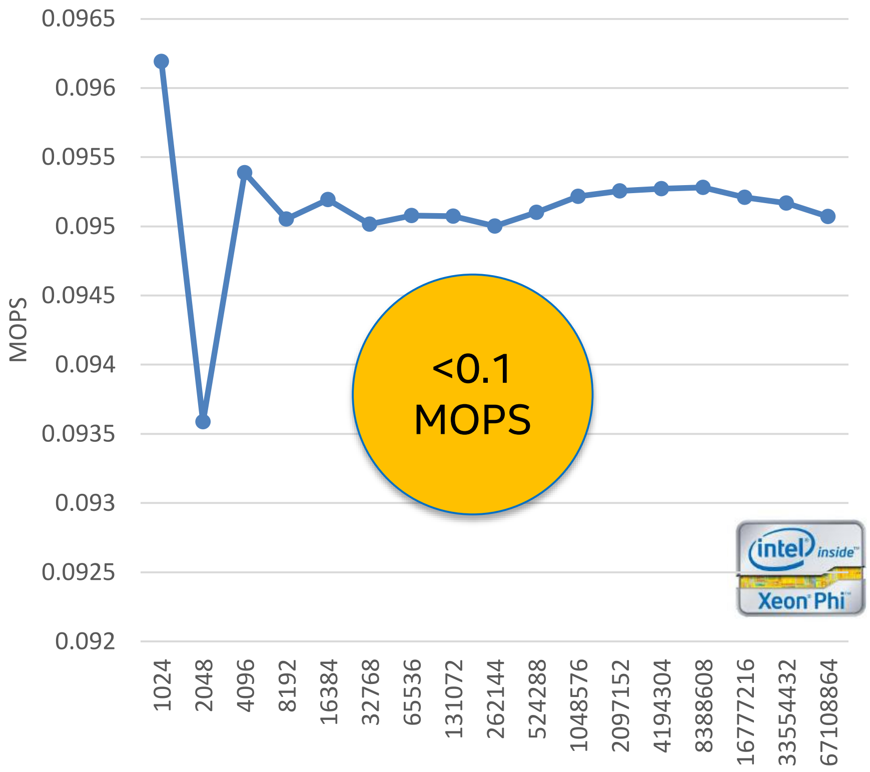
Intel® Vtune™ Amplifier

- Is **FREE** for educators and students
- Can profile mixed Python and compiled code (so you can attribute time in native code back to the Python which called it)

