# Accelerate Python Loops with the Intel AI Analytics Toolkit

Workshop

Workshop #2 in series
Module 1: Aggregations, universal functions, and broadcasting, sorting

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# Learning Objectives

- At the end of the workshop you will be able to:
  - Describe a Python loop replacement strategy using NumPy constructs which improves readability, maintainability, performs fasts on current hardware and readies code for future HW & SW accelerations that Intel builds into silicon and which are exposed via NumPy
  - Describe NumPy clause to aid sorting, aggregations, reductions, broadcasting, and “where” and “select” to significantly accelerate your Python code
  - Describe the value of the Intel oneAPI AI Analytics Toolkit
  - Describe underlying reasons for the acceleration due to NumPy powered by oneAPI

# Intel® oneAPI AI Analytics Toolkit

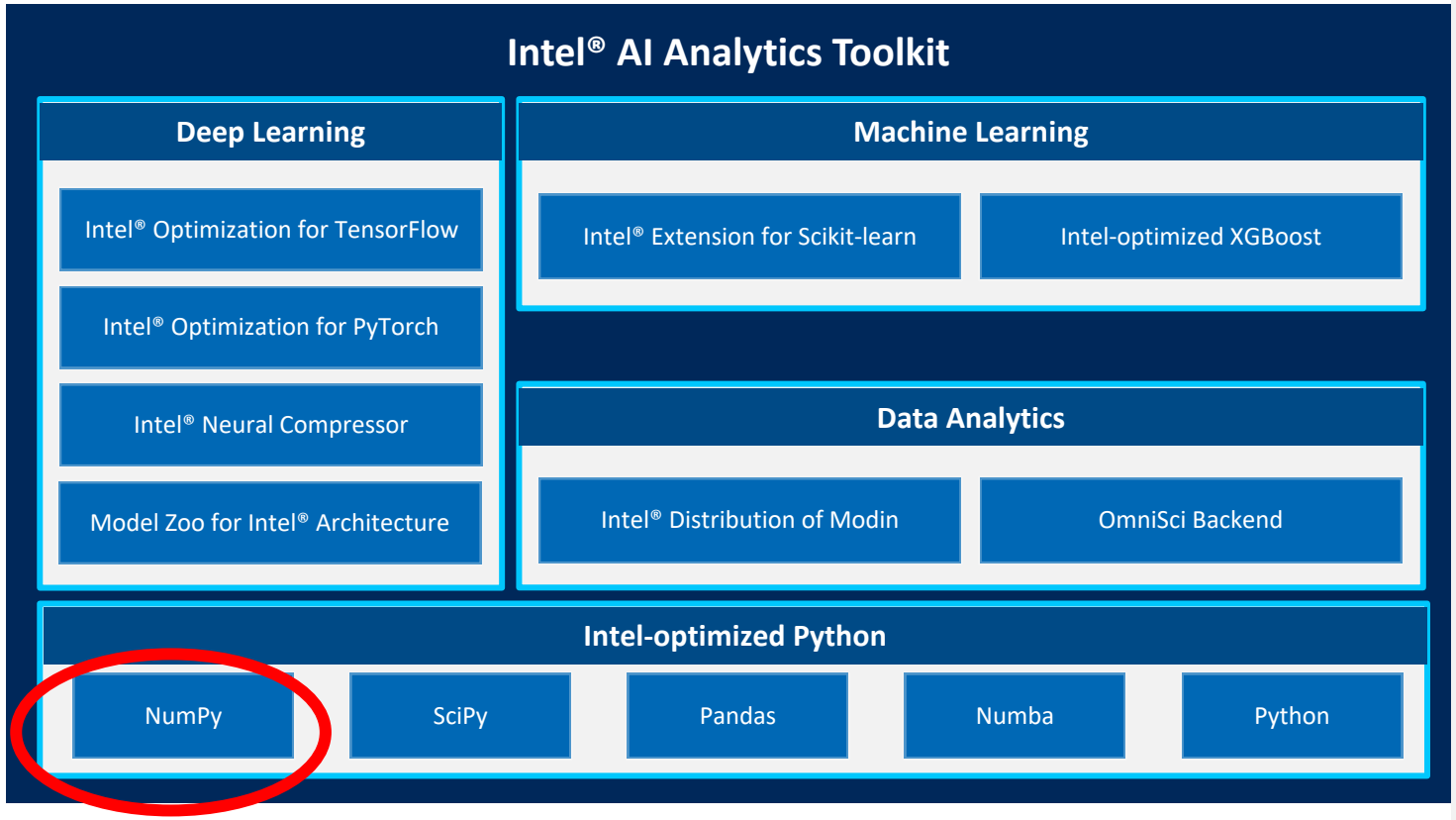
Accelerate end-to-end AI and data analytics pipelines with libraries optimized for Intel® architectures

## Who Uses It?

Data scientists, AI researchers, ML and DL developers, AI application developers

## Top Features/Benefits

- Deep learning performance for training and inference with Intel optimized DL frameworks and tools
- Drop-in acceleration for data analytics and machine learning workflows with compute-intensive Python packages




CPU GPU

Hardware support varies by individual tool. Architecture support will be expanded over time.

Get the Toolkit HERE or via these locations

Intel Installer | Docker | Apt, Yum | Conda | Intel® DevCloud

Learn More: software.intel.com/oneapi/ai-kit



Back to Domain-specific Toolkits for Specialized Workloads

# Intel® AI Analytics Toolkit

## Deep Learning

- Intel® Optimization for TensorFlow
- Intel® Optimization for PyTorch
- Intel® Neural Compressor
- Model Zoo for Intel® Architecture

## Machine Learning

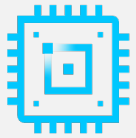
- Intel® Extension for Scikit-learn
- Intel-optimized XGBoost

## Data Analytics

- Intel® Distribution of Modin
- OmniSci Backend

## Intel-optimized Python

- NumPy
- SciPy
- Pandas
- Numba
- Python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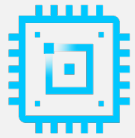
GPU

Hardware support varies by individual tool. Architecture support will be expanded over time.

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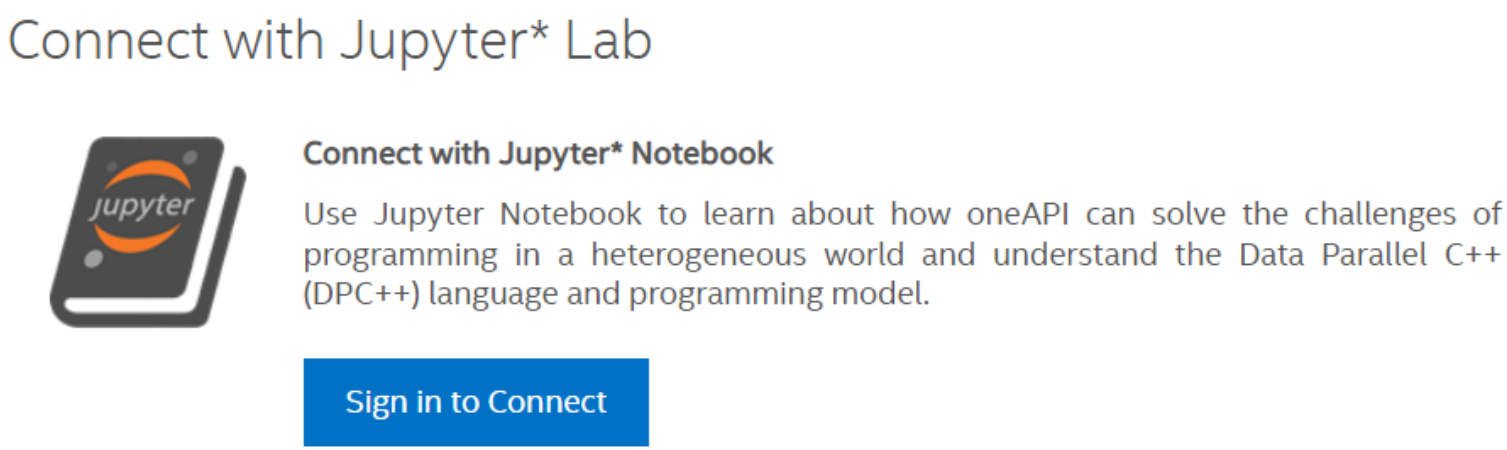
# Intel DevCloud

Register Using QR Code
Click Jupyter Icon link to sign in
**https://devcloud.intel.com/oneapi/get_started/**




- **Follow the ReadMe:**
- **github.com/IntelSoftware/Machine-Learning-using-oneAPI/blob/main/README.md**

# Numpy – powered by oneAPI

- Stock version has oneAPI included
- Download oneAPI analytics toolkit here (get latest functionality here first)
- Are you getting the performance you expect using NumPy?
- Are you using NumPy effectively?
- Note: Keep NumPy library up to date
- Are you using NumPy effectively?

# Python is Great & Fast …

- For rapidly proto typing ideas
- Tackling just about every imaginable coding task
- Getting project rolling quickly … Examples of code are everywhere
- Easy: Dynamically typed – making programming easy
- Easy & Fast: : Leverage huge number of libraries, easily installable
- For AI: fast/no porting: easy portability of models across architectures

# Python is SLOW


- **For some things:**
- **REPEATED** low level tasks
- Large loops
- Nested Loops
- List comprehensions (if large)

- **BUT**
- There are ways to mitigate its weaknesses
- Take advantage of those libraries
- **NUMPY** – this is **powered by oneAPI !**
- And others!

# Numpy Vectorization:

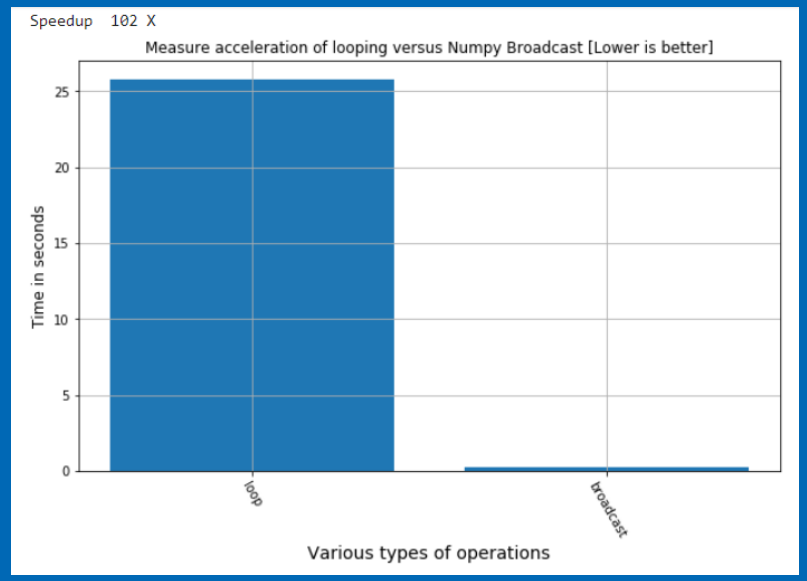
- This practice of replacing explicit loops with array expressions is commonly referred to as vectorization. In general, vectorized array operations will often be one or two (or more) orders of magnitude faster than their pure Python equivalents, with the biggest impact [seen] in any kind of numerical computations. - Wes McKinney

# Vectorization is NOT just theory!

You will **see**, **hear** about the speedups possible, then you will **experience** it in code

This is why we strongly encourage the use of libraries powered by Intel oneAPI such as Numpy, Scipy, and the rest

Get the goodness of Python but inherit vectorization speed inherent with Numpy powered by Intel oneAPI

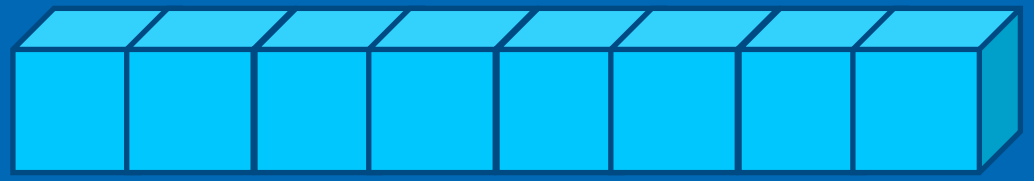



100 X speed up using Numpy broadcasting versus loop

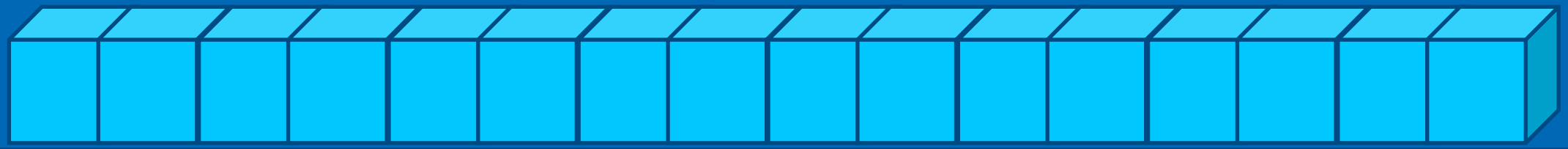
# Why are these speedup so dramatic?