THE END

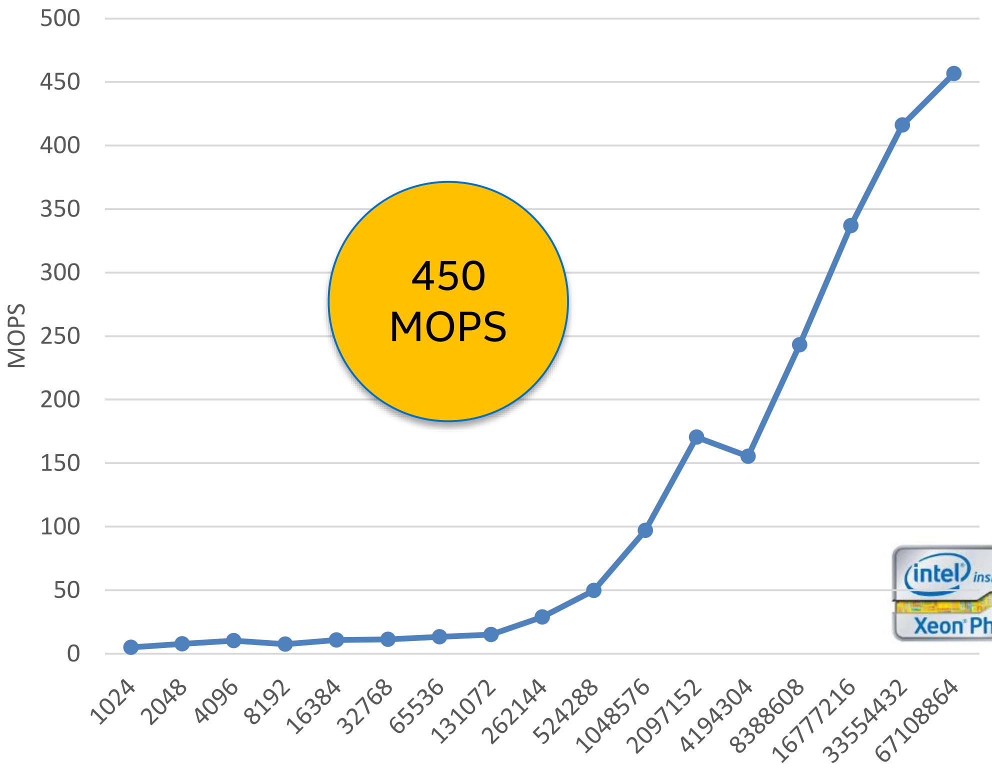
BACKUP

Variant 1: Plain Python



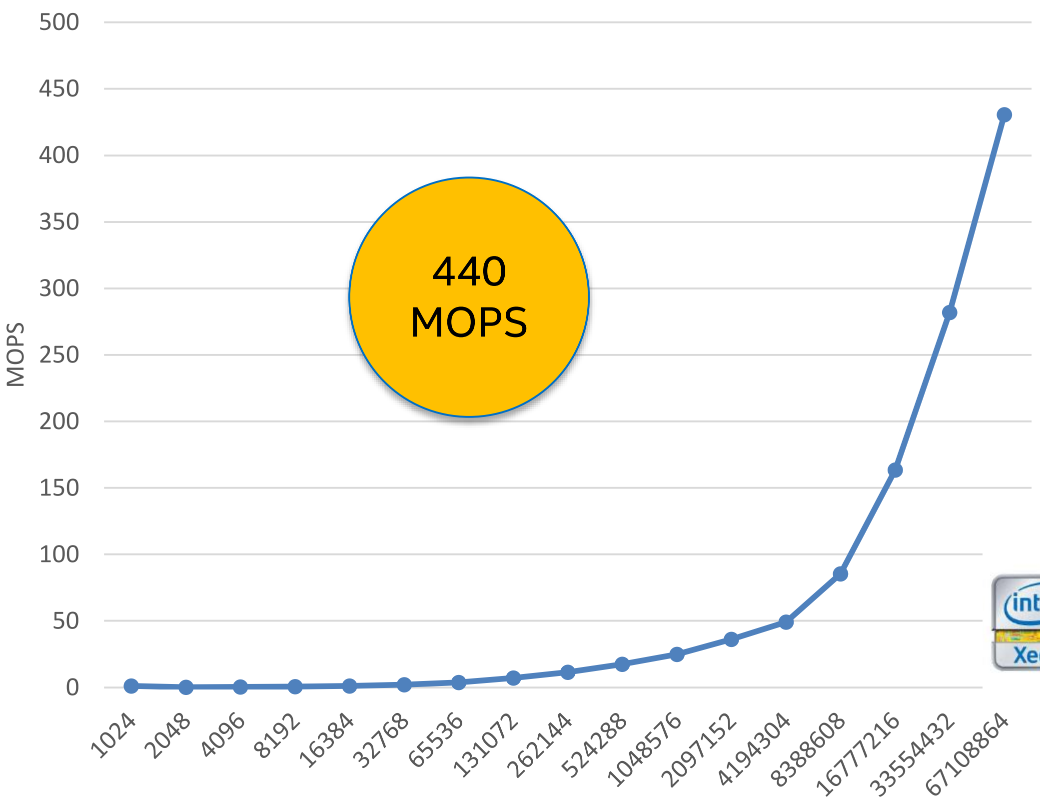

```python
def black_scholes ( nopt, price, strike, t, rate, vol, call, put ):
    mr = -rate
    sig_sig_two = vol * vol * 2

    for i in range(nopt):
        P = float( price [i] )
        S = strike [i]
        T = t [i]

        a = log(P / S)
        b = T * mr

        z = T * sig_sig_two
        c = 0.25 * z
        y = 1/sqrt(z)

        w1 = (a - b + c) * y
        w2 = (a - b - c) * y

        d1 = 0.5 + 0.5 * erf(w1)
        d2 = 0.5 + 0.5 * erf(w2)

        Se = exp(b) * S

        call [i] = P * d1 - Se * d2
        put [i] = call [i] - P + Se
```