- Numpy takes advantage of vectorization: powered by Intel oneAPI
- Specifically, oneMKL, for vectorization
- Vector width allows multiple operations in single HW instruction.
- Many FP instructions computed in single instruction

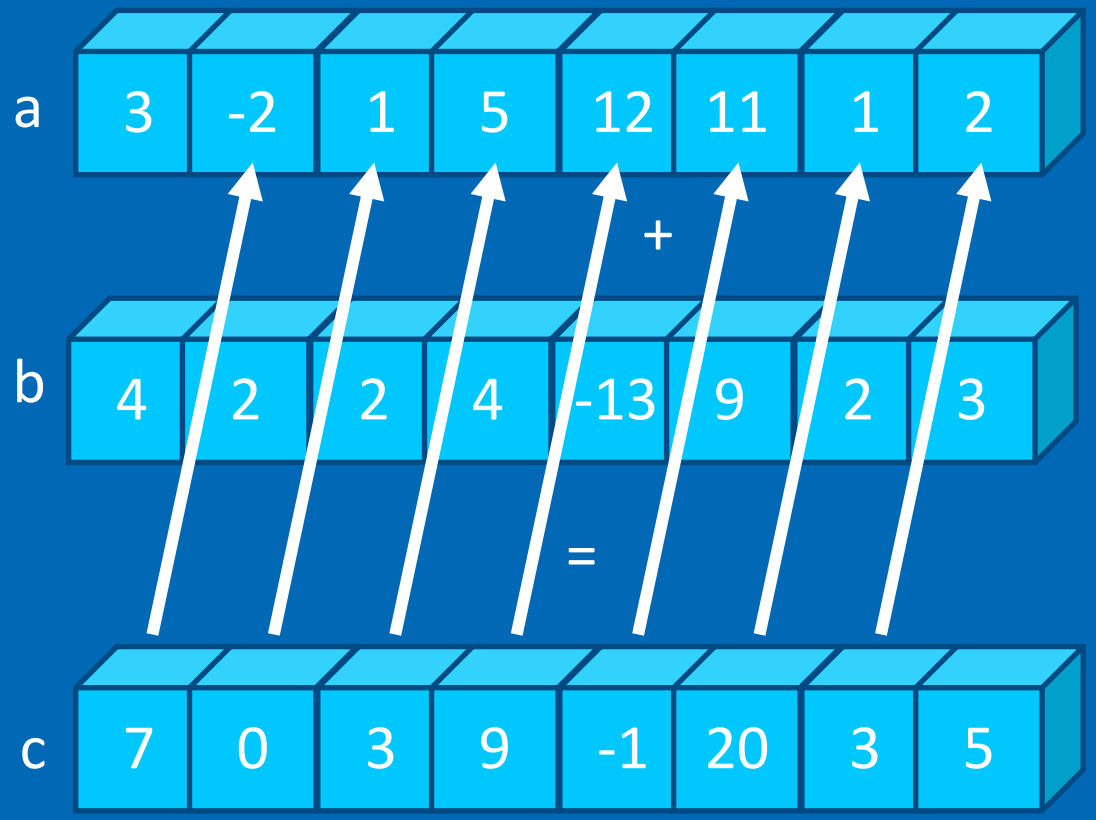
AVX2: 256 bits: 8 floats wide



AVX512: 512 bits: 16 floats wide



# SIMD in a Nutshell




Loopy: ( done one at a time)

```
for i in range(1,8):
    c[i] = a[i] + b[i]
```

SIMD: (all 8 locations done at once via SIMD instructions)

```
c = a + b
```

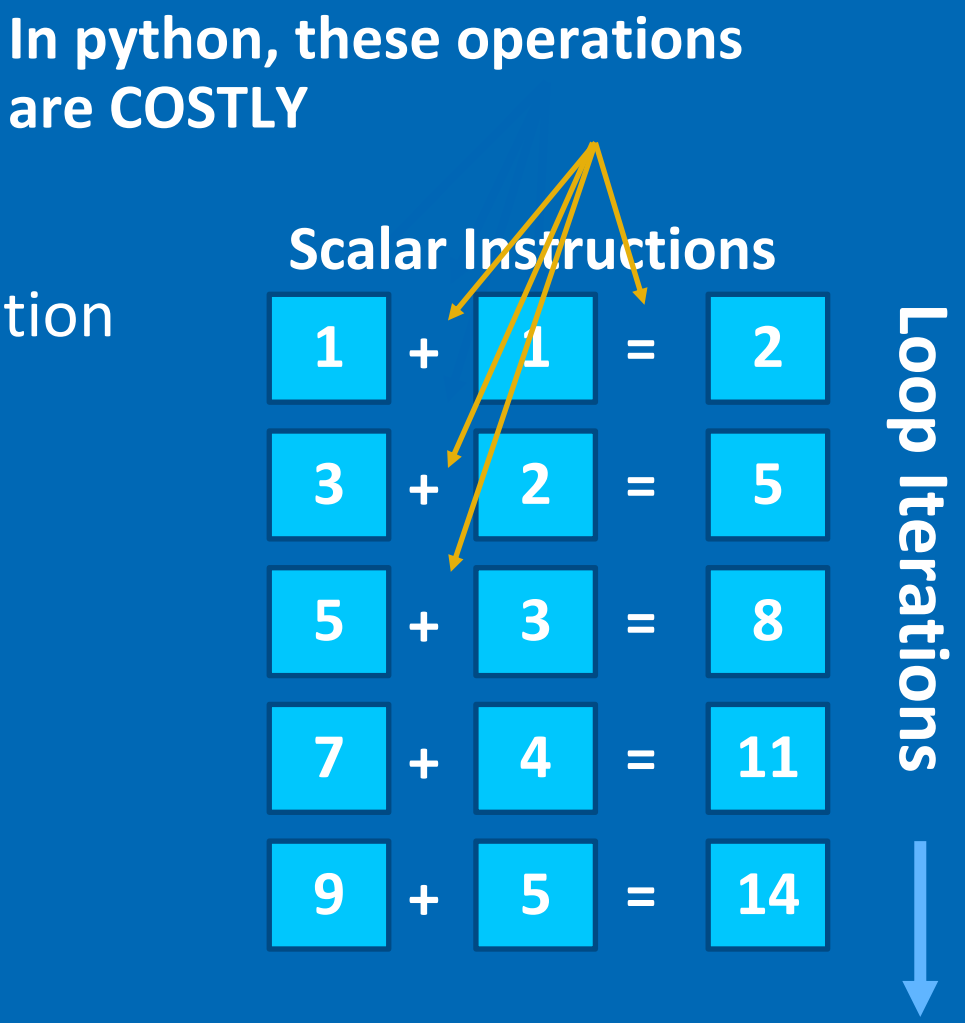
# We are comparing to simple loops in Python

Python is dynamically typed

- Has to **check** the data type before any operation to ensure correct operations are applied

Even a simple integer is not simple

- A class or structure that contains
  - reference counters and other values
  - These are updated every operation

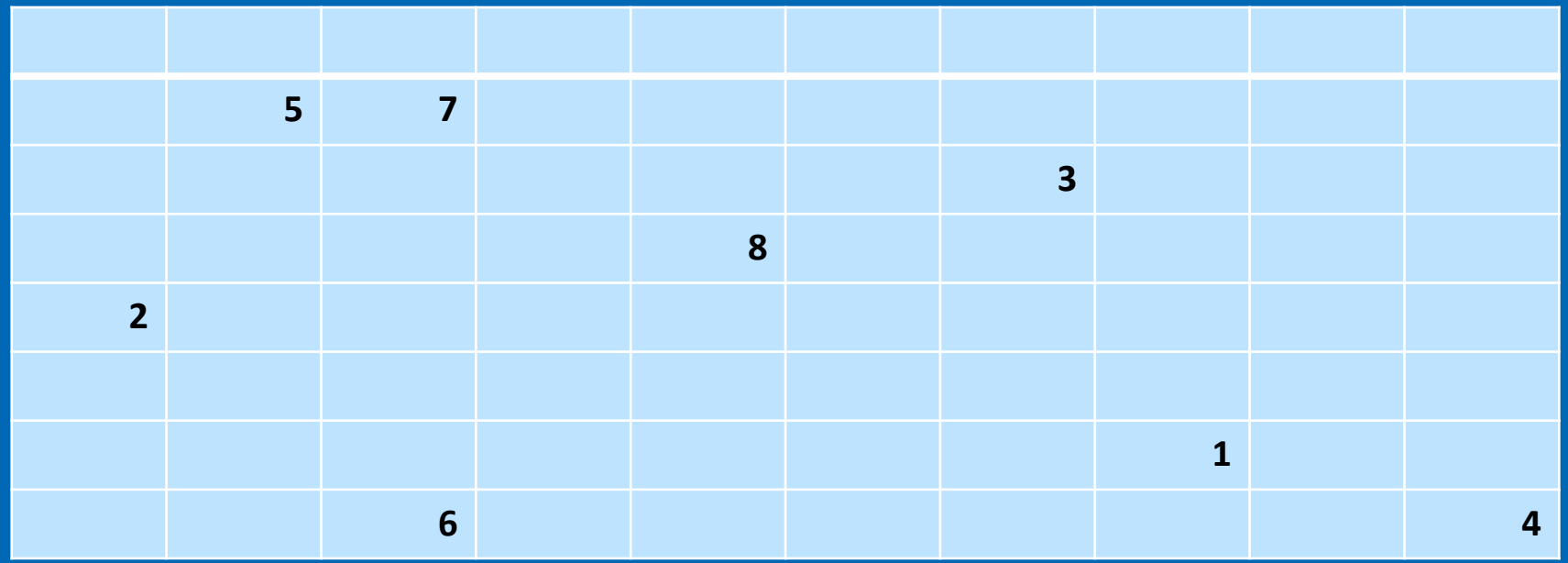


# Effect of Non Contiguous Memory Access

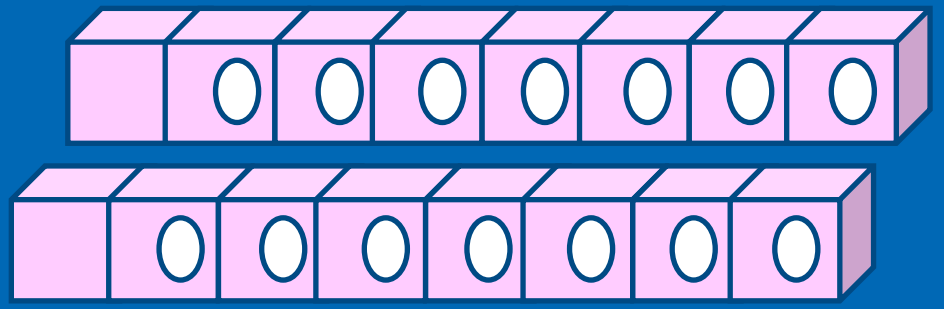
A list of integers in python are NOT generally in contiguous locations

For this list: [1, 2, 3, 4, 5, 6, 7, 8]

Accessing many of these in loops is VERY Costly (could be hundreds of clock cycles)



# Cache is used ineffectively



Random reads from all over memory hurt performance

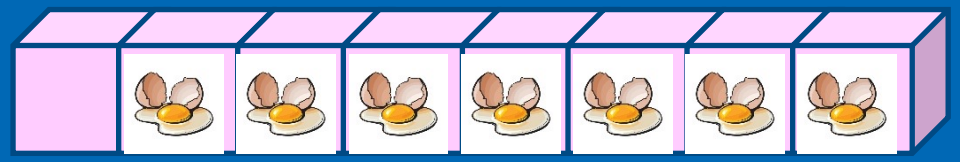
Modern Intel CPU's read in Cache line of consecutive memory  so that consecutive data is already to go when needed. The cache line may contain 16 consecutive elements or more

But with random reads, our next data element is read from a completely different place in memory – wasting the remaining elements that were ready to be served from the cache line

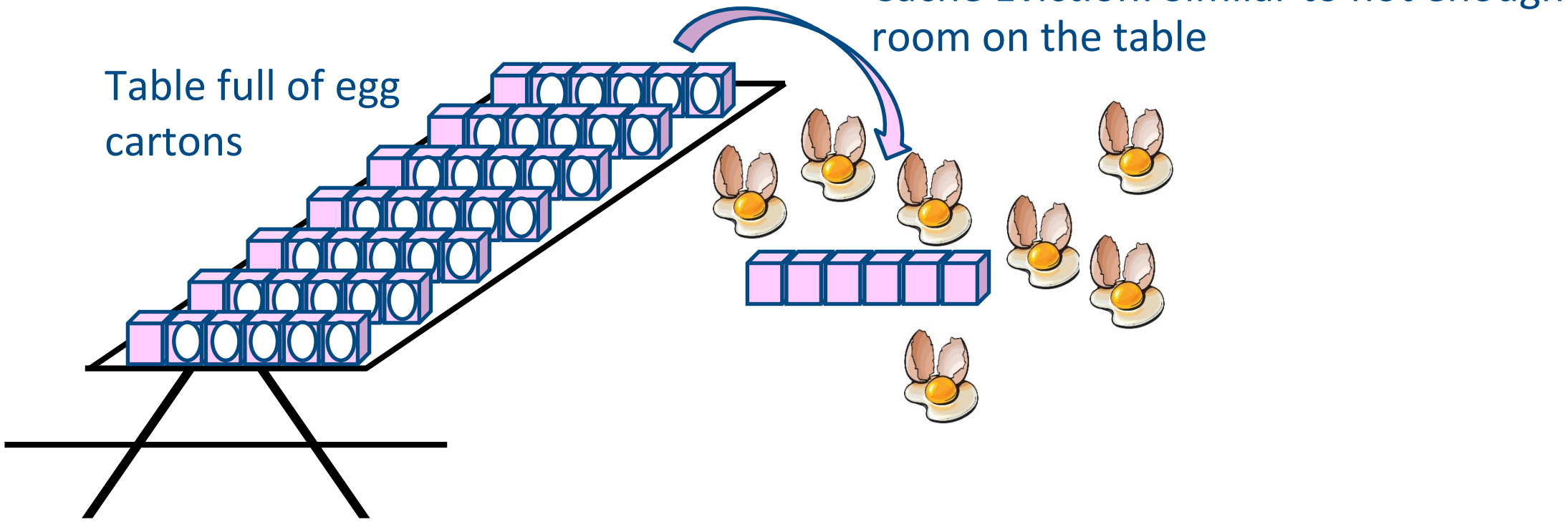
This is analogous to a chef opening and cooking a single egg from a carton of 16 to service customer number 1

Then then opening a NEW carton of eggs from a SECOND carton for customer number 2.  The other eggs get tossed out [analogous to cache line eviction ]