Variant 2: NumPy* arrays and Umath functions




```python
def black_scholes ( nopt, price, strike, t, rate, vol ):
        mr = -rate
        sig_sig_two = vol * vol * 2

        P = price
        S = strike
        T = t

        a = log(P / S)
        b = T * mr

        z = T * sig_sig_two
        c = 0.25 * z
        y = invsqrt(z)

        w1 = (a - b + c) * y
        w2 = (a - b - c) * y

        d1 = 0.5 + 0.5 * erf(w1)
        d2 = 0.5 + 0.5 * erf(w2)

        Se = exp(b) * S

        call = P * d1 - Se * d2
        put = call - P + Se

        return call, put
```

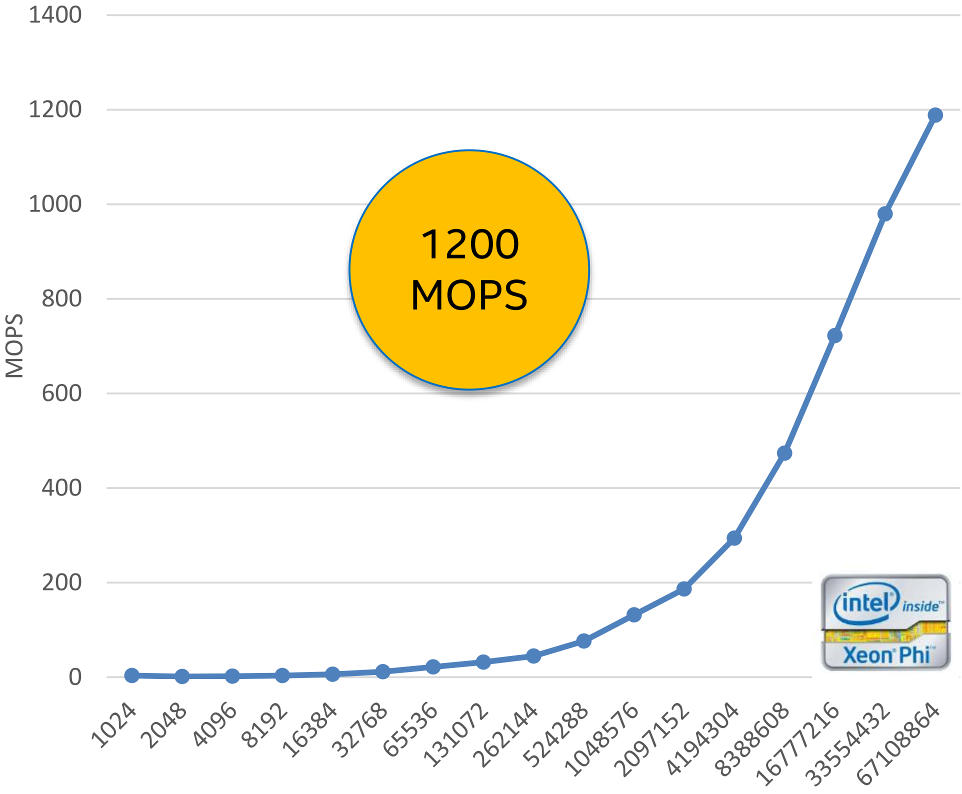
Variant 3: NumExpr* (proxy for Umath implementation)




```python
import numexpr as ne

def black_scholes ( nopt, price, strike, t, rate, vol ):
        mr = -rate
        sig_sig_two = vol * vol * 2

        P = price
        S = strike
        T = t

        a = ne.evaluate("log(P / S) ")
        b = ne.evaluate("T * mr ")

        z = ne.evaluate("T * sig_sig_two ")
        c = ne.evaluate("0.25 * z ")
        y = ne.evaluate("1/sqrt(z) ")

        w1 = ne.evaluate("(a - b + c) * y ")
        w2 = ne.evaluate("(a - b - c) * y ")

        d1 = ne.evaluate("0.5 + 0.5 * erf(w1) ")
        d2 = ne.evaluate("0.5 + 0.5 * erf(w2) ")

        Se = ne.evaluate("exp(b) * S ")

        call = ne.evaluate("P * d1 - Se * d2 ")
        put = ne.evaluate("call - P + Se ")

        return call, put

ne.set_num_threads(ne.detect_number_of_cores())
base_bs_erf.run("Numexpr", black_scholes)
```