These are SOME reasons why vectorization is better – it mitigates all the above



# Cache is used ineffectively with random memory accesses



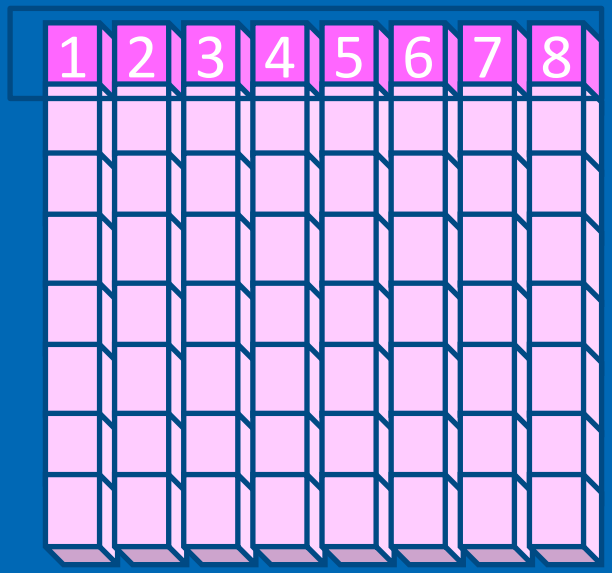
# Additionally: concerning memory

An array of integers in Numpy are contiguous locations

Modern CPU's return a cache line (like a carton of eggs) for the contiguous memory elements nearby one you chose to load initially.

The assumption is: if I just used memory address 0x12345, then likely I will use 0x12346 very soon

Contiguous memory addresses



# How do I move my code patterns to NumPy?


- NumPy Vectorization encompasses…
- NumPy Universal Functions (Ufuncs)
- Aggregations
- Fancy Indexing
- Broadcasting
- NumPy Where & Select for Conditionals
- Are ALL loops vectorizable?
  - We will give guidance

# How to create Numpy arrays

- From existing lists:

```
np.array([1, 2, 3.0])
```

- By dimensions but empty:

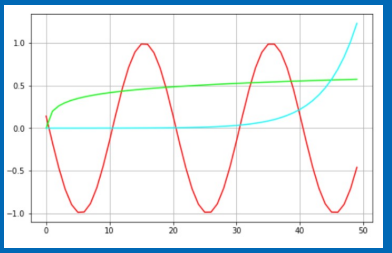
```
np.ndarray(shape=(2,2), dtype=float,
```

- By Shape – fill with zeros or ones:

```
>>> s = (2,2)
>>> np.zeros(s)
array([[ 0.,  0.],
       [ 0.,  0.]])
```

```
>>> s = (2,2)
>>> np.ones(s)
array([[1.,  1.],
       [1.,  1.]])
```

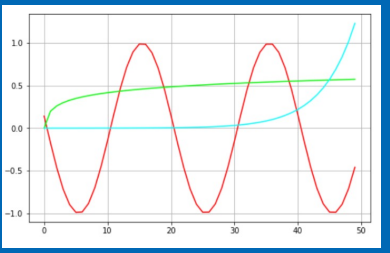
# ufuncs



ufuncs are written in C (for speed) and linked into Python with NumPy's ufunc facility

| Universal Functions | Description: These are vectorized |
|---|---|
| **Math operations** | **add, subtract, multiply, divide, reciprocal, matmul, log, exp, square, sqrt, …** |
| **Trigonometric** | sin, cos, tan, arcsin, arccos, arctan, hypot, sinh, cosh, tanh, degrees, radians |
| **Bit-twiddling** | bitwise_and, bitwise_or, bitwise_xor, invert, left_shift, right_shift |
| **Comparison Functions** | greater, greater_equal, less, less_equal, not_equal, equal, logical_and, logical_or, logical_xor, logical_not |
| **Floating Functions** | isfinite, isinf, isnan, isnat, fabs, signbit, copysign, nextafter, spacing, modf, ldexp, frexp, fmod, floor, ceil, trunc |

# NumPy Universal functions (ufunc): Vectorized!



- ufunc is a "vectorized" wrapper for a function
- Implements vectorization support in Intel AVX2 and AVX512
- Takes a fixed number of specific inputs
- Produces a fixed number of specific outputs
- Applies function in per element-wise fashion.
- For detailed information on universal functions, see Universal functions (ufunc) basics.

```
import numpy as np

arr = np.trunc([-3.1666, 3.6667])

print(arr)
out:
[-3.  3.]
```

# Sophisticated Indexing

- Slicing and Indexing can replace many common loop concepts

```
a = np.arange(100_000_000)
t1 = time.time()
b =  np.arange(50_000_002)
N = len(a)
for i in range (N):
    if i % 2 == 0:
        b[i//2] = a[i]
t2 = time.time()
```

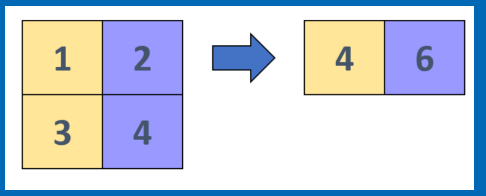
Results 4.5 X

```
b = a[::2]
```

# NumPy Aggregation & Statistics Functions

| Functions | Description: These are vectorized |
|---|---|
| **np.mean()** | Compute the arithmetic mean along the specified axis. |
| **np.std()** | Compute the standard deviation along the specified axis. |
| **np.var()** | Compute the variance along the specified axis. |
| **np.sum()** | Sum of array elements over a given axis. |
| **np.prod()** | Return the product of array elements over a given axis. |
| **np.cumsum()** | Return the cumulative sum of the elements along a given axis. |
| **np.cumprod()** | Return the cumulative product of elements along a given axis. |
| **np.min(), np.max()** | Return the minimum / maximum of an array or minimum along an axis. |
| **np.argmin(), np.argmax()** | Returns the indices of the minimum / maximum values along an axis |
| **np.all()** | Test whether all array elements along a given axis evaluate to True. |
| **np.any()** | Test whether any array element along a given axis evaluates to True. |

# NumPy Aggregations: Vectorized!

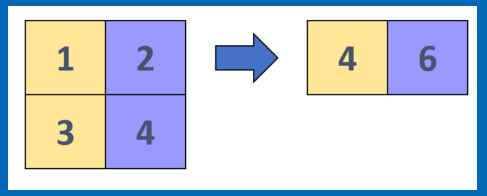



- Aggregation is an operation to reduce the dimensionality of an array or vector
- Implements vectorization support in Intel AVX2 and AVX512
- Replace loops you are using to compute averages, sums, standard deviation, min, max etc
- Use numpy aggregation instead. Its more readable, faster, and future proof

```
A = [1 2 3]
for v in  range(len(A)):
     S += v
mean = S/len(A)
```

```
A = np.array(A)
mean = A.mean()
```

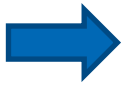
# NumPy Aggregations: Vectorized!




## Aggregations can be applied along different axes

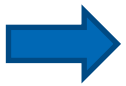
```
    A
[[1 2 3
 4 5 6]]
```

```
A.sum(axis = 0)
```



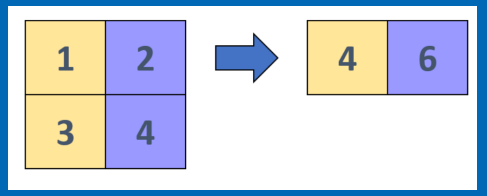
```
array([5 7 9])
```

```
A.sum(axis = 1)
```



```
array([6 15])
```

# Aggregation: Example




```
a = np.arange(1_000_000).reshape(1000,1000)
t1 = time.time()
N = len(a)
sum = 0
for i in range (N):
    for j in range(N):
        sum += a[i,j]
t2 = time.time()
```

```
sum = a.sum()
```

**100X** speed up over naïve loop

# NumPy: Aggregation & Statistics

```
a = np.arange(100_000_000)
sum = []
s = 0
for i in range (N):
    s += a[i]
    sum.append(s)
```

```
sum = a.cumsum()
```

Result: 100 Million elements: roughly **13X**

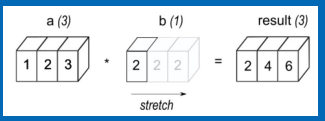
# NumPy: Sorting: Quicksort

```
def quickSort(arr, low, high):
    if low < high:
        pivotIndex = partition(arr, low, high)
        quickSort(arr, low, pivotIndex - 1)
        quickSort(arr, pivotIndex + 1, high)

def partition(arr, low, high):
    pivot = arr[high]
    i = low - 1  # Index of smaller element
    for j in range(low, high):
        # If current element is smaller than or equal to pivot
        if arr[j] <= pivot:
            i += 1
            arr[i], arr[j] = arr[j], arr[i]
    arr[i+1], arr[high] = arr[high], arr[i+1]
    return i + 1
```

```
np.sort(arr, axis=None, kind='quicksort')
```

Result: 1 Million elements: roughly **87X**

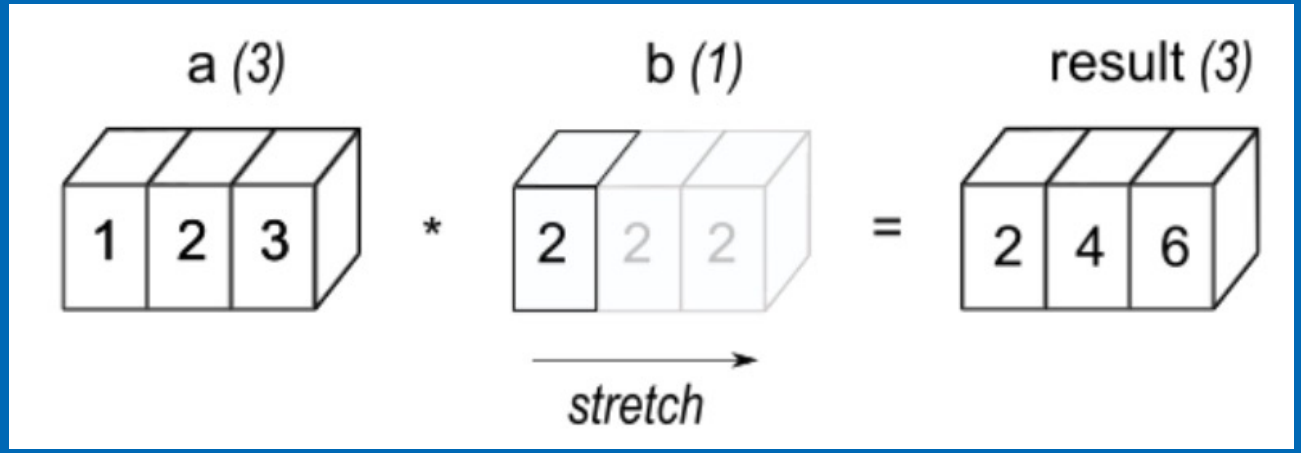
Link to Intel NumPy article

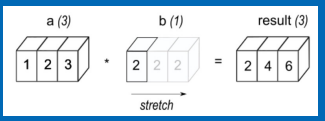



# NumPy Broadcasting: Vectorized!

- Support with AVX2 and AVX512 instructions
- Apply an operator with a scalar to each element in vector
- Also, apply operator with lower dimension vector to larger dimension

```
a = np.array([1.0 2.0 3.0])
b = 2.0
a * b
    array([ 2. 4. 6.])
```





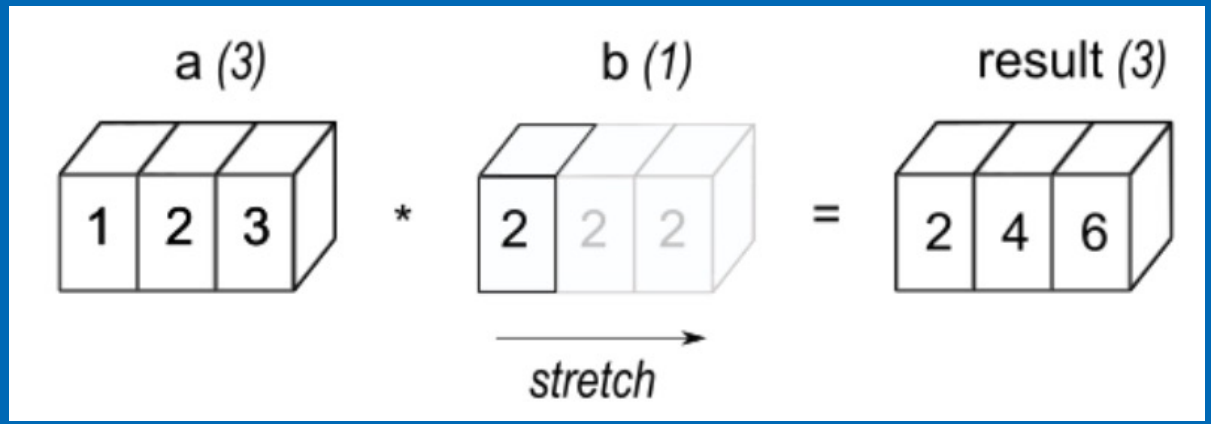

# Broadcasting Graphically

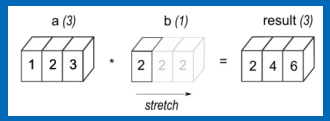
Non-matching dimensions are extended and data copied at HW level

Once dimensions match the vectors can be added, subtracted etc

First example:

- a.shape (1, 3)
- b.shape (1,1) # extend/copy to (1, 3)
- result.shape (1, 3)