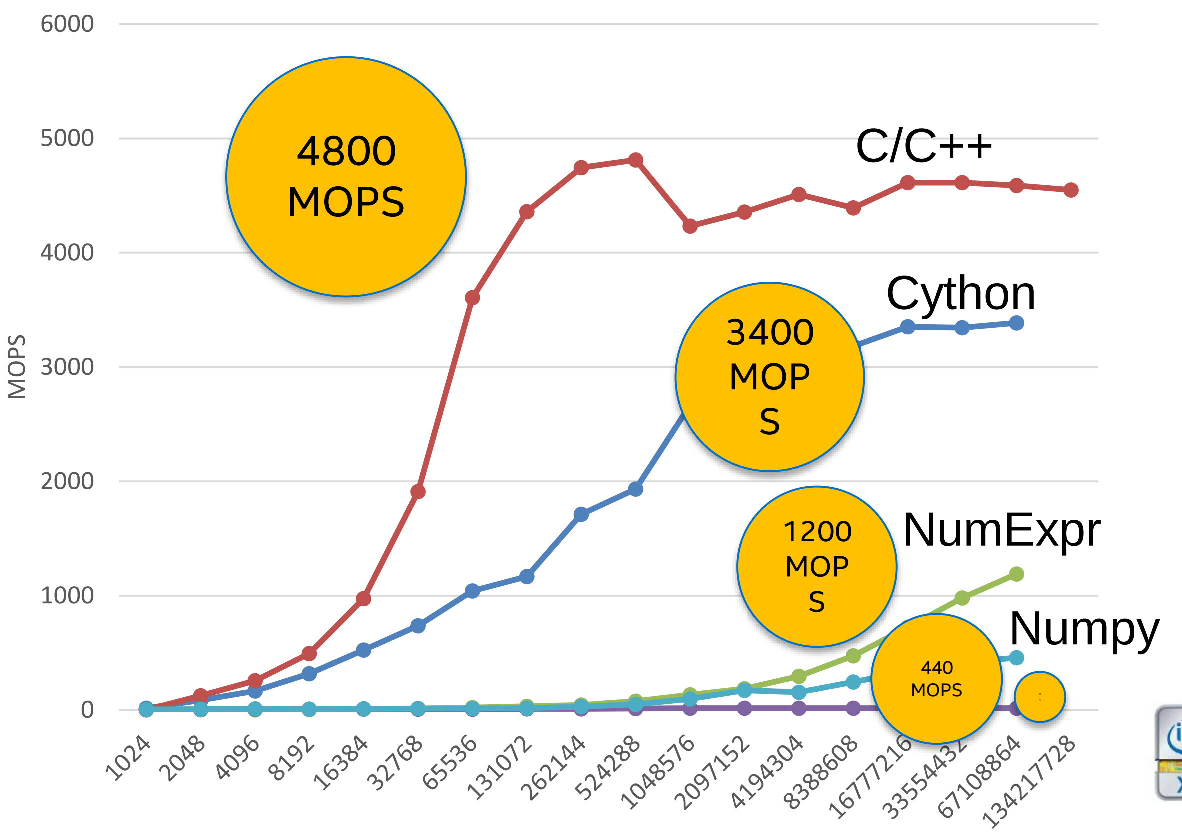
Optimization Notice

Variant 4: NumExpr* (most performant)




```python
import base_bs_erf
import numexpr as ne

def black_scholes ( nopt, price, strike, t, rate, vol ):
    mr = -rate
    sig_sig_two = vol * vol * 2

    P = price
    S = strike
    T = t

    call = ne.evaluate("P * (0.5 + 0.5 * erf((log(P / S) - T * mr +" +
    "0.25 * T * sig_sig_two) * 1/sqrt(T * sig_sig_two))) - S * exp(T * mr)*" +
    "(0.5 + 0.5 * erf((log(P / S) - T * mr - 0.25 * T * sig_sig_two) *" +
    "1/sqrt(T * sig_sig_two))) ")
    put = ne.evaluate("call - P + S * exp(T * mr) ")

    return call, put
```