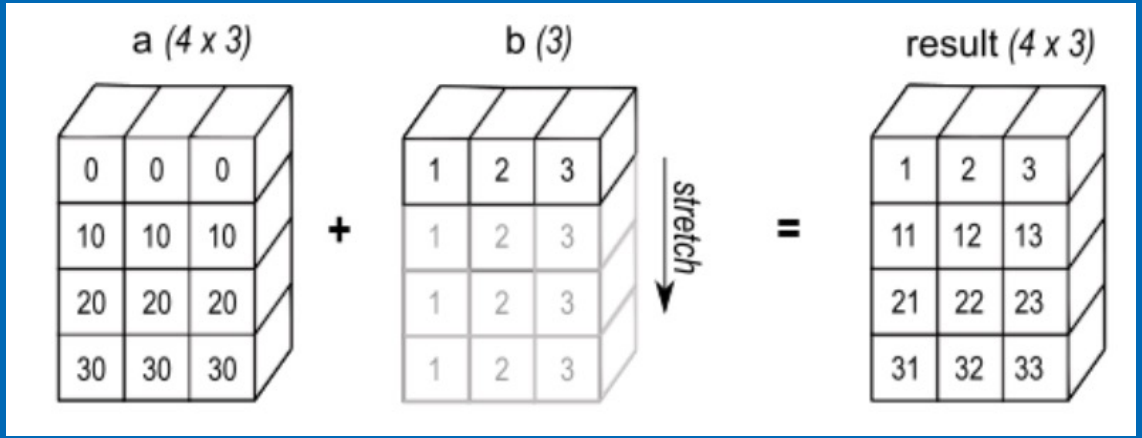

# Broadcasting Graphically

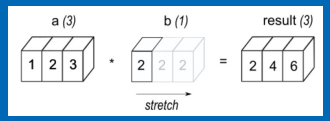
Non-matching dimensions are extended and data copied at HW level

Once dimensions match the vectors can be added, subtracted etc

Second example:

- a.shape (4, 3)
- b.shape (1, 3) # extend/copy to (4, 3)
- result.shape (4, 3)





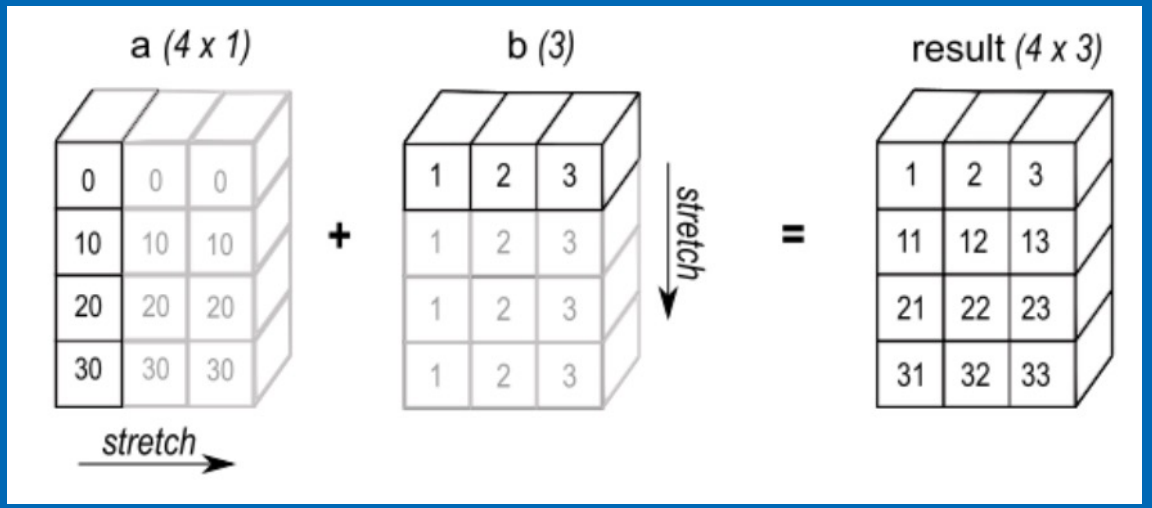

# Broadcasting Graphically

Non-matching dimensions are extended and data copied at HW level

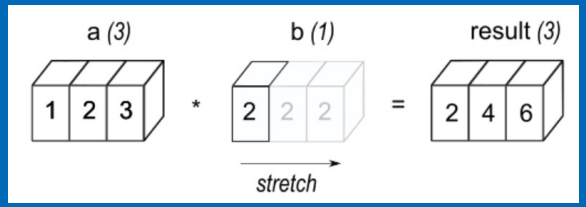
Once dimensions match the vectors can be added, subtracted etc

Third example:

- a.shape (4, 1)
- b.shape (1, 3) # extend/copy to (4, 3)
- result.shape (4, 3)
-



# Broadcasting Example

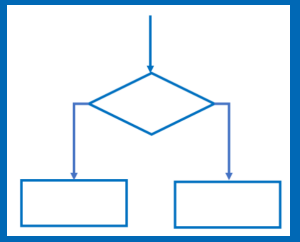



## Simple Multiplication table

```
B = np.zeros((N,N))
for i in range(N):
    for j in range(N):
        B[i,j] = (i+1)*(j+1)
```

```
B = A.reshape(N,1) * A
```

# Numpy.where

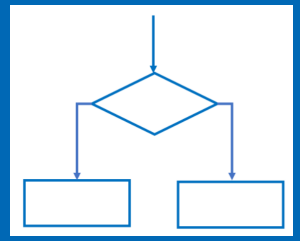


numpy.where: see : Return elements chosen from x or y depending on condition.

```
a = np.arange(10)
print("a\n",a)

np.where(a < 5, a, 10*a)
```

```
a
 [0 1 2 3 4 5 6 7 8 9]
array([ 0,  1,  2,  3,  4, 50, 60, 70, 80, 90])
```

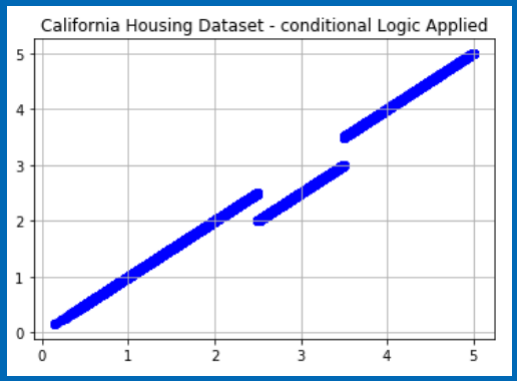
# NumPy Where, NumPy Select



- If statements (conditional logic) might severely limit performance:
- Numpy: handles conditionals quickly, efficiently

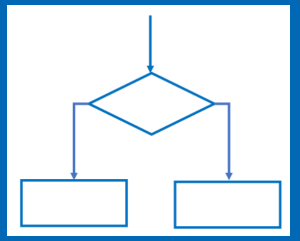
```
New = np.empty_like(T)
for i in range(len(T)):
    if ( (T[i] < buyerPriceRangeHi) & (T[i] >= buyerPriceRangeLo) ):
        New[i] = T[i] - 50_000/100_000
    else:
        New[i] = T[i]
```

Results: ~ **20 X**




```
New = np.where((T < buyerPriceRangeHi) & (T >= buyerPriceRangeLo), T - 50_000/100_000, T )
```

# Numpy Where



## Find row, col indices fast

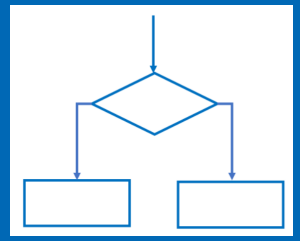
```
DBSCAN_array
 [[-1  2  1]
 [ 0  0  0]
 [ 0  1  2]
 [ 0 -1 -1]]
```

```
DBSCAN_array = np.array([[-1,2,1],[0,0,0],[0,1,2],[0,-1,-1]])

print("\nDBSCAN_array\n",DBSCAN_array)

DBSCAN_Process = np.where(DBSCAN_array < 0,"Outlier()", "ProcessNormally()")

print("\nDBSCAN_Process\n",DBSCAN_Process)

# now we can find where all the ones are by row and column
print("row index (where outliers are): ",np.where(DBSCAN_array < 0)[0])
print("col index (where outliers are): ",np.where(DBSCAN_array < 0)[1])
```

```
DBSCAN_Process
 [['Outlier()' 'ProcessNormally()' 'ProcessNormally()']
 ['ProcessNormally()' 'ProcessNormally()' 'ProcessNormally()']
 ['ProcessNormally()' 'ProcessNormally()' 'ProcessNormally()']
 ['ProcessNormally()' 'Outlier()' 'Outlier()']]
```

```
row index (where outliers are):  [0 3 3]
col index (where outliers are):  [0 1 2]
```

# Numpy.where: More Complex logic



```
## one solution - preserves the indexing edges for easy checking
res = np.where( ( MultiplicationTable%12 == 0) | ( MultiplicationTable%9 == 0) , MultiplicationTable, 0)
res[0,:] = MultiplicationTable[0,:]
res[:,0] = MultiplicationTable[:,0]
```

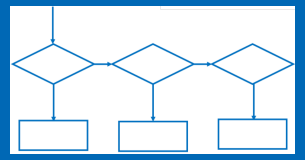
```
[[  1,   2,   3,   4,   5,   6,   7,   8,   9,  10],
 [  2,   4,   6,   8,  10,  12,  14,  16,  18,  20],
 [  3,   6,   9,  12,  15,  18,  21,  24,  27,  30],
 [  4,   8,  12,  16,  20,  24,  28,  32,  36,  40],
 [  5,  10,  15,  20,  25,  30,  35,  40,  45,  50],
 [  6,  12,  18,  24,  30,  36,  42,  48,  54,  60],
 [  7,  14,  21,  28,  35,  42,  49,  56,  63,  70],
 [  8,  16,  24,  32,  40,  48,  56,  64,  72,  80],
 [  9,  18,  27,  36,  45,  54,  63,  72,  81,  90],
 [ 10,  20,  30,  40,  50,  60,  70,  80,  90, 100]]
```

Results:

~ 20 X

```
[[ 1,  2,  3,  4,  5,  6,  7,  8,  9, 10],
 [ 2,  0,  0,  0,  0, 12,  0,  0, 18,  0],
 [ 3,  0,  9, 12,  0, 18,  0, 24, 27,  0],
 [ 4,  0, 12,  0,  0, 24,  0,  0, 36,  0],
 [ 5,  0,  0,  0,  0,  0,  0,  0, 45,  0],
 [ 6, 12, 18, 24,  0, 36,  0, 48, 54, 60],
 [ 7,  0,  0,  0,  0,  0,  0,  0, 63,  0],
 [ 8,  0, 24,  0,  0, 48,  0,  0, 72,  0],
 [ 9, 18, 27, 36, 45, 54, 63, 72, 81, 90],
 [10,  0,  0,  0,  0, 60,  0,  0, 90,  0]]
```

# Numpy Select



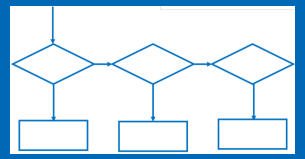
Numpy.select: see

- Return an array drawn from elements in choice list, depending on conditions.
- Great for pulling together elements or functions(elements) from different arrays, DataFrames, different parts of the same array, etc

```
x = np.arange(6)
print("X\n",x)

condlist = [x<3, x>3]

choicelist = [x, x**2]

np.select(condlist, choicelist, 42)
```

```
X
 [0 1 2 3 4 5]
array([ 0,  1,  2, 42, 16, 25])
```

# Numpy: Select Example



```
for i in range(BIG):
    if A[i,4] == 10:
        A[i,5] =  A[i,2] * A[i,3]
    elif (A[i,4] < 10) and (A[i,4] >=5):
        A[i,5] =   A[i,2] + A[i,3]
    elif A[i,4] < 5:
        A[i,5] =   A[i,0] + A[i,1]
```

```
condition = [ (A[:,4]  < 10) & (A[:,4] >= 5),
              ( A[:,4] < 5)]
choice = [ (A[:,2] + A[:,3]),
           (A[:,0] + A[:,1] ) ]
default = [(A[:,2] * A[:,3])]
A[:,5] = np.select(condition, choice, default= default )
```

Results: ~ **20 X**

# The Pandas Connection


- Pandas is built on top of Numpy
- All the methods describe before apply
- We will demonstrate alternative ways to achieve speedups when Pandas Apply is slow due to conditional logic in the custom called function

# Methods

- Use “Apply” for simple functions to apply to columns
- When things get slow, convert data to Numpy arrays
- to_numpy()
- Replace conditional logic in the Apply with Numpy.Where or Numpy.Select
- It is even possible to use Numpy. Select to manipulate Pnadas dataframes directly

# Using Numpy.Select as alternative to Pandas.Apply

```
df['new'] = df.apply(lambda x: func(x['a'], x['b'], x['c'], x['d'], x['e']), axis=1)
```

```
def my_function(x):
    return np.log(1+x)

def func(a,b,c,d,e):
    if e == 10:
        return c*d
    elif (e < 10) and (e>=7):
        return my_function(c+d)
    elif e < 7:
        return my_function(a+b+100)
```

# Using Numpy.Select as alternative to Pandas.Apply

```
df['new'] = df.apply(lambda x: func(x['a'], x['b'], x['c'], x['d'], x['e']), axis=1)
```

Results:

**200 X +**

```
npArr = df.to_numpy()  # convert to numpy

condition = [ (npArr[:,idx['e']] < 10) & (npArr[:,idx['e']] >= 7),
              (npArr[:,idx['e']] < 7)]

choice = [(my_function(npArr[:,idx['c']] + npArr[:,idx['d']]      )),
          (my_function(npArr[:,idx['a']] + npArr[:,idx['b']] + 100))]

tmp = np.select(condition, choice, default= (npArr[:,idx['c']] * npArr[:,idx['d']]) )
df.loc[:,'new'] = tmp
```

# Poll Audience
# Live Demo/Lab

https://github.com/IntelSoftware/Machine-Learning-using-oneAPI.git

Dive into Chapter 08

# Call to Action

- Loops:
- Find **large** single, double, and triple nested **loops** in your code and replace with Scipy/ Scikit-Learn*, or Numpy alternative
- Find time consuming list comprehensions and replace with a Numpy alternative .
- If statements:
- replace with Numpy.where or Numpy.select options if possible
- Using array masking that follows the conditional logic

# Thanks for attending the session

# BACKUP

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