Variant 5: Native C/C++ vs. Python variants



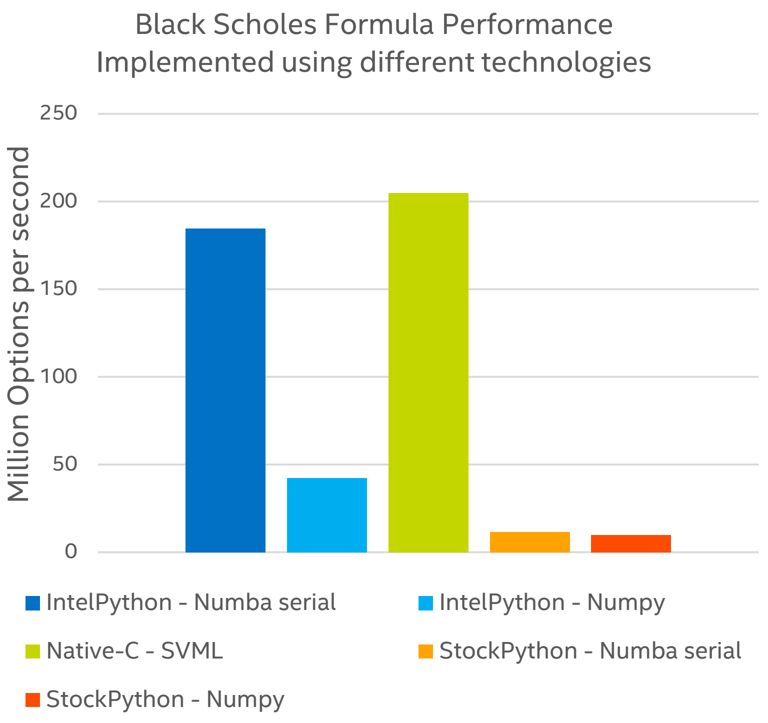
Optimizing NumPy, SciPy, NumExpr to scale

Data Analytics pipelines do not always fully match Machine Learning library functions

- Need to implement custom data transformations
- Need to provide custom optimization functions/kernels
- … And these are performance hotspots sometimes

Pure Python implementation kills performance but there are better alternatives within Python

- NumPy – array programming
- Cython – compiles Python code into native executable
- Numba – JIT compiler to accelerate performance hotspots



Configuration Info: Intel® Xeon® Gold 6140 CPU @ 2.30GHz (2 sockets, 18 cores per socket, 1 thread per core - HT is off), 256GB DDR4. Stock Python: CentOS Linux release 7.3.1611 (Core), python 3.6.4, numpy 1.14.0, numba 0.36.2, llvmlite 0.21.0. Intel® Distribution for Python 2018 Update 2 packages: python 3.6.3 intel_8, numpy 1.14.0 intel_3, numba 0.36.2 intel_2, llvmlite 0.21.1 (intel), mkl 2018.0.2 intel_1, openmp 2018.0.1 intel_0 intel®

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Notice revision #20110804

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CONFIGURATION INFORMATION

Hardware:

Intel® Core™ i7-7567U CPU @ 3.50GHz (1 socket, 2 cores per socket, 2 threads per core), 32GB DDR4 @ 2133MHz
Intel® Xeon® CPU E5-2699 v4 @ 2.20GHz (2 sockets, 22 cores per socket, 1 thread per core - HT is off), 256GB DDR4 @ 2400MHz
Intel® Xeon Phi™ CPU 7250 @ 1.40GHz (1 socket, 68 cores per socket, 4 threads per core), 192GB DDR4 @ 1200MHz, 16GB MCDRAM @ 7200MHz in cache mode

Software:

Stock: CentOS Linux release 7.3.1611 (Core), python 3.6.2, pip 9.0.1, numpy 1.13.1, scipy 0.19.1, scikit-learn 0.19.0
Intel® Distribution for Python 2018 Gold packages: mkl 2018.0.0 intel_4, daal 2018.0.0.20170814, numpy 1.13.1 py36_intel_15, openmp 2018.0.0 intel_7, scipy 0.19.1 np113py36_intel_11, scikit-learn 0.18.2 np113py36_intel_3